Supporting Information

Catalytic Selectivity Sharp Increase in Acetylene Semi-hydrogenation on Pd Achieved by Machine Learning Simulation Guided Experiment

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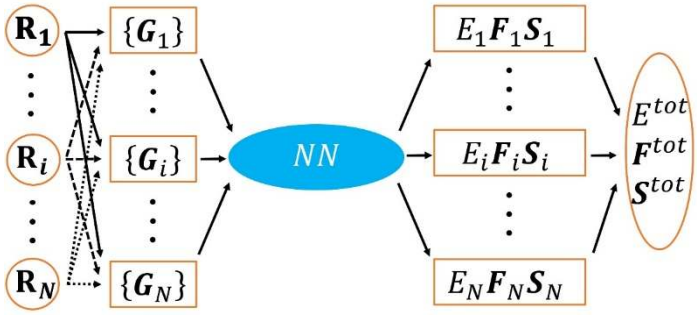
1. Theoretical methodology and the construction of the ternary Pd-C-H G-NN potential

1.1 Architecture of neural network potential



Scheme S1. Scheme for the HDNN architecture. The subscripts (1, *i* and *N*) are atom indices, representing the total number of atoms in a structure. The inputs to NN are a set of structural descriptors {**G**} constructed from the Cartesian coordinates {**R**} of the structure, and the outputs are the atomic properties { E_i, $\boldsymbol{F}_i$, $\boldsymbol{S}_i$ }, i.e. energies, forces and stresses. The overall properties E^{tot}, $\boldsymbol{F}^{tot}$, and $\boldsymbol{S}^{tot}$ are calculated from the individual atomic contribution.

In this work, we utilized the high dimensional neural network (HDNN) scheme to construct the global NN (G-NN) potential, as shown in Scheme S1. The input nodes to NN are a set of structural descriptors {$\boldsymbol{G}_i$} for a structure, as detailed discussed in our previous works.[1-3] The total energy E^{tot} is then decomposed as a linear combination of atomic energy E^i from the output of NN

$$E^{tot} = \sum_i E_i \tag{1}$$

The atomic force can be analytically derived according to Eq. 2, where the force component $F_{k,\alpha}$ (α=*x*, *y* or *z*) acting on atom *k* is the derivative of total energy with respect to the coordinate $R_{k,\alpha}$. In combination with Eq. 1, the force component could be further related to the derivatives of the atomic energy with respect to j^{th} structural descriptors of atom *i*, $G_{j,i}$

$$F_{k,\alpha} = -\frac{\partial E^{tot}}{\partial R_{k,\alpha}} = -\sum_{i,j} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial R_{k,\alpha}} \tag{2}$$

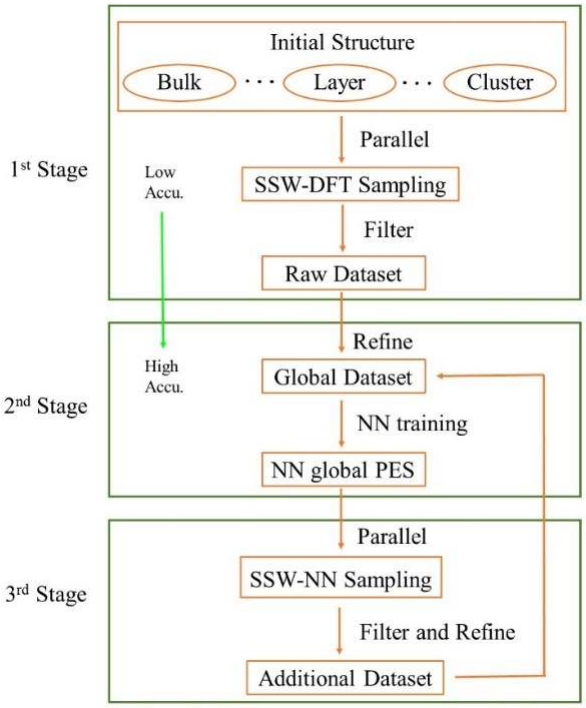
Similarly, the element $\sigma_{\alpha\beta}$ of static stress tensor matrix can be analytically derived as

$$\sigma_{\alpha\beta} = -\frac{1}{V} \sum_{i,j,d} \frac{(\boldsymbol{r}_d)_\alpha (\boldsymbol{r}_d)_\beta}{r_d} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial r_d} \tag{3}$$

where $\boldsymbol{r}_d$ and r_d are the distance vector constituting $G_{j,i}$ and its module, respectively, and *V* is the volume of the structure.

1.2 Construction of global dataset using SSW-NN

Undoubtedly, the training dataset largely determines the quality of the potential energy surface (PES) of G-NN. Our previous works have shown that, the stochastic surface walking (SSW) global optimzation[4-6] can fast generate a global dataset, which incorporates different structural patterns on the global PES. The SSW PES search is fully automated and does not need a priori knowledge on the system, such as the structure motif (e.g., bonding patterns, symmetry) of the materials. The final obtained Pd-C-H global dataset in this work is summarized in **Table S1**.



Scheme S2. Procedure for generating the training dataset using SSW global optimization. At the first stage, the SSW sampling is typically calculated by low accuracy DFT calculations. At the second stage, the global dataset is first refined with high accuracy setups, followed by the NN training on the accurate global dataset. At the third stage, an additional dataset is generated by SSW sampling utilizing the NN PES obtained previously. This additional dataset is then fed into global dataset (back to stage 2) and start a new cycle of NN training.

In brief, the SSW-NN method involves three stages for constructing the global dataset (see Scheme S2), as described in the following.

(i) **The first stage** constructs a raw dataset, which contains the most commmon atomic environment and serves as the training dataset for building an initial NN PES. This is done by performing density functional theory (DFT) SSW global optimization in a massively parallel way. The DFT calculations are typically with low accuracy setups and are restricted to small

unit cells to speed up the SSW search. By collecting and screening the structures from the SSW trajectories, a raw dataset is finally obtained.

(ii) **The second stage** trains an NN global PES. This is done by refining the dataset using DFT calculations with high accuaracy setups, followed by the NN training on the accurate global dataset (see our previous work[7] for details). The NN architecture applied in this stage utilizes a small set of structural descriptors and a small network size.

(iii) **The third stage** iteratively expands the global dataset. It targets to increase the predictive power of NN PES by incorporating more structural patterns into the dataset. This is done by carrying out SSW PES search using the NN PES obtained in the second stage, starting from a variety of initial structures. These initial structures are often randomly configurated and also include large systems with many atoms per unit cell. The structures from all SSW trajectories are collected and filtered to genereate the addtional dataset. This new dataset is then fed to the global dataset (back to stage 2) to start a new cycle of NN training.

Table S1. Structure information of the global EPS data set for G-NN potential training. The listed data is the number of structures in the data set, as distinguished by the chemical formula, the number of atoms per cell (N_{atm}) and the type of structure, including cluster (N_{cls}), layer (N_{lay}) and bulk (N_{bul}). The total numbers of the structure (N_{tot}) are also summarized.

Chem. Formula	N_{atm}	N_{cls}	N_{lay}	N_{bul}	N_{tot}
Pd4	4	0	0	23	23
Pd16	16	213	1	850	1064
Pd31	31	0	0	4	4
Pd32	32	0	0	88	88
C1-Pd12	13	0	148	0	148
C2-Pd10	12	0	173	0	173
C2-Pd25	27	0	0	51	51
C2-Pd29	31	0	5	86	91
C3-Pd16	19	14	0	0	14
C4-Pd8	12	0	0	492	492
C4-Pd25	29	0	3	48	51
C6-Pd25	31	0	175	114	289
C8-Pd16	24	8	0	0	8
C10-Pd49	59	0	20	0	20
C12-Pd50	62	0	34	2	36
H1-Pd15	16	0	0	365	365
H1-Pd16	17	0	0	1	1
H1-Pd23	24	0	33	17	50
H1-Pd26	27	0	81	0	81
H1-Pd27	28	0	32	0	32

H1-Pd31	32	1	0	16	17
H2-Pd14	16	0	69	626	695
H2-Pd16	18	0	0	1	1
H2-Pd22	24	0	29	0	29
H2-Pd27	29	3	51	74	128
H2-Pd28	30	0	64	0	64
H2-Pd30	32	2	0	16	18
H2-C2	4	2	0	0	2
H2-C4-Pd23	29	0	0	121	121
H3-Pd16	19	0	0	1	1
H3-Pd26	29	0	120	0	120
H3-Pd28	31	1	0	11	12
H3-Pd29	32	2	0	23	25
H3-C2-Pd22	27	0	0	150	150
H3-C6-Pd22	31	0	0	81	81
H4-Pd12	16	2122	0	256	2378
H4-Pd16	20	0	0	1	1
H4-Pd17	21	0	0	170	170
H4-Pd20	24	0	24	0	24
H4-Pd24	28	0	45	0	45
H4-C1-Pd36	41	0	331	0	331
H4-C4	8	429	0	0	429
H4-C7-Pd45	56	0	0	12	12
H4-C8-Pd46	58	0	0	39	39
H5-Pd16	21	0	182	39	221
H5-Pd27	32	0	101	2	103
H5-C2-Pd36	43	0	310	0	310
H5-C6-Pd20	31	0	0	78	78
H6-Pd10	16	0	0	360	360
H6-Pd15	21	0	286	5	291
H6-Pd16	22	0	0	1	1
H6-Pd25	31	0	80	0	80
H6-Pd26	32	108	77	106	291
H6-C2-Pd36	44	0	337	0	337
H6-C4	10	133	0	0	133
H6-C4-Pd43	53	0	0	17	17
H6-C4-Pd44	54	0	0	48	48
H7-Pd16	23	0	0	1	1
H7-Pd25	32	0	0	68	68
H7-C2-Pd35	44	0	200	0	200
H7-C2-Pd36	45	0	641	0	641
H8-Pd8	16	2986	0	1462	4448
H8-Pd16	24	0	53	1	54
H8-Pd20	28	0	28	0	28

H8-C2-Pd16	26	0	10	0	10
H8-C2-Pd37	47	0	10	0	10
H8-C7-Pd21	36	0	93	1	94
H9-Pd16	25	0	0	1	1
H9-Pd23	32	96	0	0	96
H9-C2-Pd16	27	0	23	0	23
H9-C2-Pd20	31	0	11	0	11
H10-Pd16	26	0	0	1	1
H10-Pd21	31	0	92	0	92
H10-Pd22	32	0	64	207	271
H10-Pd48	58	0	15	0	15
H10-Pd54	64	0	25	2	27
H10-C4	14	2	0	0	2
H10-C6-Pd40	56	0	0	18	18
H10-C8-Pd42	60	0	20	0	20
H10-C12-Pd40	62	0	0	34	34
H11-Pd5	16	0	41	1334	1375
H11-Pd16	27	0	0	1	1
H11-Pd21	32	0	0	176	176
H12-Pd16	28	0	0	1	1
H13-Pd16	29	0	0	1	1
H13-Pd19	32	0	0	53	53
H13-C2-Pd16	31	0	85	0	85
H13-C5-Pd22	40	0	28	0	28
H14-Pd16	30	0	0	124	124
H14-Pd17	31	0	0	126	126
H14-Pd18	32	0	0	84	84
H14-C2-Pd40	56	0	14	0	14
H15-Pd6	21	0	650	0	650
H15-Pd16	31	0	0	166	166
H15-Pd17	32	0	0	259	259
H15-C1-Pd16	32	0	0	99	99
H16-Pd5	21	0	950	58	1008
H16-Pd16	32	0	38	502	540
H16-Pd64	80	0	4	0	4
H16-C2-Pd16	34	0	158	0	158
H16-C2-Pd20	38	0	455	1	456
H16-C4-Pd20	40	0	184	1	185
H16-C14-Pd42	72	0	48	0	48
H17-Pd15	32	0	0	103	103
H17-C2-Pd16	35	0	188	0	188
H17-C2-Pd64	83	0	129	0	129
H17-C3-Pd20	40	0	220	0	220
H17-C5-Pd24	46	0	100	0	100

H18-Pd13	31	0	0	50	50
H18-C2-Pd16	36	0	293	1	294
H18-C2-Pd20	40	0	281	0	281
H18-C2-Pd26	46	0	72	0	72
H18-C2-Pd64	84	0	144	0	144
H19-Pd13	32	0	0	64	64
H19-Pd30	49	0	0	20	20
H19-C2-Pd20	41	0	69	0	69
H20-C2-Pd39	61	0	14	0	14
H20-C2-Pd64	86	0	147	0	147
H20-C2-Pd67	89	0	13	0	13
H20-C8-Pd44	72	0	21	0	21
H21-C2-Pd64	87	0	163	0	163
H22-C2-Pd31	55	0	0	13	13
H22-C3-Pd40	65	0	29	0	29
H22-C4-Pd48	74	0	26	0	26
H23-Pd8	31	0	149	68	217
H23-Pd9	32	0	235	139	374
H24-Pd8	32	0	41	71	112
H24-C2-Pd20	46	0	552	0	552
H25-C3-Pd51	79	0	19	0	19
H26-C2-Pd40	68	0	118	0	118
H26-C10-Pd44	80	0	46	0	46
H27-C2-Pd35	64	0	228	0	228
H27-C2-Pd36	65	0	368	0	368
H27-C2-Pd58	87	0	3	10	13
H27-C7-Pd40	74	0	35	0	35
H28-Pd32	60	0	0	55	55
H29-C2-Pd39	70	0	89	0	89
H30-C1-Pd40	71	0	17	0	17
H30-C2-Pd32	64	0	0	47	47
H32-C8-Pd40	80	0	59	0	59
H33-C2-Pd40	75	0	85	0	85
H34-C6-Pd40	80	0	49	0	49
H34-C10-Pd48	92	0	47	0	47
H35-C2-Pd30	67	0	30	0	30
H36-C4-Pd52	92	0	49	0	49
H37-C2-Pd30	69	0	29	0	29
H38-C2-Pd45	85	0	33	0	33
H40-Pd64	104	0	2	0	2
H40-C2-Pd45	87	0	40	0	40
H41-C2-Pd39	82	0	332	0	332
H41-C2-Pd64	107	0	58	0	58
H42-C2-Pd40	84	0	798	0	798

H42-C2-Pd64	108	0	67	0	67
H44-C2-Pd39	85	0	63	0	63
H44-C2-Pd64	110	0	62	0	62
H45-C2-Pd40	87	0	563	10	573
H45-C2-Pd64	111	0	56	0	56
H46-C2-Pd40	88	0	77	0	77
H47-C2-Pd40	89	0	529	0	529
H48-C2-Pd40	90	0	75	0	75
H48-C4-Pd40	92	0	43	1	44
H50-Pd64	114	0	2	0	2
H50-C2-Pd48	100	0	53	0	53
H51-C2-Pd64	117	0	107	0	107
H52-C2-Pd48	102	0	42	0	42
H52-C2-Pd64	118	0	96	0	96
H54-C2-Pd64	120	0	95	0	95
H55-C2-Pd64	121	0	86	0	86
Total	**--**	**6122**	**14187**	**9829**	**30138**

1.3 Benchmark of G-NN potential against DFT calculations

To examine the accuracy of the G-NN potential, we have selected randomly 805 PdH_x structures and computed the total energy difference between G-NN and DFT calculations (see Fig. S1), which shows a low (root mean square error) RMSE of 2.5 meV/f.u. (1 f.u.=Pd atom)

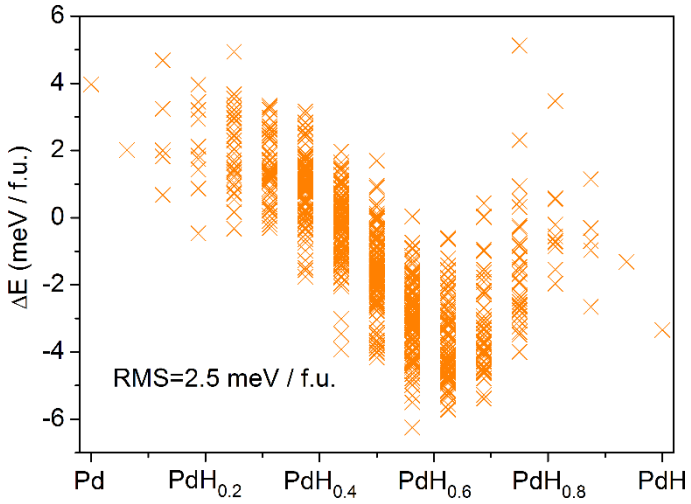


Fig. S1. Energy difference between G-NN and DFT calculations for PdH_x system with H atoms residing at the octahedral sites.

One great advantage of the G-NN potential is the predictive power to chemical reactions, i.e. those relatd to the transition state. Some key acetylene/ethene hydrogenation data on Pd(111), Pd(100), Pd_4H_3(111) and Pd_4H_3(100) from G-NN and DFT calculations have been summarized in Table S2. As shown, the energy differences between G-NN and DFT are small (< 0.12 eV), illustrating the good accuracy of G-NN for acetylene/ethene hydrogenation.

Table S2. Comparision of the energetics for acetylene/ethene hydrogenation on Pd(111), Pd(100), Pd_4H_3(111) and Pd_4H_3(100) from G-NN and DFT calculations. The listed data includes the adsorption free energy G_{ad} of acetylene and ethene, and the hydrogenation barrier G_a from acetylene to ethene G_a and from ethene to ethane G_a. Also see Table 1 in main text for the reference of the free energy.

	Surface	G-NN	VASP	Diff
G_{ad}(acetylene)	Pd (111)	0.07	0.11	0.04
	Pd (100)	-0.93	-0.92	0.01
	Pd_4H_3 (111)	-0.06	-0.16	0.10
	Pd_4H_3 (100)	-1.00	-1.02	0.02
G_{ad}(ethene)	Pd (111)	0.85	0.88	0.03
	Pd (100)	0.30	0.23	0.07
	Pd_4H_3 (111)	0.77	0.67	0.10
	Pd_4H_3 (100)	0.27	0.15	0.12
G_a(acetylene)	Pd (111)	0.62	0.66	0.04
	Pd (100)	1.00	0.91	0.09
	Pd_4H_3 (111)	0.66	0.71	0.05
	Pd_4H_3 (100)	0.93	0.87	0.06
G_a(ethene)	Pd (111)	1.31	1.38	0.07
	Pd (100)	0.88	0.89	0.01
	Pd_4H_3 (111)	1.26	1.19	0.07
	Pd_4H_3 (100)	0.83	0.79	0.04

2. Formation of Pd-C bulk phases

The possibility to form PdC_x bulk phases during the hydrogenation reactions has been considered by searching the global minimum of $Pd_{24}C_1$ bulk using SSW-NN method. As also validated by DFT calculations, the GM structure, as shown in Fig. S2, has the C in an octahedral site in fcc Pd. The structure has a positive formation energy of +0.81 eV with respect to face-centered cubic (fcc) Pd and graphite. We thus conclude that C is hard to incorporate into Pd: the formation of PdC_x bulk phases under hydrogenation conditions can be ruled out.

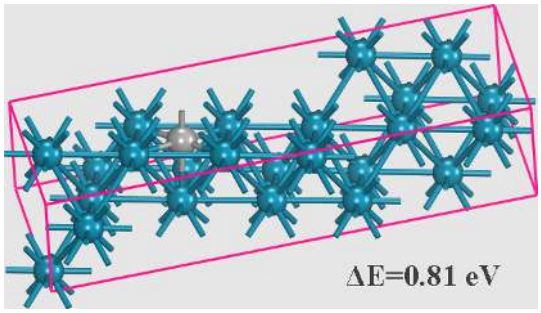


Fig. S2. Global minimum of $Pd_{24}C_1$ bulk and its formation energy (with respect to fcc Pd and graphite).

3. ZPE correction for PdH_x system

By computing the phonon of Pd and PdH_x systems, we have obtained the ZPE for bulk H at different sites, which appear to be not sensitive to the H concentraition in bulk. The value of ZPE is calculated to be 0.079 eV/atom and 0.165 eV/atom for the octahedral site H and the tetrahedral site H respectively. To test the effect of ZPE on the absorption of H, we have computed the formation energy for a series of PdH_x structures (with H atoms at octahedral or tetrahedral sites), with and without ZPE correction, as shown in Fig. S3. The formation energy with ZPE correction is calculated by

$$\Delta E = E_{\mathrm{PdH}_x} + xE_{\mathrm{ZPE}} - E_{\mathrm{Pd}} - \frac{x}{2}E_{\mathrm{H}_2} \tag{4}$$

where E_{ZPE} is the ZPE per H atom depending on its located site, while E_{Pd} and E_{H_2} are the energy of fcc Pd and H_2 as reference. The formation energy without ZPE correction is calculated by

$$\Delta E = E_{\mathrm{PdH}_x} - E_{\mathrm{Pd}} - \frac{x}{2}E_{\mathrm{H}_2} \tag{5}$$

From Fig. S3, it is obvious that, although the tetrahedral site H is energetically more stable than the octahedral site H without ZPE correction, the most stable configurations turn out to have only octahedral site H after ZPE correction. We therefore conclude that the ZPE of H is crucial, and thus is explicitly taken into account in our study.

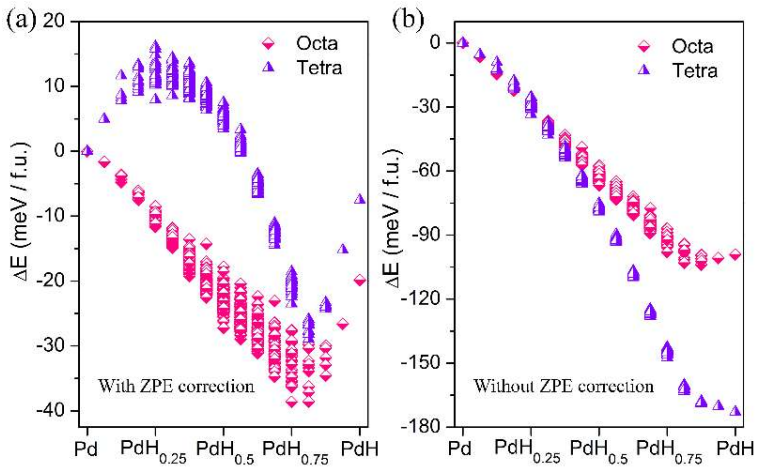


Fig. S3. Formation energy of PdH_x (**a**) with and (**b**) without ZPE correction.

4. Stability and migration of H in/on Pd bulk/surface

To examine the stability of H in Pd, we have plotted the global energy surface for 1 ML H covered Pd(111), precisely 16 H atoms in a p(4x4) Pd(111), as shown in Fig. S4. This is done by plotting the energy against the distance-weighted Steinhardt-type order parameter[8] for 21633 distinct minima collected from SSW-NN search. It shows that the GM is the 1 ML H covered Pd(111), which locates at the bottom of the funnel on the PES. With the increase of the number of H atoms (i.e. 1 to 5 H atoms) immersed into the subsurface, the energy of the minimum increases gradually, as labelled in the figure. The presence of each subsurface H will increase roughly the total energy by ~0.35 eV with no obvious H-H interaction up to five subsurface H. This demonstrates clearly that the surface H is more stable than the subsurface/bulk H.

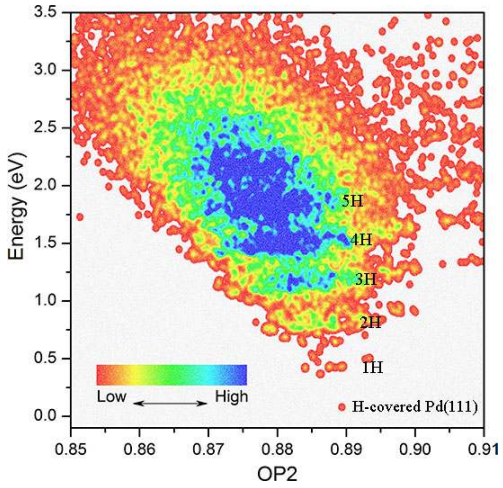


Fig. S4. Global energy surface contour plot for 1 ML H covered Pd(111), α-phase. The x-axis is the distance-weighted Steinhardt-type order parameter (OP) to distinguish different structures.[8] The colors denote the density of the structural minima.

Figure S5 provides the clue to understand how H diffusion into Pd bulk in reality. Figure S5 compares the H adsorption ability on Pd(100) with the original Pd bulk lattice (a=3.94 Å) and with an expanded lattice (a=4.10 Å). It shows that once the lattice is expanded, the H adsorption can become exothermic even when the subsurface H grows. This implies that the H diffusion to Pd is kinetically hindered for large Pd particles where the lattice should be constrained largely at the Pd bulk lattice.

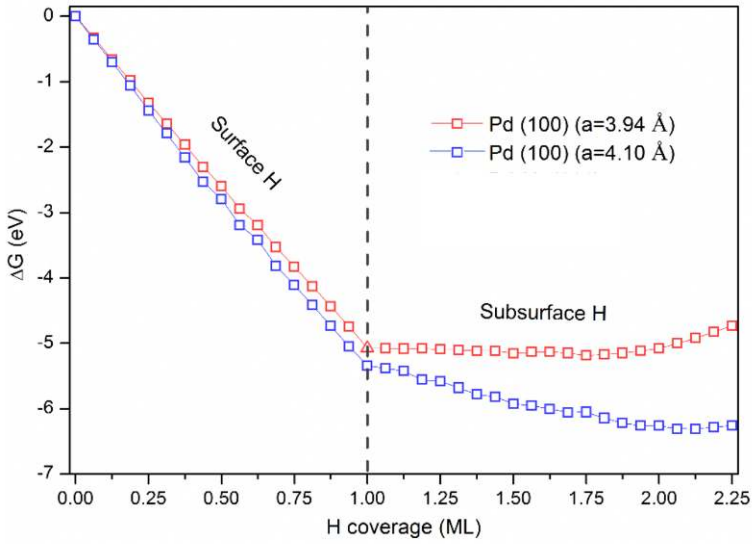


Fig. S5. The overall Gibbs free energy change for H adsorption on Pd(100) (a=3.94 Å) and Pd(100) with an expanded lattice (a=4.10 Å). The thermodynamic conditions are 298 K, $p(H_2)$=0.01 atm.

Kinetically, the migration of H from surface to subsurface and to the bulk is possible. As shown in Fig. S6, the migration barrier of H has a barrier of 0.4~0.5 eV.

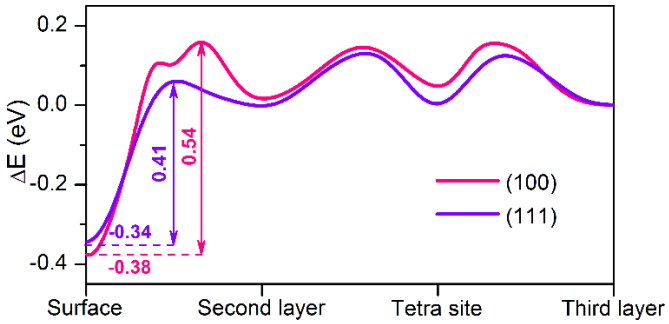


Fig. S6. Energetics profile for the migration of H in Pd, from surface to subsurface and to the bulk. H is more stable at octahedral site in bulk (after ZPE correction) and the migration of H from layer to layer needs to bypass the tetrahedral site (Tetra site).

5. Hydrogenation reactions under different conditions

5.1 Convergence check for slab thickness

We have checked the hydrogenation reactions on the five-layer slab surface with the bottom two layers fixed and the top three layers fully relaxed. The results are shown in Fig. S7, which shows that the five-layer and the four-layer results differ by less than 0.06 eV.

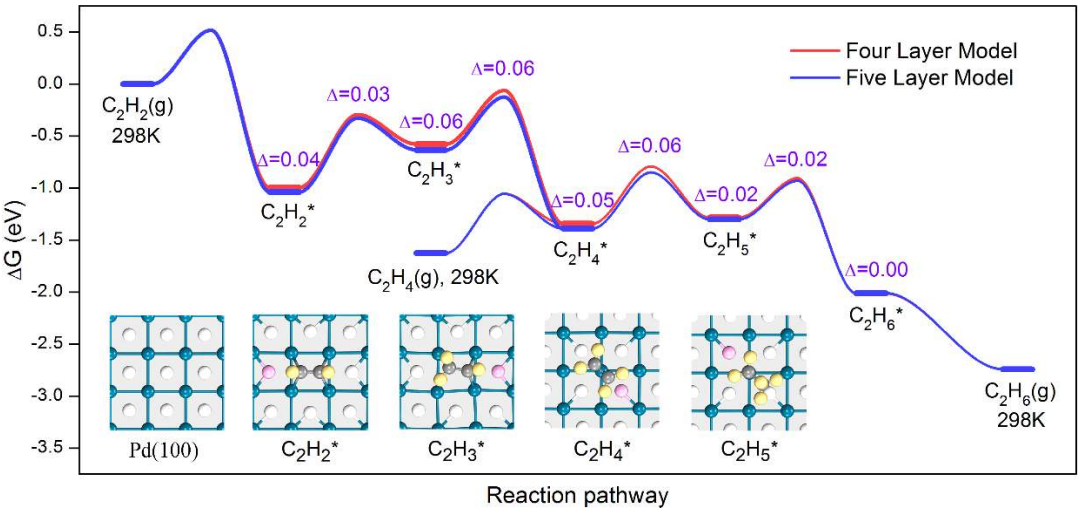


Fig. S7. The Gibbs free energy profile for acetylene/ethene hydrogenation on $Pd_4H_3(100)$ with a four-layer slab model and a five-layer slab model. The reaction conditions are 298 K, $p(H_2)$=1 atm, $p(C_2H_2)$=0.02 atm, $p(C_2H_4)$=0.02 atm.

5.2 Acetylene/ethene adsorption configurations

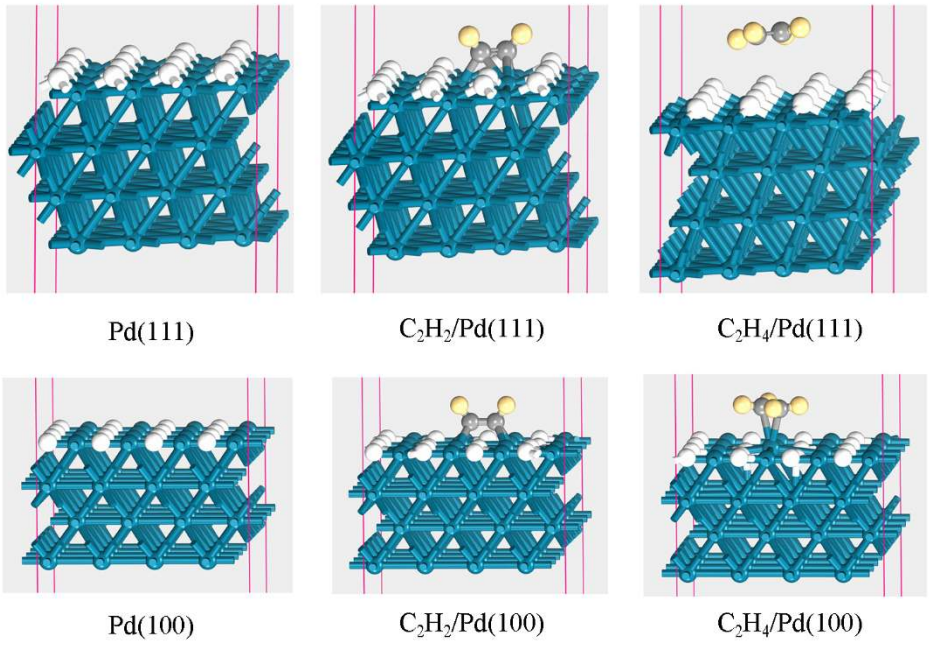


Fig. S8. The H-covered surfaces and the most stable acetylene/ethene adsorption configuration on Pd(111) and Pd(100). The H atoms may be subtracted to allow the C_2H_2/C_2H_4 adsorption and in all cases the most stable final state configuration at the thermodynamics conditions is utilized. The energetics data are shown in Table 1.

5.3 Ethene hydrogenation on Pd(111) at 15/16 ML H coverage

In the main text Fig. 3, we have reported the ethene hydrogenation on Pd(111) with no surface H vacancy (H_v), which has a high overall barrier of 1.38 eV from ethene to ethyl. In fact, we have also considered the situation with a surface H_v (i.e. 15/16 ML H coverage in a p(4×4) unit cell) as shown in Fig. S9, which yields a similar overall barrier of 1.36 eV for the hydrogenation.

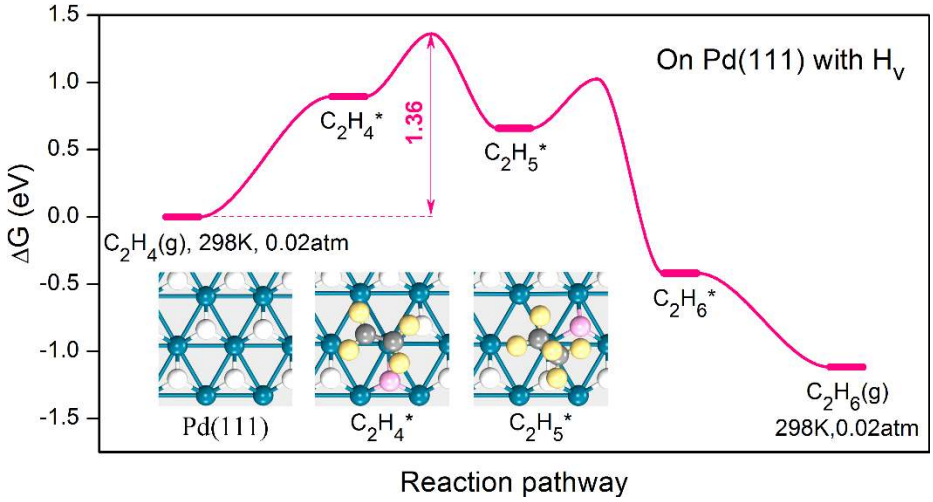


Fig. S9. Gibbs free energy profiles for ethene hydrogenation on Pd(111) with a surface H_v.

5.4 Comparison with previous literatures

We have also compared the energetics for the reactions on clean Pd(111) at 0 K (p(4x4), four-layer surface model) with the previous reported data sheth *et al.*[9] (p(2x2), three-layer surface model), as summarized in Table S3.

Table S3. Adsorption energy E_{ad} and the overall barrier for acetylene/ethene hydrogenation on Pd(111) at different conditions.

Reaction condition	Acetylene		Ethene	
	E_{ad}	E_a	E_{ad}	E_a
Clean Pd(111) (this work)	-1.91	0.77	-0.83	0.84
Clean Pd(111) by sheth *el al.*[9]	-1.79	0.88	-0.85	0.76

5.5 Examination of ethene hydrogenation on (100) surface

To resolve the origin of the poor selectivity of β phase, we have examined the ethene hydrogenation on Pd(100) and Pd_4H_3(100) with varied lattice constant. Both surfaces are pre-covered by 1 ML H atoms. We have compared the ethene hydrogenation on four different (100) surfaces, i.e. Pd (100) (a=3.94 Å), Pd (100) with expanded lattice (a=4.10 Å), Pd_4H_3 (100) with shrunk lattice (a=3.94 Å), and Pd_4H_3(100) (a=4.10 Å). As shown in Fig. S10, we found that the reaction barrier for the four surfaces are 0.89 eV, 0.64 eV, 0.96 eV and 0.79 eV respectively. Interestingly, the major difference among these surfaces lies in the ethene adsorption energy (see the dashed frame), not the elementary reaction barrier from the adsorbed ethene to ethane (being rather constantly ~0.65 eV).

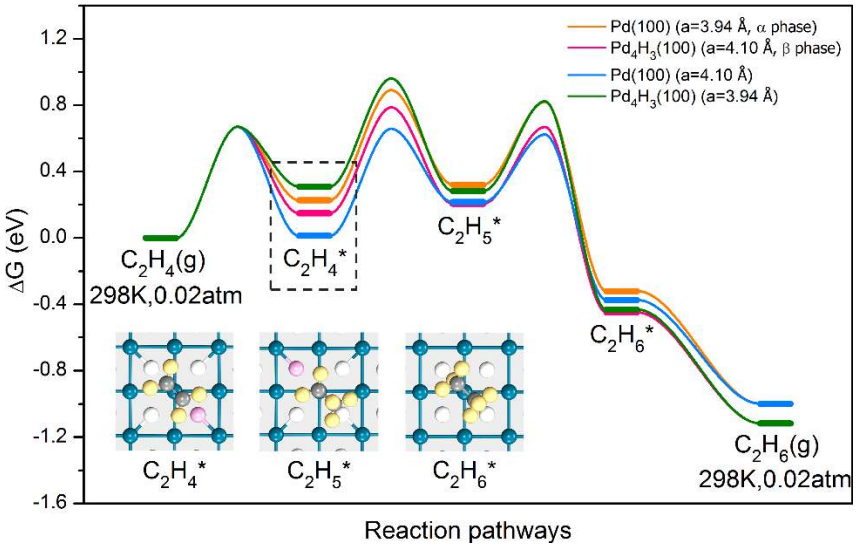


Fig. S10. Gibbs free energy profile for ethene hydrogenation on four surfaces: Pd (100) (a=3.94 Å, α phase), Pd (100) with expanded lattice (a=4.10 Å), Pd_4H_3 (100) with shrunk lattice (a=3.94 Å), and Pd_4H_3(100) (a=4.10 Å).

6. Kinetics parameters utilized in microkinetics simulation

Table S4. The Gibbs free energy barrier for acetylene/ethene hydrogenation on Pd(111), Pd(100), Pd_4H_3(111) and Pd_4H_3(100). The data is with respect to the standard state, i.e. 298 K, 1 bar, for all the gas phase molecules (e.g. hydrogen, acetylene, ethene and ethane). The effect of pressure change is explicitly taken into account in the microkinetics simulation via standard thermodynamics equation.

Elementary step		Pd(111)	Pd(100)	Pd_4H_3(111)	Pd_4H_3(100)
$H_2 + 2\# \rightleftarrows 2H\#$	Forward	0.32	0.32	0.32	0.32
	Reverse	0.62	0.92	0.62	0.92
$C_2H_2 + \# \rightleftarrows C_2H_2\#$	Forward	0.52	0.52	052	0.52
	Reverse	0.66	1.84	0.92	1.94
$C_2H_2\# + H\# \rightleftarrows C_2H_3\# + \#$	Forward	0.49	0.72	0.65	0.59
	Reverse	0.70	0.39	0.82	0.32
$C_2H_3\# + H\# \rightleftarrows C_2H_4\# + \#$	Forward	0.66	0.59	0.71	0.60
	Reverse	1.40	1.22	1.34	1.28
$C_2H_4\# + * \rightleftarrows C_2H_4* + \#$	Forward	0.30	0.35	0.30	0.35
	Reverse	0.30	0.40	0.30	0.40
$C_2H_4 + * \rightleftarrows C_2H_4*$	Forward	0.57	0.57	0.57	0.57
	Reverse	0	0.44	0	0.52
$C_2H_4* + H\# \rightleftarrows C_2H_5* + \#$	Forward	0.50	0.66	0.52	0.64
	Reverse	0.63	0.57	0.66	0.58
$C_2H_5* + H\# \rightleftarrows C_2H_6* + \#$	Forward	0.39	0.50	0.42	0.46
	Reverse	1.46	1.14	1.38	1.12
$C_2H_6* \rightleftarrows C_2H_6 + *$	Forward	0.01	0.02	0.02	0.03
	Reverse	0.60	0.60	0.60	0.60

#: Hollow site

*: Top site

7. Experimental details and characterization

7.1 Catalysts synthesis

Materials. Sodium palladium (II) chloride (Na_2PdCl_4, Pd 36.1%), L-ascorbic acid (AA, 99+%), polyvinylpyrrolidone (PVP, Mw ≈ 55000) and commercial Pd/C (10%, w/w), were obtained from Alfa Aesar. Green silicon carbide (SiC, 99.0%, average particle size of 60 mesh), quartz wool, KBr (99%), ethanol (99.7%), acetone (99.5%), formaldehyde (40% aqueous) and nitric acid (65 ~ 68%), were purchased from Sinopharm Chemical Reagent Co., Ltd. Vulcan XC-72R carbon (C) was purchased from Cabot Corporation (USA). Nitrogen (N_2, 99.99%), hydrogen (H_2, 99.999%), helium (He, 99.99%), mixed gas (5% H_2 and 95% Ar) and acetylene gas (C_2H_2, 99.9%) were supplied by Shanghai Air Liquide Co., Ltd. All the chemicals were used directly without further purification.

Synthesis of octahedral Pd/C. The octahedral Pd nanoparticles were synthesized following the previously reported method by Yang *et al.*[10] First, the Pd nanocubes were synthesized as the seeds. The aqueous solution (40 mL) containing PVP (525 mg), L-ascorbic acid (300 mg) and KBr (1.50 g) was added into a 100 mL round-bottomed flask. The solution was pre-heated at 80 °C for 5 min, and then added with 15 mL Na_2PdCl_4 (285 mg) aqueous solution. The round-bottomed flask was then capped, and the solution was maintained at 80 °C for 3 h under magnetic stirring. After centrifugation and washing by water for three times, the Pd nanocubes were dispersed in water for the following use.

Next, 3 mL Pd nanocubes aqueous suspension (1.88 mg/mL), and 80 mL aqueous solution containing HCHO (1 mL) and PVP (1050 mg), were added into a 150 mL round-bottomed flask. The solution was heated at 60 °C for 10 min under magnetic stirring. 30 mL Na_2PdCl_4 (290 mg) aqueous solution was then added to the round-bottomed flask in a short time, and maintained at 60 °C for 3 h under magnetic stirring. After centrifugation and washing by water for four times, the octahedral Pd nanoparticles were dispersed in the water.

To prepare the supported catalyst, 450 mg Vulcan XC-72R carbon was added to 350 mL deionized water (including 50 mg Pd octahedral nanoparticle), stirring for 12h. After immobilization for 12 h, the slurry was filtered, and the catalyst was washed thoroughly with deionized water.

Preparation of the Pd/C sample. Octahedral Pd/C and commercial Pd/C (10%) were reduced in the tube furnace under a flow of H_2 (5% in Ar) atmosphere with a total flow rate of 200 mL min^{-1}. The furnace was heated up to 200°C at a ramp rate of 5 °C min^{-1} and held at the final temperature for 2 hours.

7.2 Catalysts characterization

TEM image and XRD: The transmission electron microscopy (TEM) images (see Fig. 4(a-b) and Fig. S13) were taken by the Tecnai G2 F20 S-Twin (FEI, USA). The XRD (Fig. S11) was taken by the Bruker D8 Advance (Cu Kα radiation, Bruker AXS, Germany). Pd contents of the samples were determined by inductively coupled plasma optical emission spectrometer (ICP-AES, iCAP7400, USA).

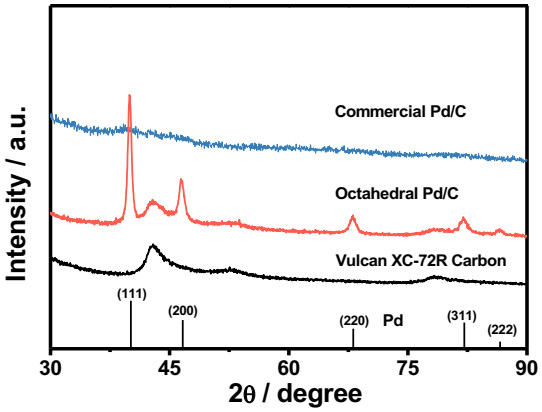


Fig. S11. X-ray diffraction (XRD) for commercial Pd/C, octahedral Pd/C and C support.

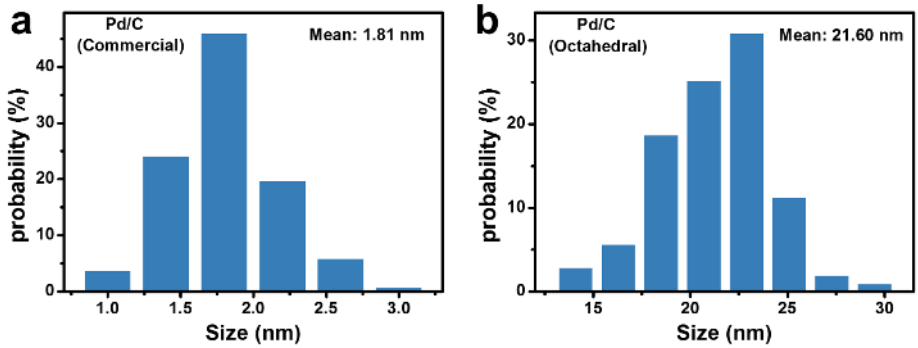


Fig. S12. Statistics of the nanoparticle size for (**a**) commercial Pd/C and (**b**) octahedral Pd/C.

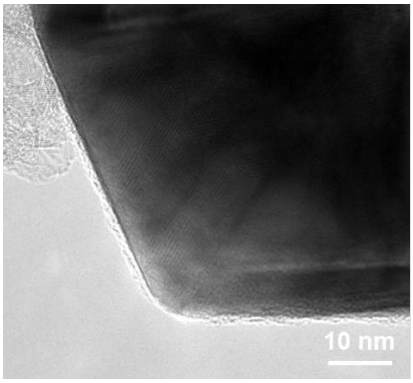


Fig. S13. HRTEM of octahedral Pd nanoparticle supported on Vulcan XC-72R carbon, showing the surface is covered with carbon overlayer.

7.3 Electrochemical experiments

Electrochemical workstation: All the electrochemical measurements were carried out on a CHI 660E electrochemical workstation (CH Instruments, Inc). In the three-electrode system, a glasscarbon electrode (GCE) was used as the working electrode (3 mm in diameter), a saturated calomel electrode (SCE, saturated KCl) as the reference electrode, and a carbon rod as the counter electrode.

Preparation of working electrode: The catalyst slurry was prepared by ultrasonically mixing 95 μL DI water, 95 μL ethanol, 10 μL nafion (5 wt %) and 1.0 mg catalyst for 40 min. The GCE was first polished with 0.05 mm alumina slurry by a Buehler micro polishing cloth, and then was droped with 10 μL catalyst slurry, and dried in air at ambient temperature.

CO stripping: Electrochemical surface area (ECSA) was estimated by CO stripping experiment. First, a cyclic voltammetry (CV) was carried out in N_2 saturated 1 M $HClO_4$ solution, at a scan rate of 100 mV s^{-1} with the potential ranging from 0.05 V to 1.30 V for ten cycles. Next, the solution was bubbled with CO at 0.2 V for 15 min, and bubbled with N_2 for 15 min. The CO stripping was then carried out at a scan rate of 10 mV s^{-1}, with the potential ranging from 0.05 V to 1.30 V. The ECSA of the Pd/C catalysts is calculated by:

$$\mathrm{ECSA} = Q / (m \cdot C) \quad (6)$$

where m is the Pd loading, Q is the reduction charge, and C is the charge of 1 ML H on Pd (420 μC·cm^{-2}). Besides, the surface normalization is performed by using the H-UPD coulometry with a charge density of *ca*. 205 μC cm^{-2} for Pd.

Table S5. Content Analysis of Pd/C Catalysts.

Catalyst	Nominal loading	Actual loading[a]	ECSA[b] (m^2*g^{-1})
	Pd (%)	Pd (%)	
Pd/C (Commercial)	10	9.47	64.87
Pd/C (Octahedral)	10	9.72	7.41

[a] Determined by ICP analysis.

[b] Calculated by CO stripping.

To identify the content of surface H and subsurface/bulk H on the Pd catalysts, we carried out the electrochemical experiments by using CV on the commercial Pd/C and the octahedral Pd/C. The CO stripping CV on the two catalysts is shown in Fig. S14. In the first scan, with CO saturated on the surface, there is a CO oxidation peak at ~1.0 V vs. RHE, from which we can estimate the ECSA for the two catalysts (see Table S5). In the second scan, as the surface CO oxidized, the proton then can deposit on the surface.

The second CV scan has been integrated and highlighted in Fig. S15 for comparison. For commercial Pd/C, there are three deposited H peaks at 0.04 V, 0.11 V and 0.24 V, respectively. The first two peaks correspond to the subsurface/bulk H deposition, while the third peaks correspond to the surface H deposition. The H:Pd ratio is calculated to be 0.82, close to the ratio of Pd_4H_3. In contrast, for octahedral Pd/C, there are two deposited H peak at 0.20 V and 0.24 V, which can be assigned to subsurface H and surface H, respectively. The H:Pd ratio is calculated to be 0.14. Since the ratio is far smaller than the ratio in Pd_4H_3, we deduce that H can only diffuse into the top few surface layers on octahedral Pd/C, and the bulk PdH_x phase does not form.

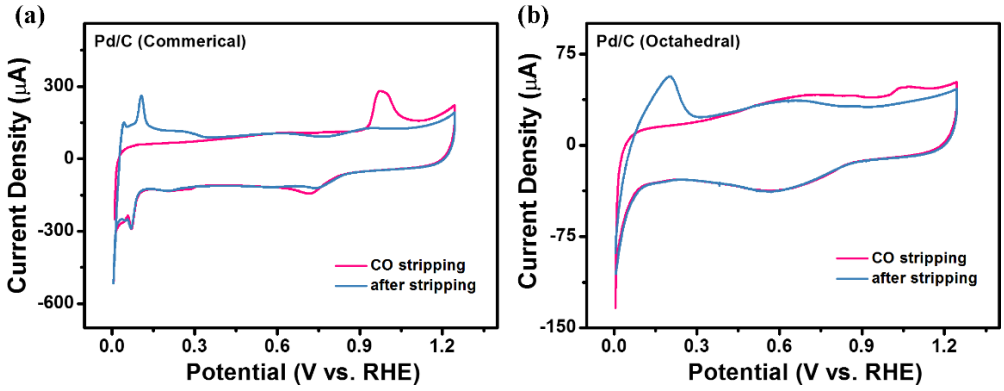


Fig. S14. CO stripping CV of (a) commercial Pd/C, (b) octahedral Pd/C. The solution is 1 M $HClO_4$, the scanning speed v=10 mV s^{-1} and T=298 K. In experiment, CO is utilized to saturate the surfaces first by pumping CO at 0.2 V vs. RHE for 15 min.

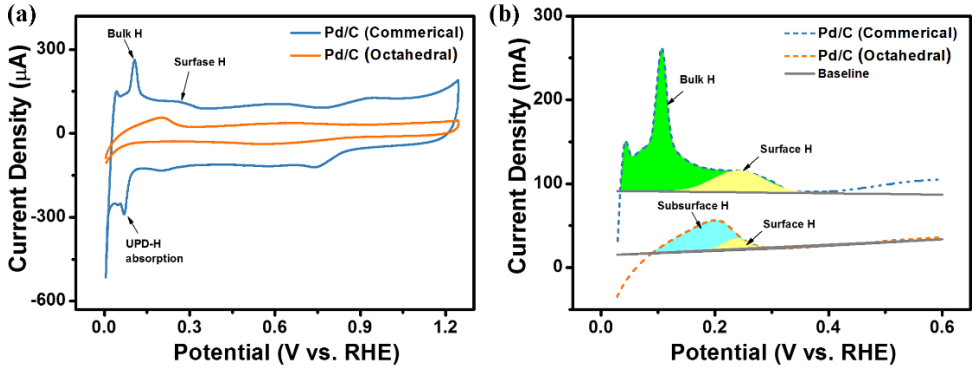


Fig. S15. (a) CV of commercial Pd/C and octahedral Pd/C in 1 M $HClO_4$ at the scanning speed of v=10 mV s^{-1}. (b) Enlarged plot of (a) to show the peaks of surface H and bulk H.

7.4 Hydrogenation reaction

The catalytic properties of octahedral Pd/C and commercial Pd/C for acetylene selective hydrogenation were evaluated by a continuous flow fixed-bed quartz tubular reactor (i.d.=10 mm) under atmospheric pressure. The catalyst containing 5 mg palladium (determined by ICP-OES measurement) was mixed with 20 g green silicon carbide, and placed in the reactor. The input gas consists of C_2H_2, H_2, and N_2 (for balance). The total flow rate was 100 ml min^{-1} in all experiments, corresponding to a gas hourly space velocity (GHSV) of 120,000 mL g^{-1} h^{-1}. The turnover frequency (TOF) of acetylene hydrogenation was measured at 20 ºC at a low acetylene conversion (<20%). The products were analyzed by using an online GC (Agilent 7890B), which is equipped with two thermal conductivity detector (TCD) and a flame ionization detector (FID). Hayesep Q and MolSieve 5Å packed columns were connected to TCD, while HP-FFAP and HP-AL/S capillary columns were connected to FID.

The activity and selectivity of the catalysts were calculated from the data of quasi-steady state (after 3 h time in stream), using the following equations:

$$C_{\text{acetylene}} = \frac{\text{C}_2\text{H}_2\ \text{(in)} - \text{C}_2\text{H}_2\ \text{(out)}}{\text{C}_2\text{H}_2\ \text{(in)}} \times 100\% \quad (7)$$

$$S_{\text{ethene}} = \frac{\text{C}_2\text{H}_4\ \text{(out)}}{\text{C}_2\text{H}_2\ \text{(in)} - \text{C}_2\text{H}_2\ \text{(out)}} \times 100\% \quad (8)$$

$$S_{\text{ethane}} = \frac{\text{C}_2\text{H}_6\ \text{(out)}}{\text{C}_2\text{H}_2\ \text{(in)} - \text{C}_2\text{H}_2\ \text{(out)}} \times 100\% \quad (9)$$

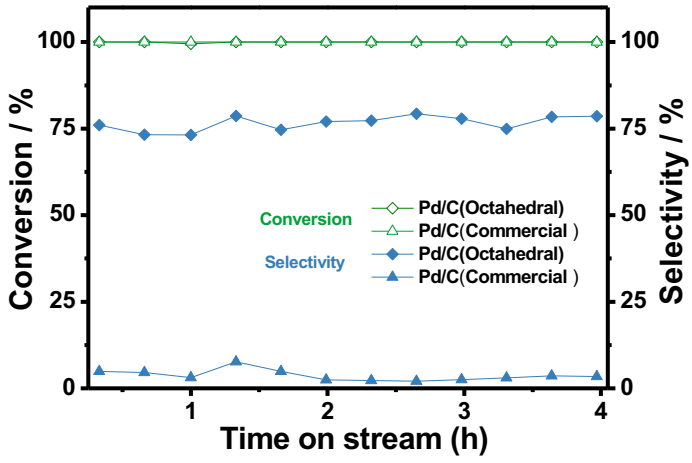


Fig. S16. Time-dependent behaviors of octahedral Pd/C ($p(H_2)$=0.60 atm) and commercial Pd/C ($p(H_2)$=0.10 atm) in acetylene selective hydrogenation. Reaction conditions: 50 mg catalyst, $p(C_2H_2)$=0.02 atm, total flow = 100 mL min^{-1} (N_2 as a diluent), GHSV = 120 000 mL g^{-1} h^{-1}.

Reference

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8. XYZ coordinates for all the structures in Fig. 3

Initial Pd(111). The energy from VASP is -378.784169 eV.

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Pd	4.022272274	5.541148999	6.343819775	CORE	2 Pd Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738	CORE	3 Pd Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485	CORE	4 Pd Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004	CORE	5 Pd Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336	CORE	6 Pd Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492	CORE	7 Pd Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712	CORE	8 Pd Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883	CORE	9 Pd Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717	CORE	10 Pd Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710	CORE	11 Pd Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199	CORE	12 Pd Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101	CORE	13 Pd Pd	0.0000	13
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Pd	9.597706838	5.541375735	6.344926776	CORE	16 Pd Pd	0.0000	16
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Pd	4.026560428	3.933717478	8.619778674	CORE	18 Pd Pd	0.0000	18
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Pd	6.814227378	8.762524945	8.620282578	CORE	28 Pd Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724	CORE	29 Pd Pd	0.0000	29
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Pd	10.995872940	6.348591411	8.621985519	CORE	32 Pd Pd	0.0000	32
Pd	8.210899551	4.740665401	10.906613112	CORE	33 Pd Pd	0.0000	33
Pd	9.604941608	2.326523430	10.906376288	CORE	34 Pd Pd	0.0000	34
Pd	6.817263019	7.154924553	10.906417497	CORE	35 Pd Pd	0.0000	35
Pd	13.786370252	9.568933039	10.906780169	CORE	36 Pd Pd	0.0000	36
Pd	6.817187292	2.326717229	10.906074821	CORE	37 Pd Pd	0.0000	37
Pd	15.179902472	7.154955798	10.906794838	CORE	38 Pd Pd	0.0000	38
Pd	5.423527817	4.740649428	10.905989725	CORE	39 Pd Pd	0.0000	39
Pd	16.573614856	9.568996816	10.906309195	CORE	40 Pd Pd	0.0000	40

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Pd      10.998447484    9.568966863    10.906569797 CORE    42 Pd Pd    0.0000    42
Pd       4.029767615    2.326600486    10.905753003 CORE    43 Pd Pd    0.0000    43
Pd      12.392567434    7.154823065    10.907355021 CORE    44 Pd Pd    0.0000    44
Pd      12.392255748    2.326655307    10.906085587 CORE    45 Pd Pd    0.0000    45
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Pd      10.998750289    4.740697529    10.906931257 CORE    47 Pd Pd    0.0000    47
Pd       9.604833063    7.154960368    10.907075113 CORE    48 Pd Pd    0.0000    48
Pd       5.425508184    3.132304821    13.228414620 CORE    49 Pd Pd    0.0000    49
Pd       9.606742504    0.718461025    13.228996144 CORE    50 Pd Pd    0.0000    50
Pd       5.425448347    7.960346715    13.228999193 CORE    51 Pd Pd    0.0000    51
Pd       8.212386584    3.132818166    13.228708031 CORE    52 Pd Pd    0.0000    52
Pd       6.819374086    5.546138785    13.228711731 CORE    53 Pd Pd    0.0000    53
Pd       6.818718113    0.718564881    13.228917886 CORE    54 Pd Pd    0.0000    54
Pd       4.031408785    5.546523426    13.228875523 CORE    55 Pd Pd    0.0000    55
Pd      13.787692078    7.960035909    13.229447319 CORE    56 Pd Pd    0.0000    56
Pd       2.637790501    3.132270253    13.228640218 CORE    57 Pd Pd    0.0000    57
Pd       9.606241244    5.546686808    13.229220003 CORE    58 Pd Pd    0.0000    58
Pd       4.031597557    0.718403947    13.228626696 CORE    59 Pd Pd    0.0000    59
Pd       1.244314017    0.718539283    13.228756309 CORE    60 Pd Pd    0.0000    60
Pd      11.000594171    3.132395339    13.228884936 CORE    61 Pd Pd    0.0000    61
Pd       8.213116770    7.960360579    13.228880584 CORE    62 Pd Pd    0.0000    62
Pd      12.394282563    5.546602539    13.229324031 CORE    63 Pd Pd    0.0000    63
Pd      11.000126927    7.960402480    13.229328221 CORE    64 Pd Pd    0.0000    64
H        6.819170630    3.937153178    14.044191024 CORE    65 H  H     0.0000    65
H        4.031792964    3.937112146    14.044325083 CORE    66 H  H     0.0000    66
H        5.425444689    1.523245817    14.044320552 CORE    67 H  H     0.0000    67
H        8.213031681    1.523193044    14.044787715 CORE    68 H  H     0.0000    68
H        5.425543816    6.351224328    14.044628896 CORE    69 H  H     0.0000    69
H        2.638053280    1.523196720    14.044409721 CORE    70 H  H     0.0000    70
H       15.181965321    8.765368570    14.045114489 CORE    71 H  H     0.0000    71
H       13.788193537    6.351134336    14.044857523 CORE    72 H  H     0.0000    72
H       12.394280033    8.765454854    14.045045932 CORE    73 H  H     0.0000    73
H        9.606725725    3.937040108    14.044714468 CORE    74 H  H     0.0000    74
H        8.212853212    6.351262526    14.044546045 CORE    75 H  H     0.0000    75
H       12.394378936    3.936997632    14.044688279 CORE    76 H  H     0.0000    76
H        9.606645124    8.765454906    14.044683949 CORE    77 H  H     0.0000    77
H       11.000653240    1.523168528    14.044755144 CORE    78 H  H     0.0000    78
H        6.819317915    8.765374710    14.044733030 CORE    79 H  H     0.0000    79
H       11.000519537    6.351231296    14.044998596 CORE    80 H  H     0.0000    80
end
end
```

Acetylene adsorbed on Pd(111). The energy from VASP is -398.672184 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	60.00000000	
Pd	6.809789092	0.713021845	6.343804094	CORE	1 Pd Pd	0.0000	1
Pd	4.022272274	5.541148999	6.343819775	CORE	2 Pd Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738	CORE	3 Pd Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485	CORE	4 Pd Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004	CORE	5 Pd Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336	CORE	6 Pd Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492	CORE	7 Pd Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712	CORE	8 Pd Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883	CORE	9 Pd Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717	CORE	10 Pd Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710	CORE	11 Pd Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199	CORE	12 Pd Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101	CORE	13 Pd Pd	0.0000	13
Pd	10.991373809	7.955436933	6.345265089	CORE	14 Pd Pd	0.0000	14
Pd	1.234428020	0.712833244	6.342029531	CORE	15 Pd Pd	0.0000	15
Pd	9.597706838	5.541375735	6.344926776	CORE	16 Pd Pd	0.0000	16
Pd	5.419869613	1.520422400	8.619780622	CORE	17 Pd Pd	0.0000	17
Pd	4.026560428	3.933717478	8.619778674	CORE	18 Pd Pd	0.0000	18
Pd	15.177210300	8.762689012	8.621082754	CORE	19 Pd Pd	0.0000	19
Pd	8.207619922	1.520449870	8.620764212	CORE	20 Pd Pd	0.0000	20
Pd	5.420456737	6.347962245	8.620778994	CORE	21 Pd Pd	0.0000	21
Pd	6.814172092	3.934277993	8.620114302	CORE	22 Pd Pd	0.0000	22
Pd	12.389417999	8.762965696	8.621923738	CORE	23 Pd Pd	0.0000	23
Pd	13.783550971	6.348239961	8.621933874	CORE	24 Pd Pd	0.0000	24
Pd	9.601765066	3.934169030	8.621232717	CORE	25 Pd Pd	0.0000	25
Pd	10.995589003	1.520212695	8.620276726	CORE	26 Pd Pd	0.0000	26
Pd	8.207876417	6.348469951	8.621233758	CORE	27 Pd Pd	0.0000	27
Pd	6.814227378	8.762524945	8.620282578	CORE	28 Pd Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724	CORE	29 Pd Pd	0.0000	29
Pd	12.389096274	3.933994969	8.621047892	CORE	30 Pd Pd	0.0000	30
Pd	9.601392037	8.762455531	8.621048992	CORE	31 Pd Pd	0.0000	31
Pd	10.995872940	6.348591411	8.621985519	CORE	32 Pd Pd	0.0000	32
Pd	8.192464588	4.744394937	10.935939972	CORE	33 Pd Pd	0.0000	33
Pd	9.580033347	2.338924454	10.913552286	CORE	34 Pd Pd	0.0000	34
Pd	6.815521148	7.120491366	10.945916620	CORE	35 Pd Pd	0.0000	35
Pd	13.782213914	9.575913410	10.897996493	CORE	36 Pd Pd	0.0000	36
Pd	6.815411493	2.339998556	10.915888506	CORE	37 Pd Pd	0.0000	37
Pd	15.180008884	7.159793521	10.890568550	CORE	38 Pd Pd	0.0000	38
Pd	5.438553061	4.744322718	10.935393755	CORE	39 Pd Pd	0.0000	39
Pd	16.572846163	9.568323743	10.894128298	CORE	40 Pd Pd	0.0000	40
Pd	13.785694498	4.741357270	10.887130474	CORE	41 Pd Pd	0.0000	41
Pd	10.998840496	9.575957339	10.897698820	CORE	42 Pd Pd	0.0000	42
Pd	4.051018645	2.338996478	10.912977368	CORE	43 Pd Pd	0.0000	43

Pd	12.390597003	7.156358934	10.899065943	CORE	44	Pd	Pd	0.0000	44
Pd	12.390542018	2.319963392	10.878235842	CORE	45	Pd	Pd	0.0000	45
Pd	8.208096839	9.568415872	10.893869617	CORE	46	Pd	Pd	0.0000	46
Pd	10.995348749	4.741467291	10.887533138	CORE	47	Pd	Pd	0.0000	47
Pd	9.601081054	7.159766977	10.890723746	CORE	48	Pd	Pd	0.0000	48
Pd	5.412361216	3.142195626	13.308191643	CORE	49	Pd	Pd	0.0000	49
Pd	9.608903491	0.716048243	13.210648514	CORE	50	Pd	Pd	0.0000	50
Pd	5.418677158	7.971246364	13.203006167	CORE	51	Pd	Pd	0.0000	51
Pd	8.219616519	3.142193316	13.308327717	CORE	52	Pd	Pd	0.0000	52
Pd	6.816004306	5.546155004	13.532811650	CORE	53	Pd	Pd	0.0000	53
Pd	6.815891906	0.732069860	13.214605548	CORE	54	Pd	Pd	0.0000	54
Pd	4.014529096	5.565633552	13.185147659	CORE	55	Pd	Pd	0.0000	55
Pd	13.780326970	7.971064327	13.218458179	CORE	56	Pd	Pd	0.0000	56
Pd	2.615581570	3.124215507	13.179378981	CORE	57	Pd	Pd	0.0000	57
Pd	9.617428652	5.565750629	13.185544732	CORE	58	Pd	Pd	0.0000	58
Pd	4.022869948	0.716106514	13.210137798	CORE	59	Pd	Pd	0.0000	59
Pd	1.240909387	0.713451986	13.211943799	CORE	60	Pd	Pd	0.0000	60
Pd	11.016447052	3.124222750	13.179568866	CORE	61	Pd	Pd	0.0000	61
Pd	8.213067113	7.971317025	13.202895581	CORE	62	Pd	Pd	0.0000	62
Pd	12.390959248	5.550848312	13.215615490	CORE	63	Pd	Pd	0.0000	63
Pd	11.001543873	7.971100754	13.218414877	CORE	64	Pd	Pd	0.0000	64
H	3.902091469	3.962956979	13.981893209	CORE	65	H	H	0.0000	65
H	5.396455808	1.459650621	14.043605729	CORE	66	H	H	0.0000	66
H	8.235273366	1.459724624	14.043834407	CORE	67	H	H	0.0000	67
H	5.341820811	6.442977129	14.069702763	CORE	68	H	H	0.0000	68
H	2.629450624	1.523322154	14.025136734	CORE	69	H	H	0.0000	69
H	15.179485761	8.769962579	14.032665689	CORE	70	H	H	0.0000	70
H	13.778783211	6.360627500	14.027616520	CORE	71	H	H	0.0000	71
H	12.391019711	8.775283131	14.034747418	CORE	72	H	H	0.0000	72
H	9.730100894	3.963018297	13.982055701	CORE	73	H	H	0.0000	73
H	8.290131812	6.443270530	14.069828725	CORE	74	H	H	0.0000	74
H	12.391146871	3.937491726	14.019326926	CORE	75	H	H	0.0000	75
H	9.602477270	8.770082905	14.032432633	CORE	76	H	H	0.0000	76
H	11.002629846	1.523372167	14.025360693	CORE	77	H	H	0.0000	77
H	6.815981931	8.762067623	14.031574055	CORE	78	H	H	0.0000	78
H	11.003440935	6.360741894	14.027726458	CORE	79	H	H	0.0000	79
C	7.483613170	3.985603665	15.006811803	CORE	80	C	C	0.0000	80
C	6.148711505	3.985543466	15.006823132	CORE	81	C	C	0.0000	81
H	8.191365569	4.180624306	15.812983845	CORE	82	H	H	0.0000	82
H	5.441014105	4.180621758	15.812854940	CORE	83	H	H	0.0000	83

end

end

TS from acetylene to vinyl on Pd(111). The energy from VASP is -398.092782 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	60.00000000	
Pd	6.809789092	0.713021845	6.343804094	CORE	1 Pd Pd	0.0000	1
Pd	4.022272274	5.541148999	6.343819775	CORE	2 Pd Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738	CORE	3 Pd Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485	CORE	4 Pd Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004	CORE	5 Pd Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336	CORE	6 Pd Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492	CORE	7 Pd Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712	CORE	8 Pd Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883	CORE	9 Pd Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717	CORE	10 Pd Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710	CORE	11 Pd Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199	CORE	12 Pd Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101	CORE	13 Pd Pd	0.0000	13
Pd	10.991373809	7.955436933	6.345265089	CORE	14 Pd Pd	0.0000	14
Pd	1.234428020	0.712833244	6.342029531	CORE	15 Pd Pd	0.0000	15
Pd	9.597706838	5.541375735	6.344926776	CORE	16 Pd Pd	0.0000	16
Pd	5.419869613	1.520422400	8.619780622	CORE	17 Pd Pd	0.0000	17
Pd	4.026560428	3.933717478	8.619778674	CORE	18 Pd Pd	0.0000	18
Pd	15.177210300	8.762689012	8.621082754	CORE	19 Pd Pd	0.0000	19
Pd	8.207619922	1.520449870	8.620764212	CORE	20 Pd Pd	0.0000	20
Pd	5.420456737	6.347962245	8.620778994	CORE	21 Pd Pd	0.0000	21
Pd	6.814172092	3.934277993	8.620114302	CORE	22 Pd Pd	0.0000	22
Pd	12.389417999	8.762965696	8.621923738	CORE	23 Pd Pd	0.0000	23
Pd	13.783550971	6.348239961	8.621933874	CORE	24 Pd Pd	0.0000	24
Pd	9.601765066	3.934169030	8.621232717	CORE	25 Pd Pd	0.0000	25
Pd	10.995589003	1.520212695	8.620276726	CORE	26 Pd Pd	0.0000	26
Pd	8.207876417	6.348469951	8.621233758	CORE	27 Pd Pd	0.0000	27
Pd	6.814227378	8.762524945	8.620282578	CORE	28 Pd Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724	CORE	29 Pd Pd	0.0000	29
Pd	12.389096274	3.933994969	8.621047892	CORE	30 Pd Pd	0.0000	30
Pd	9.601392037	8.762455531	8.621048992	CORE	31 Pd Pd	0.0000	31
Pd	10.995872940	6.348591411	8.621985519	CORE	32 Pd Pd	0.0000	32
Pd	8.210648179	4.725664968	10.948366879	CORE	33 Pd Pd	0.0000	33
Pd	9.585050889	2.339061617	10.952635127	CORE	34 Pd Pd	0.0000	34
Pd	6.822429559	7.130850751	10.940785484	CORE	35 Pd Pd	0.0000	35
Pd	13.795651552	9.564260000	10.914891539	CORE	36 Pd Pd	0.0000	36
Pd	6.826330287	2.330808679	10.941092734	CORE	37 Pd Pd	0.0000	37
Pd	15.190051054	7.143958822	10.923552239	CORE	38 Pd Pd	0.0000	38
Pd	5.438707329	4.737652729	10.925415734	CORE	39 Pd Pd	0.0000	39
Pd	16.573697129	9.570355615	10.915465920	CORE	40 Pd Pd	0.0000	40
Pd	13.798786091	4.735948700	10.921692127	CORE	41 Pd Pd	0.0000	41
Pd	11.003433303	9.566016532	10.911340006	CORE	42 Pd Pd	0.0000	42
Pd	4.041669851	2.329538919	10.922180256	CORE	43 Pd Pd	0.0000	43

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Pd      12.401565714    7.150697003    10.922267351 CORE    44 Pd Pd    0.0000    44
Pd      12.388745968    2.324334064    10.910506290 CORE    45 Pd Pd    0.0000    45
Pd       8.204242656    9.565583874    10.903266193 CORE    46 Pd Pd    0.0000    46
Pd      11.007551717    4.737958704    10.913620121 CORE    47 Pd Pd    0.0000    47
Pd       9.610294632    7.153812235    10.911747957 CORE    48 Pd Pd    0.0000    48
Pd       5.401831075    3.097787243    13.274871889 CORE    49 Pd Pd    0.0000    49
Pd       9.607790134    0.729226765    13.246888729 CORE    50 Pd Pd    0.0000    50
Pd       5.434359059    7.978334700    13.234459247 CORE    51 Pd Pd    0.0000    51
Pd       8.180811252    3.168910633    13.457284823 CORE    52 Pd Pd    0.0000    52
Pd       6.862092212    5.548904301    13.346216769 CORE    53 Pd Pd    0.0000    53
Pd       6.834046404    0.704162908    13.226888169 CORE    54 Pd Pd    0.0000    54
Pd       4.065725820    5.519642743    13.274606795 CORE    55 Pd Pd    0.0000    55
Pd      13.806501501    7.946658430    13.264384889 CORE    56 Pd Pd    0.0000    56
Pd       2.644293237    3.133712455    13.234811211 CORE    57 Pd Pd    0.0000    57
Pd       9.640117201    5.553150353    13.223714373 CORE    58 Pd Pd    0.0000    58
Pd       4.021512832    0.698481745    13.223137465 CORE    59 Pd Pd    0.0000    59
Pd       1.246240124    0.725755556    13.248709136 CORE    60 Pd Pd    0.0000    60
Pd      11.008069086    3.135848468    13.252092527 CORE    61 Pd Pd    0.0000    61
Pd       8.224801888    7.974560656    13.234172582 CORE    62 Pd Pd    0.0000    62
Pd      12.421585389    5.540365736    13.256833096 CORE    63 Pd Pd    0.0000    63
Pd      11.017429901    7.955532057    13.256927007 CORE    64 Pd Pd    0.0000    64
H        4.586818846    4.186314346    14.407024837 CORE    65 H  H     0.0000    65
H        5.401518756    1.409555066    14.035080544 CORE    66 H  H     0.0000    66
H        8.235657637    1.462238206    14.097311848 CORE    67 H  H     0.0000    67
H        5.384975075    6.457213287    14.075634576 CORE    68 H  H     0.0000    68
H        2.645093102    1.545269901    14.061734665 CORE    69 H  H     0.0000    69
H       15.193209389    8.775710732    14.073243700 CORE    70 H  H     0.0000    70
H       13.809044775    6.331270318    14.090442074 CORE    71 H  H     0.0000    71
H       12.412005795    8.762030019    14.074596819 CORE    72 H  H     0.0000    72
H        9.683590050    3.961959284    14.097511442 CORE    73 H  H     0.0000    73
H        8.294235867    6.414634247    14.063956330 CORE    74 H  H     0.0000    74
H       12.427485252    3.920256898    14.073737253 CORE    75 H  H     0.0000    75
H        9.617061893    8.759795764    14.072599702 CORE    76 H  H     0.0000    76
H       11.003584231    1.528913817    14.076326007 CORE    77 H  H     0.0000    77
H        6.834042710    8.777209994    14.068281681 CORE    78 H  H     0.0000    78
H       11.026644213    6.348162725    14.072969006 CORE    79 H  H     0.0000    79
C        7.054687835    4.320236437    15.016742547 CORE    80 C  C     0.0000    80
C        5.913191347    3.637704252    15.188324070 CORE    81 C  C     0.0000    81
H        7.740369587    4.637450103    15.807988709 CORE    82 H  H     0.0000    82
H        5.500701313    3.160552568    16.080315019 CORE    83 H  H     0.0000    83
end
end
```

Vinyl adsorbed on Pd(111). The energy from VASP is -402.599071 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	60.00000000	
Pd	6.809789092	0.713021845	6.343804094	CORE	1 Pd Pd	0.0000	1
Pd	4.022272274	5.541148999	6.343819775	CORE	2 Pd Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738	CORE	3 Pd Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485	CORE	4 Pd Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004	CORE	5 Pd Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336	CORE	6 Pd Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492	CORE	7 Pd Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712	CORE	8 Pd Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883	CORE	9 Pd Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717	CORE	10 Pd Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710	CORE	11 Pd Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199	CORE	12 Pd Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101	CORE	13 Pd Pd	0.0000	13
Pd	10.991373809	7.955436933	6.345265089	CORE	14 Pd Pd	0.0000	14
Pd	1.234428020	0.712833244	6.342029531	CORE	15 Pd Pd	0.0000	15
Pd	9.597706838	5.541375735	6.344926776	CORE	16 Pd Pd	0.0000	16
Pd	5.419869613	1.520422400	8.619780622	CORE	17 Pd Pd	0.0000	17
Pd	4.026560428	3.933717478	8.619778674	CORE	18 Pd Pd	0.0000	18
Pd	15.177210300	8.762689012	8.621082754	CORE	19 Pd Pd	0.0000	19
Pd	8.207619922	1.520449870	8.620764212	CORE	20 Pd Pd	0.0000	20
Pd	5.420456737	6.347962245	8.620778994	CORE	21 Pd Pd	0.0000	21
Pd	6.814172092	3.934277993	8.620114302	CORE	22 Pd Pd	0.0000	22
Pd	12.389417999	8.762965696	8.621923738	CORE	23 Pd Pd	0.0000	23
Pd	13.783550971	6.348239961	8.621933874	CORE	24 Pd Pd	0.0000	24
Pd	9.601765066	3.934169030	8.621232717	CORE	25 Pd Pd	0.0000	25
Pd	10.995589003	1.520212695	8.620276726	CORE	26 Pd Pd	0.0000	26
Pd	8.207876417	6.348469951	8.621233758	CORE	27 Pd Pd	0.0000	27
Pd	6.814227378	8.762524945	8.620282578	CORE	28 Pd Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724	CORE	29 Pd Pd	0.0000	29
Pd	12.389096274	3.933994969	8.621047892	CORE	30 Pd Pd	0.0000	30
Pd	9.601392037	8.762455531	8.621048992	CORE	31 Pd Pd	0.0000	31
Pd	10.995872940	6.348591411	8.621985519	CORE	32 Pd Pd	0.0000	32
Pd	8.198062942	4.735010975	10.920405699	CORE	33 Pd Pd	0.0000	33
Pd	9.578810508	2.334636022	10.924642642	CORE	34 Pd Pd	0.0000	34
Pd	6.809583327	7.131233485	10.924635242	CORE	35 Pd Pd	0.0000	35
Pd	13.783790442	9.571935249	10.895863630	CORE	36 Pd Pd	0.0000	36
Pd	6.813661700	2.339183705	10.929978033	CORE	37 Pd Pd	0.0000	37
Pd	15.179683632	7.154334726	10.895638613	CORE	38 Pd Pd	0.0000	38
Pd	5.430877871	4.734237972	10.929795770	CORE	39 Pd Pd	0.0000	39
Pd	16.563557057	9.565042918	10.903855638	CORE	40 Pd Pd	0.0000	40
Pd	13.786938609	4.739136534	10.892726108	CORE	41 Pd Pd	0.0000	41
Pd	10.996023683	9.573329330	10.892941734	CORE	42 Pd Pd	0.0000	42
Pd	4.046857813	2.338467784	10.920132967	CORE	43 Pd Pd	0.0000	43

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Pd        12.390112244    7.155420944    10.898707850 CORE    44 Pd Pd    0.0000    44
Pd        12.383826527    2.320993610    10.887975520 CORE    45 Pd Pd    0.0000    45
Pd         8.200344843    9.567266385    10.888031545 CORE    46 Pd Pd    0.0000    46
Pd        10.998281880    4.736677095    10.887185976 CORE    47 Pd Pd    0.0000    47
Pd         9.599554645    7.159445137    10.887172849 CORE    48 Pd Pd    0.0000    48
Pd         5.405187957    3.124480412    13.370765646 CORE    49 Pd Pd    0.0000    49
Pd         9.595043116    0.725868044    13.223095664 CORE    50 Pd Pd    0.0000    50
Pd         5.423208743    7.951953562    13.222855006 CORE    51 Pd Pd    0.0000    51
Pd         8.185449502    3.169269914    13.361691734 CORE    52 Pd Pd    0.0000    52
Pd         6.834820174    5.510213505    13.360375342 CORE    53 Pd Pd    0.0000    53
Pd         6.816234010    0.720832940    13.195469401 CORE    54 Pd Pd    0.0000    54
Pd         4.029322346    5.547883766    13.194717385 CORE    55 Pd Pd    0.0000    55
Pd        13.787463294    7.963624645    13.220014838 CORE    56 Pd Pd    0.0000    56
Pd         2.613076434    3.121971319    13.192849090 CORE    57 Pd Pd    0.0000    57
Pd         9.628912797    5.562500927    13.171021336 CORE    58 Pd Pd    0.0000    58
Pd         4.007623254    0.707196555    13.193205373 CORE    59 Pd Pd    0.0000    59
Pd         1.227069990    0.711795143    13.212187806 CORE    60 Pd Pd    0.0000    60
Pd        10.997902568    3.128440160    13.201146071 CORE    61 Pd Pd    0.0000    61
Pd         8.205630907    7.965591068    13.201141372 CORE    62 Pd Pd    0.0000    62
Pd        12.397563602    5.547662190    13.216219254 CORE    63 Pd Pd    0.0000    63
Pd        11.000429737    7.967769649    13.216261748 CORE    64 Pd Pd    0.0000    64
H          5.387991537    1.415887458    14.013111188 CORE    65 H  H     0.0000    65
H          8.207460619    1.466855451    14.065535039 CORE    66 H  H     0.0000    66
H          5.370801113    6.380000144    14.064715199 CORE    67 H  H     0.0000    67
H          2.617365631    1.514532832    14.023117560 CORE    68 H  H     0.0000    68
H         15.182038759    8.768851700    14.034748051 CORE    69 H  H     0.0000    69
H         13.789312244    6.354457909    14.027125680 CORE    70 H  H     0.0000    70
H         12.394801353    8.769787326    14.027341469 CORE    71 H  H     0.0000    71
H          9.709690346    3.975659757    14.027351008 CORE    72 H  H     0.0000    72
H          8.294949556    6.426288619    14.027172548 CORE    73 H  H     0.0000    73
H         12.385064041    3.935541718    14.024851237 CORE    74 H  H     0.0000    74
H          9.598164431    8.763287116    14.025035340 CORE    75 H  H     0.0000    75
H         10.995823237    1.523253035    14.037194403 CORE    76 H  H     0.0000    76
H          6.814210967    8.766194819    14.037152799 CORE    77 H  H     0.0000    77
H         11.008517430    6.359114383    14.025986213 CORE    78 H  H     0.0000    78
H          3.916153204    3.963646231    14.012336328 CORE    79 H  H     0.0000    79
C          7.240846840    4.185733574    14.870842192 CORE    80 C  C     0.0000    80
C          6.065172204    3.509219313    15.343891011 CORE    81 C  C     0.0000    81
H          7.976180845    4.608787615    15.568856521 CORE    82 H  H     0.0000    82
H          6.216637757    2.544895394    15.843720984 CORE    83 H  H     0.0000    83
H          5.305722149    4.126635844    15.839456711 CORE    84 H  H     0.0000    84
end
end
```

TS from vinyl to ethene on Pd(111). The energy from VASP is -401.898406 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	60.00000000	
Pd	6.809789092	0.713021845	6.343804094	CORE	1 Pd Pd	0.0000	1
Pd	4.022272274	5.541148999	6.343819775	CORE	2 Pd Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738	CORE	3 Pd Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485	CORE	4 Pd Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004	CORE	5 Pd Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336	CORE	6 Pd Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492	CORE	7 Pd Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712	CORE	8 Pd Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883	CORE	9 Pd Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717	CORE	10 Pd Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710	CORE	11 Pd Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199	CORE	12 Pd Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101	CORE	13 Pd Pd	0.0000	13
Pd	10.991373809	7.955436933	6.345265089	CORE	14 Pd Pd	0.0000	14
Pd	1.234428020	0.712833244	6.342029531	CORE	15 Pd Pd	0.0000	15
Pd	9.597706838	5.541375735	6.344926776	CORE	16 Pd Pd	0.0000	16
Pd	5.419869613	1.520422400	8.619780622	CORE	17 Pd Pd	0.0000	17
Pd	4.026560428	3.933717478	8.619778674	CORE	18 Pd Pd	0.0000	18
Pd	15.177210300	8.762689012	8.621082754	CORE	19 Pd Pd	0.0000	19
Pd	8.207619922	1.520449870	8.620764212	CORE	20 Pd Pd	0.0000	20
Pd	5.420456737	6.347962245	8.620778994	CORE	21 Pd Pd	0.0000	21
Pd	6.814172092	3.934277993	8.620114302	CORE	22 Pd Pd	0.0000	22
Pd	12.389417999	8.762965696	8.621923738	CORE	23 Pd Pd	0.0000	23
Pd	13.783550971	6.348239961	8.621933874	CORE	24 Pd Pd	0.0000	24
Pd	9.601765066	3.934169030	8.621232717	CORE	25 Pd Pd	0.0000	25
Pd	10.995589003	1.520212695	8.620276726	CORE	26 Pd Pd	0.0000	26
Pd	8.207876417	6.348469951	8.621233758	CORE	27 Pd Pd	0.0000	27
Pd	6.814227378	8.762524945	8.620282578	CORE	28 Pd Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724	CORE	29 Pd Pd	0.0000	29
Pd	12.389096274	3.933994969	8.621047892	CORE	30 Pd Pd	0.0000	30
Pd	9.601392037	8.762455531	8.621048992	CORE	31 Pd Pd	0.0000	31
Pd	10.995872940	6.348591411	8.621985519	CORE	32 Pd Pd	0.0000	32
Pd	8.206929759	4.737239508	10.917747333	CORE	33 Pd Pd	0.0000	33
Pd	9.590773573	2.333767867	10.942440090	CORE	34 Pd Pd	0.0000	34
Pd	6.811719646	7.131015341	10.933917500	CORE	35 Pd Pd	0.0000	35
Pd	13.790527043	9.563215276	10.906604558	CORE	36 Pd Pd	0.0000	36
Pd	6.826202482	2.340871158	10.954224143	CORE	37 Pd Pd	0.0000	37
Pd	15.179027529	7.146244510	10.918081082	CORE	38 Pd Pd	0.0000	38
Pd	5.429810324	4.725909928	10.948163120	CORE	39 Pd Pd	0.0000	39
Pd	16.574279734	9.563626480	10.915411723	CORE	40 Pd Pd	0.0000	40
Pd	13.790376472	4.733869801	10.918269465	CORE	41 Pd Pd	0.0000	41
Pd	10.992777131	9.569290935	10.904990457	CORE	42 Pd Pd	0.0000	42

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Pd      4.054971773   2.342292595   10.956002249 CORE   43 Pd Pd   0.0000   43
Pd     12.389780716   7.152108449   10.923763732 CORE   44 Pd Pd   0.0000   44
Pd     12.387215586   2.323537570   10.922743753 CORE   45 Pd Pd   0.0000   45
Pd      8.206257477   9.575250371   10.905854088 CORE   46 Pd Pd   0.0000   46
Pd     11.005697770   4.727987043   10.913982331 CORE   47 Pd Pd   0.0000   47
Pd      9.604295449   7.157832299   10.901400372 CORE   48 Pd Pd   0.0000   48
Pd      5.436040215   3.140897826   13.477001511 CORE   49 Pd Pd   0.0000   49
Pd      9.608525227   0.705488748   13.237837112 CORE   50 Pd Pd   0.0000   50
Pd      5.424163075   7.949390655   13.251650188 CORE   51 Pd Pd   0.0000   51
Pd      8.254608040   3.160613925   13.331305316 CORE   52 Pd Pd   0.0000   52
Pd      6.828359938   5.506621414   13.344334190 CORE   53 Pd Pd   0.0000   53
Pd      6.813914344   0.700796845   13.191426313 CORE   54 Pd Pd   0.0000   54
Pd      4.031271159   5.538240552   13.245520422 CORE   55 Pd Pd   0.0000   55
Pd     13.787559762   7.950610754   13.260992601 CORE   56 Pd Pd   0.0000   56
Pd      2.622395531   3.128491093   13.258349230 CORE   57 Pd Pd   0.0000   57
Pd      9.632530661   5.551641876   13.188209620 CORE   58 Pd Pd   0.0000   58
Pd      4.014854131   0.714140114   13.226981508 CORE   59 Pd Pd   0.0000   59
Pd      1.231792983   0.715900142   13.254604324 CORE   60 Pd Pd   0.0000   60
Pd     10.992561931   3.135519470   13.282692961 CORE   61 Pd Pd   0.0000   61
Pd      8.207308919   7.975555562   13.221088037 CORE   62 Pd Pd   0.0000   62
Pd     12.395583891   5.539512484   13.256551521 CORE   63 Pd Pd   0.0000   63
Pd     10.997300587   7.956228895   13.264722457 CORE   64 Pd Pd   0.0000   64
H       5.400148605   1.399487109   14.044301416 CORE   65 H  H    0.0000   65
H       8.203419339   1.444904877   14.028343441 CORE   66 H  H    0.0000   66
H       5.401157761   6.360912658   14.077624615 CORE   67 H  H    0.0000   67
H       2.623364317   1.517477389   14.073769324 CORE   68 H  H    0.0000   68
H      15.185984853   8.759487324   14.078442736 CORE   69 H  H    0.0000   69
H      13.791501566   6.338698431   14.076010944 CORE   70 H  H    0.0000   70
H      12.395338173   8.770271547   14.067559638 CORE   71 H  H    0.0000   71
H       9.022921137   3.744413003   14.640135694 CORE   72 H  H    0.0000   72
H       8.323806145   6.431598457   14.007888200 CORE   73 H  H    0.0000   73
H      12.370823655   3.926157950   14.094894984 CORE   74 H  H    0.0000   74
H       9.594264422   8.767840576   14.067568742 CORE   75 H  H    0.0000   75
H      10.996295534   1.531405399   14.082464133 CORE   76 H  H    0.0000   76
H       6.809266370   8.764178204   14.073498557 CORE   77 H  H    0.0000   77
H      10.988818796   6.325822911   14.073946742 CORE   78 H  H    0.0000   78
H       3.951408092   3.957193299   14.106616557 CORE   79 H  H    0.0000   79
C       7.407310928   4.175013377   14.943594549 CORE   80 C  C    0.0000   80
C       6.312560939   3.405720820   15.445944309 CORE   81 C  C    0.0000   81
H       7.792832422   5.001610784   15.554985090 CORE   82 H  H    0.0000   82
H       6.462551331   2.354606518   15.705700469 CORE   83 H  H    0.0000   83
H       5.630902184   3.933254249   16.125822869 CORE   84 H  H    0.0000   84
end
end
```

Ethene adsorbed on Pd(111). The energy from VASP is -410.547990 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	60.00000000	
Pd	6.809789092	0.713021845	6.343804094	CORE	1 Pd Pd	0.0000	1
Pd	4.022272274	5.541148999	6.343819775	CORE	2 Pd Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738	CORE	3 Pd Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485	CORE	4 Pd Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004	CORE	5 Pd Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336	CORE	6 Pd Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492	CORE	7 Pd Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712	CORE	8 Pd Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883	CORE	9 Pd Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717	CORE	10 Pd Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710	CORE	11 Pd Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199	CORE	12 Pd Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101	CORE	13 Pd Pd	0.0000	13
Pd	10.991373809	7.955436933	6.345265089	CORE	14 Pd Pd	0.0000	14
Pd	1.234428020	0.712833244	6.342029531	CORE	15 Pd Pd	0.0000	15
Pd	9.597706838	5.541375735	6.344926776	CORE	16 Pd Pd	0.0000	16
Pd	5.419869613	1.520422400	8.619780622	CORE	17 Pd Pd	0.0000	17
Pd	4.026560428	3.933717478	8.619778674	CORE	18 Pd Pd	0.0000	18
Pd	15.177210300	8.762689012	8.621082754	CORE	19 Pd Pd	0.0000	19
Pd	8.207619922	1.520449870	8.620764212	CORE	20 Pd Pd	0.0000	20
Pd	5.420456737	6.347962245	8.620778994	CORE	21 Pd Pd	0.0000	21
Pd	6.814172092	3.934277993	8.620114302	CORE	22 Pd Pd	0.0000	22
Pd	12.389417999	8.762965696	8.621923738	CORE	23 Pd Pd	0.0000	23
Pd	13.783550971	6.348239961	8.621933874	CORE	24 Pd Pd	0.0000	24
Pd	9.601765066	3.934169030	8.621232717	CORE	25 Pd Pd	0.0000	25
Pd	10.995589003	1.520212695	8.620276726	CORE	26 Pd Pd	0.0000	26
Pd	8.207876417	6.348469951	8.621233758	CORE	27 Pd Pd	0.0000	27
Pd	6.814227378	8.762524945	8.620282578	CORE	28 Pd Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724	CORE	29 Pd Pd	0.0000	29
Pd	12.389096274	3.933994969	8.621047892	CORE	30 Pd Pd	0.0000	30
Pd	9.601392037	8.762455531	8.621048992	CORE	31 Pd Pd	0.0000	31
Pd	10.995872940	6.348591411	8.621985519	CORE	32 Pd Pd	0.0000	32
Pd	8.210854121	4.712446251	10.941457854	CORE	33 Pd Pd	0.0000	33
Pd	9.580950810	2.337210567	10.941484901	CORE	34 Pd Pd	0.0000	34
Pd	6.818484579	7.149380458	10.897025860	CORE	35 Pd Pd	0.0000	35
Pd	13.785082995	9.572987233	10.898043514	CORE	36 Pd Pd	0.0000	36
Pd	6.839664752	2.336477688	10.940417609	CORE	37 Pd Pd	0.0000	37
Pd	15.180454327	7.153035684	10.898042627	CORE	38 Pd Pd	0.0000	38
Pd	5.428977664	4.735025067	10.896922254	CORE	39 Pd Pd	0.0000	39
Pd	16.570802133	9.569697517	10.896625471	CORE	40 Pd Pd	0.0000	40
Pd	13.785461435	4.737012936	10.897554306	CORE	41 Pd Pd	0.0000	41

Pd	10.999191396	9.569799156	10.897028725	CORE	42	Pd	Pd	0.0000	42
Pd	4.032999965	2.324248999	10.896137866	CORE	43	Pd	Pd	0.0000	43
Pd	12.390155035	7.153271838	10.898647707	CORE	44	Pd	Pd	0.0000	44
Pd	12.387634200	2.324355065	10.896146642	CORE	45	Pd	Pd	0.0000	45
Pd	8.210065276	9.566575688	10.899480466	CORE	46	Pd	Pd	0.0000	46
Pd	10.991820967	4.735649112	10.897890290	CORE	47	Pd	Pd	0.0000	47
Pd	9.601844448	7.149924005	10.897404012	CORE	48	Pd	Pd	0.0000	48
Pd	5.439271849	3.129281467	13.195909416	CORE	49	Pd	Pd	0.0000	49
Pd	9.596133285	0.722060856	13.200489668	CORE	50	Pd	Pd	0.0000	50
Pd	5.425528035	7.956254967	13.215646413	CORE	51	Pd	Pd	0.0000	51
Pd	8.216616810	3.124730468	14.088658259	CORE	52	Pd	Pd	0.0000	52
Pd	6.823890145	5.530315638	13.198439681	CORE	53	Pd	Pd	0.0000	53
Pd	6.824326670	0.721133620	13.201916695	CORE	54	Pd	Pd	0.0000	54
Pd	4.031986766	5.541065197	13.213696029	CORE	55	Pd	Pd	0.0000	55
Pd	13.786637863	7.955347740	13.213772722	CORE	56	Pd	Pd	0.0000	56
Pd	2.637112190	3.127134532	13.214299309	CORE	57	Pd	Pd	0.0000	57
Pd	9.601152485	5.533514067	13.200805466	CORE	58	Pd	Pd	0.0000	58
Pd	4.032131158	0.715462756	13.213538773	CORE	59	Pd	Pd	0.0000	59
Pd	1.239341688	0.715893379	13.212469370	CORE	60	Pd	Pd	0.0000	60
Pd	10.985623053	3.131074763	13.197225640	CORE	61	Pd	Pd	0.0000	61
Pd	8.211128446	7.953698084	13.215354067	CORE	62	Pd	Pd	0.0000	62
Pd	12.392635482	5.541853776	13.214063580	CORE	63	Pd	Pd	0.0000	63
Pd	10.997046381	7.957155641	13.216194077	CORE	64	Pd	Pd	0.0000	64
H	5.428430670	1.520515767	14.019069942	CORE	65	H	H	0.0000	65
H	8.204134219	1.328018233	14.122693471	CORE	66	H	H	0.0000	66
H	5.432134779	6.344912322	14.016434304	CORE	67	H	H	0.0000	67
H	2.635809643	1.515581469	14.030889700	CORE	68	H	H	0.0000	68
H	15.183064105	8.765880975	14.017452235	CORE	69	H	H	0.0000	69
H	13.787788409	6.345450854	14.031782750	CORE	70	H	H	0.0000	70
H	12.390670801	8.765265247	14.018730307	CORE	71	H	H	0.0000	71
H	8.211626726	6.338879242	14.024447546	CORE	72	H	H	0.0000	72
H	12.389297253	3.927168704	14.015450438	CORE	73	H	H	0.0000	73
H	9.601532511	8.763349049	14.031869901	CORE	74	H	H	0.0000	74
H	10.994959961	1.520901754	14.015596608	CORE	75	H	H	0.0000	75
H	6.820631573	8.763623729	14.031566669	CORE	76	H	H	0.0000	76
H	10.993323741	6.346157989	14.018286836	CORE	77	H	H	0.0000	77
H	4.036197927	3.926413372	14.014774115	CORE	78	H	H	0.0000	78
H	9.766783966	4.036826266	14.119498336	CORE	79	H	H	0.0000	79
H	6.655972668	4.029169610	14.119731200	CORE	80	H	H	0.0000	80
C	8.904377405	2.876879321	16.330885921	CORE	81	C	C	0.0000	81
C	7.576999255	3.224616427	16.347440928	CORE	82	C	C	0.0000	82
H	9.684878474	3.624982105	16.469545862	CORE	83	H	H	0.0000	83
H	6.794799541	2.467751115	16.413687080	CORE	84	H	H	0.0000	84
H	7.268088819	4.259125659	16.500156188	CORE	85	H	H	0.0000	85

H	9.217550524	1.834116590	16.383134457 CORE	86 H	H	0.0000	86

end

end

TS from ethene to ethyl on Pd(111). The energy from VASP is -410.067736 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	60.00000000	
Pd	6.809789092	0.713021845	6.343804094 CORE	1 Pd	Pd	0.0000	1
Pd	4.022272274	5.541148999	6.343819775 CORE	2 Pd	Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738 CORE	3 Pd	Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485 CORE	4 Pd	Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004 CORE	5 Pd	Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336 CORE	6 Pd	Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492 CORE	7 Pd	Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712 CORE	8 Pd	Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883 CORE	9 Pd	Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717 CORE	10 Pd	Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710 CORE	11 Pd	Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199 CORE	12 Pd	Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101 CORE	13 Pd	Pd	0.0000	13
Pd	10.991373809	7.955436933	6.345265089 CORE	14 Pd	Pd	0.0000	14
Pd	1.234428020	0.712833244	6.342029531 CORE	15 Pd	Pd	0.0000	15
Pd	9.597706838	5.541375735	6.344926776 CORE	16 Pd	Pd	0.0000	16
Pd	5.419869613	1.520422400	8.619780622 CORE	17 Pd	Pd	0.0000	17
Pd	4.026560428	3.933717478	8.619778674 CORE	18 Pd	Pd	0.0000	18
Pd	15.177210300	8.762689012	8.621082754 CORE	19 Pd	Pd	0.0000	19
Pd	8.207619922	1.520449870	8.620764212 CORE	20 Pd	Pd	0.0000	20
Pd	5.420456737	6.347962245	8.620778994 CORE	21 Pd	Pd	0.0000	21
Pd	6.814172092	3.934277993	8.620114302 CORE	22 Pd	Pd	0.0000	22
Pd	12.389417999	8.762965696	8.621923738 CORE	23 Pd	Pd	0.0000	23
Pd	13.783550971	6.348239961	8.621933874 CORE	24 Pd	Pd	0.0000	24
Pd	9.601765066	3.934169030	8.621232717 CORE	25 Pd	Pd	0.0000	25
Pd	10.995589003	1.520212695	8.620276726 CORE	26 Pd	Pd	0.0000	26
Pd	8.207876417	6.348469951	8.621233758 CORE	27 Pd	Pd	0.0000	27
Pd	6.814227378	8.762524945	8.620282578 CORE	28 Pd	Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724 CORE	29 Pd	Pd	0.0000	29
Pd	12.389096274	3.933994969	8.621047892 CORE	30 Pd	Pd	0.0000	30
Pd	9.601392037	8.762455531	8.621048992 CORE	31 Pd	Pd	0.0000	31
Pd	10.995872940	6.348591411	8.621985519 CORE	32 Pd	Pd	0.0000	32
Pd	8.210470827	4.718975483	10.947798514 CORE	33 Pd	Pd	0.0000	33
Pd	9.584276623	2.334046074	10.946938970 CORE	34 Pd	Pd	0.0000	34
Pd	6.817734538	7.158614872	10.908032927 CORE	35 Pd	Pd	0.0000	35
Pd	13.786352541	9.569488968	10.908846619 CORE	36 Pd	Pd	0.0000	36
Pd	6.842393315	2.344681032	10.962800609 CORE	37 Pd	Pd	0.0000	37
Pd	15.180255423	7.153236450	10.919698701 CORE	38 Pd	Pd	0.0000	38

Pd	5.425920310	4.735989021	10.912494724	CORE	39	Pd	Pd	0.0000	39
Pd	16.573860900	9.567631119	10.915560428	CORE	40	Pd	Pd	0.0000	40
Pd	13.785844943	4.735469617	10.917637094	CORE	41	Pd	Pd	0.0000	41
Pd	10.998550904	9.571766543	10.910144452	CORE	42	Pd	Pd	0.0000	42
Pd	4.032430755	2.323647548	10.913909989	CORE	43	Pd	Pd	0.0000	43
Pd	12.390836343	7.153531509	10.918815619	CORE	44	Pd	Pd	0.0000	44
Pd	12.392230009	2.321828238	10.913476655	CORE	45	Pd	Pd	0.0000	45
Pd	8.209760326	9.567469162	10.917190904	CORE	46	Pd	Pd	0.0000	46
Pd	10.996670002	4.737508166	10.906380514	CORE	47	Pd	Pd	0.0000	47
Pd	9.603208012	7.159577310	10.909233778	CORE	48	Pd	Pd	0.0000	48
Pd	5.443703859	3.137909382	13.245435100	CORE	49	Pd	Pd	0.0000	49
Pd	9.607600771	0.707523503	13.222427839	CORE	50	Pd	Pd	0.0000	50
Pd	5.427421909	7.947823699	13.261369327	CORE	51	Pd	Pd	0.0000	51
Pd	8.228123416	3.153334965	13.877921964	CORE	52	Pd	Pd	0.0000	52
Pd	6.814739383	5.525699241	13.202388969	CORE	53	Pd	Pd	0.0000	53
Pd	6.818725845	0.706261093	13.212423711	CORE	54	Pd	Pd	0.0000	54
Pd	4.032990062	5.538054331	13.248282161	CORE	55	Pd	Pd	0.0000	55
Pd	13.787118197	7.950407861	13.251226320	CORE	56	Pd	Pd	0.0000	56
Pd	2.641303096	3.124885723	13.251897967	CORE	57	Pd	Pd	0.0000	57
Pd	9.607874655	5.556893374	13.199984152	CORE	58	Pd	Pd	0.0000	58
Pd	4.023712217	0.709235460	13.240265358	CORE	59	Pd	Pd	0.0000	59
Pd	1.244119982	0.709066364	13.249718116	CORE	60	Pd	Pd	0.0000	60
Pd	10.994593862	3.120290658	13.210103231	CORE	61	Pd	Pd	0.0000	61
Pd	8.207235813	7.951547734	13.257831052	CORE	62	Pd	Pd	0.0000	62
Pd	12.394237055	5.539300403	13.250470031	CORE	63	Pd	Pd	0.0000	63
Pd	10.997723628	7.958412262	13.255826469	CORE	64	Pd	Pd	0.0000	64
H	5.406975144	1.500147793	14.030233089	CORE	65	H	H	0.0000	65
H	8.217011391	1.313967250	14.102695531	CORE	66	H	H	0.0000	66
H	5.451896097	6.317010628	14.060100267	CORE	67	H	H	0.0000	67
H	2.635745649	1.512863092	14.077883510	CORE	68	H	H	0.0000	68
H	15.183114594	8.758302307	14.063770675	CORE	69	H	H	0.0000	69
H	13.787033033	6.340260707	14.074735289	CORE	70	H	H	0.0000	70
H	12.391715551	8.765843261	14.064792265	CORE	71	H	H	0.0000	71
H	8.186264660	6.315290446	14.040334436	CORE	72	H	H	0.0000	72
H	12.392218538	3.922137175	14.054046276	CORE	73	H	H	0.0000	73
H	9.598968056	8.760187156	14.078020164	CORE	74	H	H	0.0000	74
H	10.996105414	1.516568635	14.051268512	CORE	75	H	H	0.0000	75
H	6.818639036	8.760948365	14.085733682	CORE	76	H	H	0.0000	76
H	10.991178222	6.344542318	14.059511356	CORE	77	H	H	0.0000	77
H	4.041014520	3.935243961	14.070519442	CORE	78	H	H	0.0000	78
H	9.791000819	4.045178569	14.091333776	CORE	79	H	H	0.0000	79
H	6.585746423	3.445126609	14.637895261	CORE	80	H	H	0.0000	80
C	8.553391980	3.250483612	16.029663489	CORE	81	C	C	0.0000	81
C	7.138456749	3.355462512	16.021826538	CORE	82	C	C	0.0000	82

H	9.153205961	4.140146778	16.225019735 CORE	83 H	H	0.0000	83
H	6.552946814	2.470115931	16.279224956 CORE	84 H	H	0.0000	84
H	6.688902504	4.314714615	16.291071365 CORE	85 H	H	0.0000	85
H	9.032964071	2.298769741	16.262538137 CORE	86 H	H	0.0000	86

end

end

Ethyl adsorbed on Pd(111). The energy from VASP is -414.496037 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	60.00000000	
Pd	6.809789092	0.713021845	6.343804094 CORE	1 Pd	Pd	0.0000	1
Pd	4.022272274	5.541148999	6.343819775 CORE	2 Pd	Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738 CORE	3 Pd	Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485 CORE	4 Pd	Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004 CORE	5 Pd	Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336 CORE	6 Pd	Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492 CORE	7 Pd	Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712 CORE	8 Pd	Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883 CORE	9 Pd	Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717 CORE	10 Pd	Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710 CORE	11 Pd	Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199 CORE	12 Pd	Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101 CORE	13 Pd	Pd	0.0000	13
Pd	10.991373809	7.955436933	6.345265089 CORE	14 Pd	Pd	0.0000	14
Pd	1.234428020	0.712833244	6.342029531 CORE	15 Pd	Pd	0.0000	15
Pd	9.597706838	5.541375735	6.344926776 CORE	16 Pd	Pd	0.0000	16
Pd	5.419869613	1.520422400	8.619780622 CORE	17 Pd	Pd	0.0000	17
Pd	4.026560428	3.933717478	8.619778674 CORE	18 Pd	Pd	0.0000	18
Pd	15.177210300	8.762689012	8.621082754 CORE	19 Pd	Pd	0.0000	19
Pd	8.207619922	1.520449870	8.620764212 CORE	20 Pd	Pd	0.0000	20
Pd	5.420456737	6.347962245	8.620778994 CORE	21 Pd	Pd	0.0000	21
Pd	6.814172092	3.934277993	8.620114302 CORE	22 Pd	Pd	0.0000	22
Pd	12.389417999	8.762965696	8.621923738 CORE	23 Pd	Pd	0.0000	23
Pd	13.783550971	6.348239961	8.621933874 CORE	24 Pd	Pd	0.0000	24
Pd	9.601765066	3.934169030	8.621232717 CORE	25 Pd	Pd	0.0000	25
Pd	10.995589003	1.520212695	8.620276726 CORE	26 Pd	Pd	0.0000	26
Pd	8.207876417	6.348469951	8.621233758 CORE	27 Pd	Pd	0.0000	27
Pd	6.814227378	8.762524945	8.620282578 CORE	28 Pd	Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724 CORE	29 Pd	Pd	0.0000	29
Pd	12.389096274	3.933994969	8.621047892 CORE	30 Pd	Pd	0.0000	30
Pd	9.601392037	8.762455531	8.621048992 CORE	31 Pd	Pd	0.0000	31
Pd	10.995872940	6.348591411	8.621985519 CORE	32 Pd	Pd	0.0000	32
Pd	8.207688926	4.718329327	10.938609242 CORE	33 Pd	Pd	0.0000	33
Pd	9.583530972	2.335447054	10.938475257 CORE	34 Pd	Pd	0.0000	34
Pd	6.815405561	7.150239761	10.897321521 CORE	35 Pd	Pd	0.0000	35

Pd	13.783960291	9.572165445	10.899215686	CORE	36 Pd Pd	0.0000	36
Pd	6.835468383	2.337255085	10.942556715	CORE	37 Pd Pd	0.0000	37
Pd	15.177080138	7.153950271	10.900618407	CORE	38 Pd Pd	0.0000	38
Pd	5.424907507	4.738177076	10.897626252	CORE	39 Pd Pd	0.0000	39
Pd	16.567730510	9.570757576	10.897630656	CORE	40 Pd Pd	0.0000	40
Pd	13.783782352	4.739480931	10.899685223	CORE	41 Pd Pd	0.0000	41
Pd	10.998716475	9.571251201	10.895590148	CORE	42 Pd Pd	0.0000	42
Pd	4.031392784	2.325930469	10.894044490	CORE	43 Pd Pd	0.0000	43
Pd	12.389841254	7.154008090	10.900643516	CORE	44 Pd Pd	0.0000	44
Pd	12.388011087	2.324387323	10.892993165	CORE	45 Pd Pd	0.0000	45
Pd	8.207842046	9.567424695	10.897796931	CORE	46 Pd Pd	0.0000	46
Pd	10.992587829	4.737589160	10.895943086	CORE	47 Pd Pd	0.0000	47
Pd	9.600402280	7.152503808	10.894123500	CORE	48 Pd Pd	0.0000	48
Pd	5.417586778	3.128632168	13.200314919	CORE	49 Pd Pd	0.0000	49
Pd	9.603626039	0.716485315	13.209661034	CORE	50 Pd Pd	0.0000	50
Pd	5.420941642	7.959309298	13.215917126	CORE	51 Pd Pd	0.0000	51
Pd	8.207538347	3.130557915	13.695469900	CORE	52 Pd Pd	0.0000	52
Pd	6.815704812	5.548115060	13.207820508	CORE	53 Pd Pd	0.0000	53
Pd	6.810034508	0.714420810	13.204229494	CORE	54 Pd Pd	0.0000	54
Pd	4.025966547	5.545362727	13.220393652	CORE	55 Pd Pd	0.0000	55
Pd	13.783006253	7.957381417	13.221459868	CORE	56 Pd Pd	0.0000	56
Pd	2.633457960	3.128437541	13.213099123	CORE	57 Pd Pd	0.0000	57
Pd	9.599561573	5.551235474	13.196032038	CORE	58 Pd Pd	0.0000	58
Pd	4.023547528	0.714611725	13.213195985	CORE	59 Pd Pd	0.0000	59
Pd	1.242027409	0.713718649	13.215637030	CORE	60 Pd Pd	0.0000	60
Pd	11.001566019	3.123947084	13.194851482	CORE	61 Pd Pd	0.0000	61
Pd	8.207537762	7.962127063	13.216034621	CORE	62 Pd Pd	0.0000	62
Pd	12.389896882	5.544418425	13.219593949	CORE	63 Pd Pd	0.0000	63
Pd	10.993872263	7.959045690	13.214382674	CORE	64 Pd Pd	0.0000	64
H	5.410718018	1.517173939	14.016497128	CORE	65 H H	0.0000	65
H	8.202977866	1.351673408	14.090889266	CORE	66 H H	0.0000	66
H	5.419285024	6.354953022	14.028295276	CORE	67 H H	0.0000	67
H	2.633271763	1.519378978	14.032772339	CORE	68 H H	0.0000	68
H	15.180896394	8.759633444	14.029129903	CORE	69 H H	0.0000	69
H	13.782049806	6.348212486	14.038447119	CORE	70 H H	0.0000	70
H	12.384233019	8.758141432	14.027047715	CORE	71 H H	0.0000	71
H	8.208871024	6.359697326	14.024179216	CORE	72 H H	0.0000	72
H	12.394046085	3.931862393	14.023902317	CORE	73 H H	0.0000	73
H	9.600581859	8.764597493	14.033246944	CORE	74 H H	0.0000	74
H	11.005169644	1.515719561	14.023772716	CORE	75 H H	0.0000	75
H	6.814949116	8.763318363	14.034911680	CORE	76 H H	0.0000	76
H	10.995226817	6.353628845	14.024573515	CORE	77 H H	0.0000	77
H	4.020690142	3.933429268	14.024717119	CORE	78 H H	0.0000	78
H	9.756589999	4.020853292	14.052419266	CORE	79 H H	0.0000	79

H	6.669275535	4.020196633	14.085295230	CORE	80 H	H	0.0000	80
C	8.329070099	3.189250143	15.820461462	CORE	81 C	C	0.0000	81
C	7.126070917	2.648338630	16.541744001	CORE	82 C	C	0.0000	82
H	8.502202924	4.256298995	15.999504243	CORE	83 H	H	0.0000	83
H	6.925333698	1.594406602	16.312240410	CORE	84 H	H	0.0000	84
H	7.334249338	2.715539419	17.627613166	CORE	85 H	H	0.0000	85
H	9.243990991	2.613295585	15.997534609	CORE	86 H	H	0.0000	86
H	6.215029619	3.228174616	16.346958661	CORE	87 H	H	0.0000	87

end

end

TS from ethyl to ethane on Pd(111). The energy from VASP is -414.035996 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	60.00000000		
Pd	6.809789092	0.713021845	6.343804094	CORE	1 Pd	Pd	0.0000	1
Pd	4.022272274	5.541148999	6.343819775	CORE	2 Pd	Pd	0.0000	2
Pd	5.415961487	3.127044139	6.342212738	CORE	3 Pd	Pd	0.0000	3
Pd	9.597174486	0.712978286	6.343400485	CORE	4 Pd	Pd	0.0000	4
Pd	5.415925548	7.955113833	6.343415004	CORE	5 Pd	Pd	0.0000	5
Pd	8.203765107	3.127145561	6.343736336	CORE	6 Pd	Pd	0.0000	6
Pd	6.809950930	5.541303822	6.343741492	CORE	7 Pd	Pd	0.0000	7
Pd	2.628220285	3.126962857	6.342391712	CORE	8 Pd	Pd	0.0000	8
Pd	4.022019879	0.712831413	6.342397883	CORE	9 Pd	Pd	0.0000	9
Pd	13.778678714	7.955260923	6.345043717	CORE	10 Pd	Pd	0.0000	10
Pd	10.991074815	3.127126895	6.343972710	CORE	11 Pd	Pd	0.0000	11
Pd	8.203590998	7.955194679	6.343976199	CORE	12 Pd	Pd	0.0000	12
Pd	12.385177994	5.541295461	6.345270101	CORE	13 Pd	Pd	0.0000	13
Pd	10.991373809	7.955436933	6.345265089	CORE	14 Pd	Pd	0.0000	14
Pd	1.234428020	0.712833244	6.342029531	CORE	15 Pd	Pd	0.0000	15
Pd	9.597706838	5.541375735	6.344926776	CORE	16 Pd	Pd	0.0000	16
Pd	5.419869613	1.520422400	8.619780622	CORE	17 Pd	Pd	0.0000	17
Pd	4.026560428	3.933717478	8.619778674	CORE	18 Pd	Pd	0.0000	18
Pd	15.177210300	8.762689012	8.621082754	CORE	19 Pd	Pd	0.0000	19
Pd	8.207619922	1.520449870	8.620764212	CORE	20 Pd	Pd	0.0000	20
Pd	5.420456737	6.347962245	8.620778994	CORE	21 Pd	Pd	0.0000	21
Pd	6.814172092	3.934277993	8.620114302	CORE	22 Pd	Pd	0.0000	22
Pd	12.389417999	8.762965696	8.621923738	CORE	23 Pd	Pd	0.0000	23
Pd	13.783550971	6.348239961	8.621933874	CORE	24 Pd	Pd	0.0000	24
Pd	9.601765066	3.934169030	8.621232717	CORE	25 Pd	Pd	0.0000	25
Pd	10.995589003	1.520212695	8.620276726	CORE	26 Pd	Pd	0.0000	26
Pd	8.207876417	6.348469951	8.621233758	CORE	27 Pd	Pd	0.0000	27
Pd	6.814227378	8.762524945	8.620282578	CORE	28 Pd	Pd	0.0000	28
Pd	2.632951829	1.520252666	8.619441724	CORE	29 Pd	Pd	0.0000	29
Pd	12.389096274	3.933994969	8.621047892	CORE	30 Pd	Pd	0.0000	30
Pd	9.601392037	8.762455531	8.621048992	CORE	31 Pd	Pd	0.0000	31

Pd	10.995872940	6.348591411	8.621985519	CORE	32	Pd	Pd	0.0000	32
Pd	8.196511454	4.733135011	10.927496133	CORE	33	Pd	Pd	0.0000	33
Pd	9.574968980	2.344169112	10.936435591	CORE	34	Pd	Pd	0.0000	34
Pd	6.799878274	7.164055859	10.892075960	CORE	35	Pd	Pd	0.0000	35
Pd	13.768274585	9.578229088	10.901020833	CORE	36	Pd	Pd	0.0000	36
Pd	6.829114498	2.351161655	10.960397189	CORE	37	Pd	Pd	0.0000	37
Pd	15.159220100	7.159954551	10.901474518	CORE	38	Pd	Pd	0.0000	38
Pd	5.404792837	4.744435991	10.893268906	CORE	39	Pd	Pd	0.0000	39
Pd	16.553434317	9.578750845	10.899113822	CORE	40	Pd	Pd	0.0000	40
Pd	13.766216884	4.744332723	10.903125329	CORE	41	Pd	Pd	0.0000	41
Pd	10.979995833	9.577634389	10.898809286	CORE	42	Pd	Pd	0.0000	42
Pd	4.009495408	2.328773311	10.894681471	CORE	43	Pd	Pd	0.0000	43
Pd	12.373618200	7.160565090	10.904218773	CORE	44	Pd	Pd	0.0000	44
Pd	12.364642757	2.334705570	10.903485598	CORE	45	Pd	Pd	0.0000	45
Pd	8.192215532	9.577684224	10.900473996	CORE	46	Pd	Pd	0.0000	46
Pd	10.976727676	4.742935308	10.908905496	CORE	47	Pd	Pd	0.0000	47
Pd	9.586059919	7.156128711	10.900825379	CORE	48	Pd	Pd	0.0000	48
Pd	5.366648769	3.138394226	13.196269638	CORE	49	Pd	Pd	0.0000	49
Pd	9.572765554	0.726581890	13.212960880	CORE	50	Pd	Pd	0.0000	50
Pd	5.391434553	7.974538071	13.216303076	CORE	51	Pd	Pd	0.0000	51
Pd	8.176863770	3.164550302	13.579101124	CORE	52	Pd	Pd	0.0000	52
Pd	6.775277392	5.568405071	13.188051428	CORE	53	Pd	Pd	0.0000	53
Pd	6.779468974	0.717508721	13.206806771	CORE	54	Pd	Pd	0.0000	54
Pd	3.991484021	5.556808928	13.224801246	CORE	55	Pd	Pd	0.0000	55
Pd	13.754086393	7.966616815	13.228041911	CORE	56	Pd	Pd	0.0000	56
Pd	2.586228826	3.140967261	13.223677995	CORE	57	Pd	Pd	0.0000	57
Pd	9.569883512	5.541289519	13.223027726	CORE	58	Pd	Pd	0.0000	58
Pd	3.994645778	0.725341244	13.221740414	CORE	59	Pd	Pd	0.0000	59
Pd	1.208294036	0.731474704	13.223773234	CORE	60	Pd	Pd	0.0000	60
Pd	10.939657432	3.150997163	13.239843814	CORE	61	Pd	Pd	0.0000	61
Pd	8.179776727	7.975793927	13.215420240	CORE	62	Pd	Pd	0.0000	62
Pd	12.356527095	5.553199168	13.226434918	CORE	63	Pd	Pd	0.0000	63
Pd	10.963344209	7.960220685	13.224534656	CORE	64	Pd	Pd	0.0000	64
H	5.393493894	1.532543206	14.024564754	CORE	65	H	H	0.0000	65
H	8.172268883	1.396610435	14.062533341	CORE	66	H	H	0.0000	66
H	5.389545988	6.367726496	14.026930623	CORE	67	H	H	0.0000	67
H	2.604322763	1.532068200	14.041684373	CORE	68	H	H	0.0000	68
H	15.151084665	8.773314625	14.034615341	CORE	69	H	H	0.0000	69
H	13.750083643	6.358149416	14.045523222	CORE	70	H	H	0.0000	70
H	12.351578686	8.765334524	14.034685190	CORE	71	H	H	0.0000	71
H	8.182332213	6.376025288	14.006246381	CORE	72	H	H	0.0000	72
H	12.333573708	3.940290824	14.041624656	CORE	73	H	H	0.0000	73
H	9.575178301	8.772899558	14.039934867	CORE	74	H	H	0.0000	74
H	10.972233465	1.543379880	14.032490999	CORE	75	H	H	0.0000	75

H	6.786829770	8.777846245	14.033338612	CORE	76 H	H	0.0000	76
H	10.951917138	6.344187070	14.039618006	CORE	77 H	H	0.0000	77
H	3.976825524	3.942106889	14.031018175	CORE	78 H	H	0.0000	78
H	9.393895585	3.908585186	14.477851536	CORE	79 H	H	0.0000	79
H	6.623871746	4.021412170	14.039465572	CORE	80 H	H	0.0000	80
C	8.566953924	3.662975420	15.832618868	CORE	81 C	C	0.0000	81
C	7.572141635	2.725260012	16.494863111	CORE	82 C	C	0.0000	82
H	8.290494553	4.715546288	15.946063896	CORE	83 H	H	0.0000	83
H	7.837117982	1.666852684	16.388035068	CORE	84 H	H	0.0000	84
H	7.578687102	2.960504870	17.576244561	CORE	85 H	H	0.0000	85
H	9.579923008	3.503160212	16.221185059	CORE	86 H	H	0.0000	86
H	6.544422275	2.863310422	16.136701686	CORE	87 H	H	0.0000	87

end

end

Initial Pd_4H_3(111). The energy from VASP is -462.910922 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	60.00000000
Pd	6.747338531	0.544541613	6.403267290	CORE	1 Pd Pd	0.0000 1
Pd	3.845151399	5.571142423	6.403290684	CORE	2 Pd Pd	0.0000 2
Pd	5.298982544	3.059410650	6.403296328	CORE	3 Pd Pd	0.0000 3
Pd	9.648025542	0.547773874	6.403201805	CORE	4 Pd Pd	0.0000 4
Pd	5.298282266	8.081617720	6.403218683	CORE	5 Pd Pd	0.0000 5
Pd	8.196069754	3.060087698	6.403506017	CORE	6 Pd Pd	0.0000 6
Pd	6.748041394	5.568042339	6.403528135	CORE	7 Pd Pd	0.0000 7
Pd	2.396203981	3.056086329	6.403974639	CORE	8 Pd Pd	0.0000 8
Pd	3.844692371	0.547193572	6.403980644	CORE	9 Pd Pd	0.0000 9
Pd	13.995599937	8.080432901	6.403915026	CORE	10 Pd Pd	0.0000 10
Pd	11.097339485	3.057320193	6.404178400	CORE	11 Pd Pd	0.0000 11
Pd	8.196252877	8.082018112	6.404201419	CORE	12 Pd Pd	0.0000 12
Pd	12.547118135	5.570172821	6.404809441	CORE	13 Pd Pd	0.0000 13
Pd	11.097374320	8.081197886	6.404806864	CORE	14 Pd Pd	0.0000 14
Pd	0.947647213	0.547191260	6.404240481	CORE	15 Pd Pd	0.0000 15
Pd	9.647863113	5.570318755	6.404626518	CORE	16 Pd Pd	0.0000 16
Pd	5.296345229	1.383774072	8.598645002	CORE	17 Pd Pd	0.0000 17
Pd	3.846430041	3.895121361	8.598650689	CORE	18 Pd Pd	0.0000 18
Pd	15.446747886	8.918407968	8.598673994	CORE	19 Pd Pd	0.0000 19
Pd	8.196524484	1.383846907	8.598440679	CORE	20 Pd Pd	0.0000 20
Pd	5.296487130	6.406750055	8.598478119	CORE	21 Pd Pd	0.0000 21
Pd	6.746726050	3.895397354	8.597899801	CORE	22 Pd Pd	0.0000 22
Pd	12.546601356	8.918351911	8.598885115	CORE	23 Pd Pd	0.0000 23
Pd	13.996646681	6.406823241	8.598891508	CORE	24 Pd Pd	0.0000 24
Pd	9.646822887	3.895276415	8.599334404	CORE	25 Pd Pd	0.0000 25
Pd	11.096261310	1.383436470	8.598996838	CORE	26 Pd Pd	0.0000 26
Pd	8.196560479	6.407055489	8.599357814	CORE	27 Pd Pd	0.0000 27

Pd	6.745960494	8.918219637	8.599027684	CORE	28	Pd	Pd	0.0000	28
Pd	2.396365455	1.383718188	8.599138079	CORE	29	Pd	Pd	0.0000	29
Pd	12.546369931	3.894993974	8.599714782	CORE	30	Pd	Pd	0.0000	30
Pd	9.646092187	8.918242765	8.599728379	CORE	31	Pd	Pd	0.0000	31
Pd	11.096426310	6.406760277	8.599885411	CORE	32	Pd	Pd	0.0000	32
H	13.966125551	4.748953754	7.090172091	CORE	33	H	H	0.0000	33
H	11.095843995	9.720660436	7.090205342	CORE	34	H	H	0.0000	34
H	3.762469203	2.172306700	7.151879904	CORE	35	H	H	0.0000	35
H	11.088054196	4.720768041	7.106096184	CORE	36	H	H	0.0000	36
H	9.632236062	7.242354712	7.106403093	CORE	37	H	H	0.0000	37
H	9.656494872	2.239241128	7.061700226	CORE	38	H	H	0.0000	38
H	6.767328375	7.243231015	7.061730988	CORE	39	H	H	0.0000	39
H	5.362474569	4.720515917	7.163971161	CORE	40	H	H	0.0000	40
H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.190540377	4.728793648	10.926207701	CORE	45	Pd	Pd	0.0000	45
Pd	9.636844757	2.218260463	10.928822638	CORE	46	Pd	Pd	0.0000	46
Pd	6.739331029	7.237303247	10.928976166	CORE	47	Pd	Pd	0.0000	47
Pd	14.004947361	9.749279380	10.935681715	CORE	48	Pd	Pd	0.0000	48
Pd	6.733568561	2.227661996	10.927141614	CORE	49	Pd	Pd	0.0000	49
Pd	15.445629622	7.254087557	10.935541042	CORE	50	Pd	Pd	0.0000	50
Pd	5.295797800	4.717699510	10.927211354	CORE	51	Pd	Pd	0.0000	51
Pd	16.875717337	9.743351224	10.932223704	CORE	52	Pd	Pd	0.0000	52
Pd	13.995078595	4.726125952	10.929693345	CORE	53	Pd	Pd	0.0000	53
Pd	11.090644221	9.756813300	10.929879756	CORE	54	Pd	Pd	0.0000	54
Pd	3.846777630	2.221081280	10.934522595	CORE	55	Pd	Pd	0.0000	55
Pd	12.531297677	7.235046133	10.919237186	CORE	56	Pd	Pd	0.0000	56
Pd	12.539149454	2.213798633	10.921715610	CORE	57	Pd	Pd	0.0000	57
Pd	8.186681680	9.752436714	10.921776339	CORE	58	Pd	Pd	0.0000	58
Pd	11.084924605	4.728525118	10.929877688	CORE	59	Pd	Pd	0.0000	59
Pd	9.637466719	7.235670405	10.929919210	CORE	60	Pd	Pd	0.0000	60
Pd	5.288811116	3.053877627	13.206607437	CORE	61	Pd	Pd	0.0000	61
Pd	9.643585099	0.544854877	13.206234053	CORE	62	Pd	Pd	0.0000	62
Pd	5.293612976	8.079108449	13.206424676	CORE	63	Pd	Pd	0.0000	63
Pd	8.190901733	3.052945822	13.222221516	CORE	64	Pd	Pd	0.0000	64
Pd	6.739130297	5.567194433	13.222246662	CORE	65	Pd	Pd	0.0000	65
Pd	6.739910352	0.543799134	13.215705820	CORE	66	Pd	Pd	0.0000	66
Pd	3.841798139	5.564411475	13.215691315	CORE	67	Pd	Pd	0.0000	67
Pd	13.988112625	8.076814242	13.223935146	CORE	68	Pd	Pd	0.0000	68
Pd	2.389538734	3.051903186	13.219149286	CORE	69	Pd	Pd	0.0000	69
Pd	9.643013019	5.567495364	13.205986011	CORE	70	Pd	Pd	0.0000	70
Pd	3.837768620	0.543324874	13.219267007	CORE	71	Pd	Pd	0.0000	71

Pd 0.937652128 0.541526897 13.216846898 CORE 72 Pd Pd 0.0000 72
Pd 11.088453171 3.057095329 13.218115351 CORE 73 Pd Pd 0.0000 73
Pd 8.191847263 8.074118303 13.218223075 CORE 74 Pd Pd 0.0000 74
Pd 12.541186649 5.563940166 13.217954572 CORE 75 Pd Pd 0.0000 75
Pd 11.089713475 8.079349254 13.218009725 CORE 76 Pd Pd 0.0000 76
H 2.639049226 3.199440221 9.878127119 CORE 77 H H 0.0000 77
H 4.090211366 0.685354999 9.877722553 CORE 78 H H 0.0000 78
H 7.024673598 0.720196163 9.910170242 CORE 79 H H 0.0000 79
H 4.135811047 5.723267804 9.910137354 CORE 80 H H 0.0000 80
H 7.000872755 5.671440489 9.830145983 CORE 81 H H 0.0000 81
H 8.408718698 3.228696974 9.827643382 CORE 82 H H 0.0000 82
H 0.694956062 0.402100849 9.747381356 CORE 83 H H 0.0000 83
H 14.267803719 8.237422859 9.854078579 CORE 84 H H 0.0000 84
H 11.097453574 2.823648022 9.902281630 CORE 85 H H 0.0000 85
H 7.994128300 8.200013238 9.901463288 CORE 86 H H 0.0000 86
H 11.022982511 7.877377738 9.872208968 CORE 87 H H 0.0000 87
H 12.331992579 5.608116497 9.870993079 CORE 88 H H 0.0000 88
H 6.735292718 3.888687929 13.898151955 CORE 89 H H 0.0000 89
H 3.841794664 3.893404891 13.900431104 CORE 90 H H 0.0000 90
H 5.292687011 1.380416124 13.900580150 CORE 91 H H 0.0000 91
H 8.191912583 1.372330257 13.902125968 CORE 92 H H 0.0000 92
H 5.284345180 6.408217598 13.902042771 CORE 93 H H 0.0000 93
H 2.384590824 1.376748658 13.906865598 CORE 94 H H 0.0000 94
H 15.444674285 8.917168608 13.894194977 CORE 95 H H 0.0000 95
H 13.990097922 6.395406892 13.905024673 CORE 96 H H 0.0000 96
H 12.533660489 8.918082467 13.904813228 CORE 97 H H 0.0000 97
H 9.639395004 3.898039465 13.904515657 CORE 98 H H 0.0000 98
H 8.195513430 6.398905900 13.904503546 CORE 99 H H 0.0000 99
H 12.542239061 3.887637417 13.905628024 CORE 100 H H 0.0000 100
H 9.638000017 8.918050712 13.905737927 CORE 101 H H 0.0000 101
H 11.091650758 1.389184106 13.901719162 CORE 102 H H 0.0000 102
H 6.748883165 8.911085417 13.901826230 CORE 103 H H 0.0000 103
H 11.099366385 6.408120632 13.900054301 CORE 104 H H 0.0000 104
end
end

Acetylene adsorbed on Pd_4H_3(111). The energy from VASP is -483.125295 eV.

PBC 11.60000000 11.60000000 20.00000000 90.00000000 90.00000000 60.00000000
Pd 6.747338531 0.544541613 6.403267290 CORE 1 Pd Pd 0.0000 1
Pd 3.845151399 5.571142423 6.403290684 CORE 2 Pd Pd 0.0000 2
Pd 5.298982544 3.059410650 6.403296328 CORE 3 Pd Pd 0.0000 3
Pd 9.648025542 0.547773874 6.403201805 CORE 4 Pd Pd 0.0000 4
Pd 5.298282266 8.081617720 6.403218683 CORE 5 Pd Pd 0.0000 5
Pd 8.196069754 3.060087698 6.403506017 CORE 6 Pd Pd 0.0000 6

Pd	6.748041394	5.568042339	6.403528135	CORE	7	Pd	Pd	0.0000	7
Pd	2.396203981	3.056086329	6.403974639	CORE	8	Pd	Pd	0.0000	8
Pd	3.844692371	0.547193572	6.403980644	CORE	9	Pd	Pd	0.0000	9
Pd	13.995599937	8.080432901	6.403915026	CORE	10	Pd	Pd	0.0000	10
Pd	11.097339485	3.057320193	6.404178400	CORE	11	Pd	Pd	0.0000	11
Pd	8.196252877	8.082018112	6.404201419	CORE	12	Pd	Pd	0.0000	12
Pd	12.547118135	5.570172821	6.404809441	CORE	13	Pd	Pd	0.0000	13
Pd	11.097374320	8.081197886	6.404806864	CORE	14	Pd	Pd	0.0000	14
Pd	0.947647213	0.547191260	6.404240481	CORE	15	Pd	Pd	0.0000	15
Pd	9.647863113	5.570318755	6.404626518	CORE	16	Pd	Pd	0.0000	16
Pd	5.296345229	1.383774072	8.598645002	CORE	17	Pd	Pd	0.0000	17
Pd	3.846430041	3.895121361	8.598650689	CORE	18	Pd	Pd	0.0000	18
Pd	15.446747886	8.918407968	8.598673994	CORE	19	Pd	Pd	0.0000	19
Pd	8.196524484	1.383846907	8.598440679	CORE	20	Pd	Pd	0.0000	20
Pd	5.296487130	6.406750055	8.598478119	CORE	21	Pd	Pd	0.0000	21
Pd	6.746726050	3.895397354	8.597899801	CORE	22	Pd	Pd	0.0000	22
Pd	12.546601356	8.918351911	8.598885115	CORE	23	Pd	Pd	0.0000	23
Pd	13.996646681	6.406823241	8.598891508	CORE	24	Pd	Pd	0.0000	24
Pd	9.646822887	3.895276415	8.599334404	CORE	25	Pd	Pd	0.0000	25
Pd	11.096261310	1.383436470	8.598996838	CORE	26	Pd	Pd	0.0000	26
Pd	8.196560479	6.407055489	8.599357814	CORE	27	Pd	Pd	0.0000	27
Pd	6.745960494	8.918219637	8.599027684	CORE	28	Pd	Pd	0.0000	28
Pd	2.396365455	1.383718188	8.599138079	CORE	29	Pd	Pd	0.0000	29
Pd	12.546369931	3.894993974	8.599714782	CORE	30	Pd	Pd	0.0000	30
Pd	9.646092187	8.918242765	8.599728379	CORE	31	Pd	Pd	0.0000	31
Pd	11.096426310	6.406760277	8.599885411	CORE	32	Pd	Pd	0.0000	32
H	13.966125551	4.748953754	7.090172091	CORE	33	H	H	0.0000	33
H	11.095843995	9.720660436	7.090205342	CORE	34	H	H	0.0000	34
H	3.762469203	2.172306700	7.151879904	CORE	35	H	H	0.0000	35
H	11.088054196	4.720768041	7.106096184	CORE	36	H	H	0.0000	36
H	9.632236062	7.242354712	7.106403093	CORE	37	H	H	0.0000	37
H	9.656494872	2.239241128	7.061700226	CORE	38	H	H	0.0000	38
H	6.767328375	7.243231015	7.061730988	CORE	39	H	H	0.0000	39
H	5.362474569	4.720515917	7.163971161	CORE	40	H	H	0.0000	40
H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.192149083	4.740228648	10.938999197	CORE	45	Pd	Pd	0.0000	45
Pd	9.640684008	2.212393326	10.932181035	CORE	46	Pd	Pd	0.0000	46
Pd	6.746004936	7.214783272	10.964310440	CORE	47	Pd	Pd	0.0000	47
Pd	14.008105283	9.770090887	10.932424794	CORE	48	Pd	Pd	0.0000	48
Pd	6.740367540	2.241917439	10.928445345	CORE	49	Pd	Pd	0.0000	49
Pd	15.454704617	7.270595918	10.924071748	CORE	50	Pd	Pd	0.0000	50

Pd	5.305046987	4.732115819	10.947539999	CORE	51 Pd Pd	0.0000	51
Pd	16.883915843	9.750952002	10.915545230	CORE	52 Pd Pd	0.0000	52
Pd	14.005327330	4.735417641	10.922344631	CORE	53 Pd Pd	0.0000	53
Pd	11.093908595	9.773401434	10.927750198	CORE	54 Pd Pd	0.0000	54
Pd	3.873033751	2.223833891	10.936972411	CORE	55 Pd Pd	0.0000	55
Pd	12.531844699	7.251472131	10.918511292	CORE	56 Pd Pd	0.0000	56
Pd	12.544661268	2.196538852	10.902721056	CORE	57 Pd Pd	0.0000	57
Pd	8.179146559	9.751822413	10.902977284	CORE	58 Pd Pd	0.0000	58
Pd	11.093079885	4.735261346	10.918745370	CORE	59 Pd Pd	0.0000	59
Pd	9.643299703	7.251308045	10.917908515	CORE	60 Pd Pd	0.0000	60
Pd	5.278863363	3.079027088	13.272141010	CORE	61 Pd Pd	0.0000	61
Pd	9.658628791	0.553472021	13.196312967	CORE	62 Pd Pd	0.0000	62
Pd	5.289797324	8.114389394	13.189549084	CORE	63 Pd Pd	0.0000	63
Pd	8.215514051	3.081099935	13.271063244	CORE	64 Pd Pd	0.0000	64
Pd	6.749215859	5.575965312	13.419399021	CORE	65 Pd Pd	0.0000	65
Pd	6.744804683	0.576451313	13.212325547	CORE	66 Pd Pd	0.0000	66
Pd	3.820535277	5.602855363	13.197035948	CORE	67 Pd Pd	0.0000	67
Pd	13.988205932	8.104129077	13.218615435	CORE	68 Pd Pd	0.0000	68
Pd	2.369835610	3.052385328	13.186106592	CORE	69 Pd Pd	0.0000	69
Pd	9.675641177	5.605461369	13.178301440	CORE	70 Pd Pd	0.0000	70
Pd	3.830942612	0.554793701	13.201155921	CORE	71 Pd Pd	0.0000	71
Pd	0.942856321	0.549130772	13.204279154	CORE	72 Pd Pd	0.0000	72
Pd	11.123285836	3.055313810	13.184530736	CORE	73 Pd Pd	0.0000	73
Pd	8.206683695	8.114921185	13.197869803	CORE	74 Pd Pd	0.0000	74
Pd	12.546607159	5.584752158	13.207760828	CORE	75 Pd Pd	0.0000	75
Pd	11.101237348	8.105929791	13.217511836	CORE	76 Pd Pd	0.0000	76
H	2.682465161	3.222380310	9.889280440	CORE	77 H H	0.0000	77
H	4.053588417	0.641093229	9.853763277	CORE	78 H H	0.0000	78
H	7.003249462	0.736743918	9.910949737	CORE	79 H H	0.0000	79
H	4.096472419	5.729367423	9.916465751	CORE	80 H H	0.0000	80
H	6.760908637	5.373786948	9.935095127	CORE	81 H H	0.0000	81
H	8.477421599	3.220234168	9.908960060	CORE	82 H H	0.0000	82
H	0.776911110	0.395403232	9.777992977	CORE	83 H H	0.0000	83
H	14.263429037	8.259778589	9.844917415	CORE	84 H H	0.0000	84
H	11.328932613	3.172608575	9.887961084	CORE	85 H H	0.0000	85
H	8.149638930	7.858104745	9.877180709	CORE	86 H H	0.0000	86
H	11.032302994	7.978648391	9.849031976	CORE	87 H H	0.0000	87
H	12.398704359	5.727153338	9.822585969	CORE	88 H H	0.0000	88
H	3.741299144	3.918609689	13.848283656	CORE	89 H H	0.0000	89
H	5.263867612	1.345126092	13.899862491	CORE	90 H H	0.0000	90
H	8.227385610	1.345809427	13.896898018	CORE	91 H H	0.0000	91
H	5.243591222	6.491383308	13.892763933	CORE	92 H H	0.0000	92
H	2.380665146	1.383887768	13.905146342	CORE	93 H H	0.0000	93
H	15.443792413	8.931601285	13.906074117	CORE	94 H H	0.0000	94

H	13.977358513	6.429671947	13.911425202	CORE	95 H	H	0.0000	95
H	12.542501242	8.941635351	13.907525188	CORE	96 H	H	0.0000	96
H	9.751479402	3.920171404	13.841987988	CORE	97 H	H	0.0000	97
H	8.253745629	6.489633056	13.890878792	CORE	98 H	H	0.0000	98
H	12.549296070	3.909352603	13.901608139	CORE	99 H	H	0.0000	99
H	9.649549461	8.938370082	13.915600010	CORE	100 H	H	0.0000	100
H	11.106412269	1.394671441	13.903953794	CORE	101 H	H	0.0000	101
H	6.754360419	8.927635090	13.899345671	CORE	102 H	H	0.0000	102
H	11.119592657	6.438774490	13.906453832	CORE	103 H	H	0.0000	103
C	7.423539127	4.030585783	14.880504768	CORE	104 C	C	0.0000	104
C	6.082549385	4.032074485	14.878876602	CORE	105 C	C	0.0000	105
H	8.114322855	4.247264915	15.696863734	CORE	106 H	H	0.0000	106
H	5.390920074	4.248575365	15.694624412	CORE	107 H	H	0.0000	107

end

end

TS from acetylene to vinyl on Pd_4H_3(111). The energy from VASP is -482.390181 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	60.00000000		
Pd	6.747338531	0.544541613	6.403267290	CORE	1 Pd	Pd	0.0000	1
Pd	3.845151399	5.571142423	6.403290684	CORE	2 Pd	Pd	0.0000	2
Pd	5.298982544	3.059410650	6.403296328	CORE	3 Pd	Pd	0.0000	3
Pd	9.648025542	0.547773874	6.403201805	CORE	4 Pd	Pd	0.0000	4
Pd	5.298282266	8.081617720	6.403218683	CORE	5 Pd	Pd	0.0000	5
Pd	8.196069754	3.060087698	6.403506017	CORE	6 Pd	Pd	0.0000	6
Pd	6.748041394	5.568042339	6.403528135	CORE	7 Pd	Pd	0.0000	7
Pd	2.396203981	3.056086329	6.403974639	CORE	8 Pd	Pd	0.0000	8
Pd	3.844692371	0.547193572	6.403980644	CORE	9 Pd	Pd	0.0000	9
Pd	13.995599937	8.080432901	6.403915026	CORE	10 Pd	Pd	0.0000	10
Pd	11.097339485	3.057320193	6.404178400	CORE	11 Pd	Pd	0.0000	11
Pd	8.196252877	8.082018112	6.404201419	CORE	12 Pd	Pd	0.0000	12
Pd	12.547118135	5.570172821	6.404809441	CORE	13 Pd	Pd	0.0000	13
Pd	11.097374320	8.081197886	6.404806864	CORE	14 Pd	Pd	0.0000	14
Pd	0.947647213	0.547191260	6.404240481	CORE	15 Pd	Pd	0.0000	15
Pd	9.647863113	5.570318755	6.404626518	CORE	16 Pd	Pd	0.0000	16
Pd	5.296345229	1.383774072	8.598645002	CORE	17 Pd	Pd	0.0000	17
Pd	3.846430041	3.895121361	8.598650689	CORE	18 Pd	Pd	0.0000	18
Pd	15.446747886	8.918407968	8.598673994	CORE	19 Pd	Pd	0.0000	19
Pd	8.196524484	1.383846907	8.598440679	CORE	20 Pd	Pd	0.0000	20
Pd	5.296487130	6.406750055	8.598478119	CORE	21 Pd	Pd	0.0000	21
Pd	6.746726050	3.895397354	8.597899801	CORE	22 Pd	Pd	0.0000	22
Pd	12.546601356	8.918351911	8.598885115	CORE	23 Pd	Pd	0.0000	23
Pd	13.996646681	6.406823241	8.598891508	CORE	24 Pd	Pd	0.0000	24
Pd	9.646822887	3.895276415	8.599334404	CORE	25 Pd	Pd	0.0000	25
Pd	11.096261310	1.383436470	8.598996838	CORE	26 Pd	Pd	0.0000	26

Pd	8.196560479	6.407055489	8.599357814	CORE	27	Pd	Pd	0.0000	27
Pd	6.745960494	8.918219637	8.599027684	CORE	28	Pd	Pd	0.0000	28
Pd	2.396365455	1.383718188	8.599138079	CORE	29	Pd	Pd	0.0000	29
Pd	12.546369931	3.894993974	8.599714782	CORE	30	Pd	Pd	0.0000	30
Pd	9.646092187	8.918242765	8.599728379	CORE	31	Pd	Pd	0.0000	31
Pd	11.096426310	6.406760277	8.599885411	CORE	32	Pd	Pd	0.0000	32
H	13.966125551	4.748953754	7.090172091	CORE	33	H	H	0.0000	33
H	11.095843995	9.720660436	7.090205342	CORE	34	H	H	0.0000	34
H	3.762469203	2.172306700	7.151879904	CORE	35	H	H	0.0000	35
H	11.088054196	4.720768041	7.106096184	CORE	36	H	H	0.0000	36
H	9.632236062	7.242354712	7.106403093	CORE	37	H	H	0.0000	37
H	9.656494872	2.239241128	7.061700226	CORE	38	H	H	0.0000	38
H	6.767328375	7.243231015	7.061730988	CORE	39	H	H	0.0000	39
H	5.362474569	4.720515917	7.163971161	CORE	40	H	H	0.0000	40
H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.185331512	4.719078948	10.934769539	CORE	45	Pd	Pd	0.0000	45
Pd	9.623144703	2.234661777	10.952798680	CORE	46	Pd	Pd	0.0000	46
Pd	6.744703096	7.228219246	10.938950641	CORE	47	Pd	Pd	0.0000	47
Pd	14.010829166	9.749818229	10.928847640	CORE	48	Pd	Pd	0.0000	48
Pd	6.746815618	2.213917360	10.926070447	CORE	49	Pd	Pd	0.0000	49
Pd	15.462879370	7.238041433	10.934671112	CORE	50	Pd	Pd	0.0000	50
Pd	5.312507729	4.720150288	10.926945432	CORE	51	Pd	Pd	0.0000	51
Pd	16.872442332	9.749563406	10.922818617	CORE	52	Pd	Pd	0.0000	52
Pd	14.028971756	4.709959798	10.939462826	CORE	53	Pd	Pd	0.0000	53
Pd	11.094551701	9.770547684	10.930415496	CORE	54	Pd	Pd	0.0000	54
Pd	3.850784375	2.212384560	10.923268486	CORE	55	Pd	Pd	0.0000	55
Pd	12.538755570	7.226019459	10.933806612	CORE	56	Pd	Pd	0.0000	56
Pd	12.529708941	2.213154220	10.918488155	CORE	57	Pd	Pd	0.0000	57
Pd	8.175317530	9.745166637	10.912198746	CORE	58	Pd	Pd	0.0000	58
Pd	11.098134323	4.722485216	10.937161103	CORE	59	Pd	Pd	0.0000	59
Pd	9.640460593	7.239476924	10.934488720	CORE	60	Pd	Pd	0.0000	60
Pd	5.236223730	2.985506412	13.218045055	CORE	61	Pd	Pd	0.0000	61
Pd	9.642884923	0.552593373	13.206831631	CORE	62	Pd	Pd	0.0000	62
Pd	5.302320124	8.108792304	13.195853520	CORE	63	Pd	Pd	0.0000	63
Pd	8.138727914	3.106115344	13.363577602	CORE	64	Pd	Pd	0.0000	64
Pd	6.808089018	5.590182436	13.303443106	CORE	65	Pd	Pd	0.0000	65
Pd	6.751593304	0.522819002	13.220717567	CORE	66	Pd	Pd	0.0000	66
Pd	3.886226613	5.537694351	13.250501017	CORE	67	Pd	Pd	0.0000	67
Pd	14.007674350	8.058818986	13.239389438	CORE	68	Pd	Pd	0.0000	68
Pd	2.379171285	3.040905452	13.209193603	CORE	69	Pd	Pd	0.0000	69
Pd	9.682979647	5.579497909	13.198399079	CORE	70	Pd	Pd	0.0000	70

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Pd        3.812987903    0.512881366    13.210735943 CORE    71 Pd Pd    0.0000    71
Pd        0.932849619    0.547625795    13.222195212 CORE    72 Pd Pd    0.0000    72
Pd        11.099089447   3.056617392    13.238090610 CORE    73 Pd Pd    0.0000    73
Pd        8.203718541    8.100680848    13.225292013 CORE    74 Pd Pd    0.0000    74
Pd        12.574192544   5.554035103    13.238921370 CORE    75 Pd Pd    0.0000    75
Pd        11.107030838   8.073194375    13.237728813 CORE    76 Pd Pd    0.0000    76
H         2.434053842    3.096844788    9.872900575 CORE     77 H  H     0.0000    77
H         3.901752582    0.525417077    9.850717203 CORE     78 H  H     0.0000    78
H         6.777024887    0.585375201    9.949586525 CORE     79 H  H     0.0000    79
H         3.902078240    5.542768476    9.974735150 CORE     80 H  H     0.0000    80
H         6.789229216    5.543563169    9.895544306 CORE     81 H  H     0.0000    81
H         8.192379686    3.096685787    9.907657066 CORE     82 H  H     0.0000    82
H         0.711465997    0.420025961    9.749474047 CORE     83 H  H     0.0000    83
H         14.270966288   8.211279697    9.840444356 CORE     84 H  H     0.0000    84
H         11.045362977   3.095510809    9.897847337 CORE     85 H  H     0.0000    85
H         8.206495091    7.998303105    9.871771678 CORE     86 H  H     0.0000    86
H         11.071668963   7.858142229    9.852730221 CORE     87 H  H     0.0000    87
H         12.326461474   5.648097303    9.824071235 CORE     88 H  H     0.0000    88
H         4.602098121    4.227431275    14.289652808 CORE    89 H  H     0.0000    89
H         5.248838491    1.269818765    13.902231041 CORE    90 H  H     0.0000    90
H         8.217664630    1.343025458    13.909495090 CORE    91 H  H     0.0000    91
H         5.239374814    6.521608054    13.908512379 CORE    92 H  H     0.0000    92
H         2.377120062    1.395797226    13.923644777 CORE    93 H  H     0.0000    93
H         15.444299548   8.926584823    13.920848639 CORE    94 H  H     0.0000    94
H         14.011964764   6.385831475    13.945734201 CORE    95 H  H     0.0000    95
H         12.558610935   8.899531199    13.937027279 CORE    96 H  H     0.0000    96
H         9.693894814    3.906910939    13.920897874 CORE    97 H  H     0.0000    97
H         8.256790027    6.459162596    13.934108748 CORE    98 H  H     0.0000    98
H         12.573995470   3.865712205    13.942939495 CORE    99 H  H     0.0000    99
H         9.651935869    8.908328668    13.950036858 CORE   100 H  H     0.0000   100
H         11.090358562   1.385806211    13.933742115 CORE   101 H  H     0.0000   101
H         6.756298332    8.930760603    13.930137079 CORE   102 H  H     0.0000   102
H         11.131336923   6.405251706    13.934237600 CORE   103 H  H     0.0000   103
C         7.073304936    4.235030290    14.871806039 CORE   104 C  C     0.0000   104
C         5.884581354    3.624455292    15.051422605 CORE   105 C  C     0.0000   105
H         7.763751955    4.507897775    15.676049289 CORE   106 H  H     0.0000   106
H         5.447794311    3.255760383    15.984517440 CORE   107 H  H     0.0000   107
end
end
```

Vinyl adsorbed on Pd_4H_3(111). The energy from VASP is -486.962038 eV.

```
PBC    11.60000000    11.60000000    20.00000000    90.00000000    90.00000000    60.00000000
Pd        6.747338531    0.544541613    6.403267290 CORE     1 Pd Pd    0.0000     1
Pd        3.845151399    5.571142423    6.403290684 CORE     2 Pd Pd    0.0000     2
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Pd	5.298982544	3.059410650	6.403296328	CORE	3	Pd	Pd	0.0000	3
Pd	9.648025542	0.547773874	6.403201805	CORE	4	Pd	Pd	0.0000	4
Pd	5.298282266	8.081617720	6.403218683	CORE	5	Pd	Pd	0.0000	5
Pd	8.196069754	3.060087698	6.403506017	CORE	6	Pd	Pd	0.0000	6
Pd	6.748041394	5.568042339	6.403528135	CORE	7	Pd	Pd	0.0000	7
Pd	2.396203981	3.056086329	6.403974639	CORE	8	Pd	Pd	0.0000	8
Pd	3.844692371	0.547193572	6.403980644	CORE	9	Pd	Pd	0.0000	9
Pd	13.995599937	8.080432901	6.403915026	CORE	10	Pd	Pd	0.0000	10
Pd	11.097339485	3.057320193	6.404178400	CORE	11	Pd	Pd	0.0000	11
Pd	8.196252877	8.082018112	6.404201419	CORE	12	Pd	Pd	0.0000	12
Pd	12.547118135	5.570172821	6.404809441	CORE	13	Pd	Pd	0.0000	13
Pd	11.097374320	8.081197886	6.404806864	CORE	14	Pd	Pd	0.0000	14
Pd	0.947647213	0.547191260	6.404240481	CORE	15	Pd	Pd	0.0000	15
Pd	9.647863113	5.570318755	6.404626518	CORE	16	Pd	Pd	0.0000	16
Pd	5.296345229	1.383774072	8.598645002	CORE	17	Pd	Pd	0.0000	17
Pd	3.846430041	3.895121361	8.598650689	CORE	18	Pd	Pd	0.0000	18
Pd	15.446747886	8.918407968	8.598673994	CORE	19	Pd	Pd	0.0000	19
Pd	8.196524484	1.383846907	8.598440679	CORE	20	Pd	Pd	0.0000	20
Pd	5.296487130	6.406750055	8.598478119	CORE	21	Pd	Pd	0.0000	21
Pd	6.746726050	3.895397354	8.597899801	CORE	22	Pd	Pd	0.0000	22
Pd	12.546601356	8.918351911	8.598885115	CORE	23	Pd	Pd	0.0000	23
Pd	13.996646681	6.406823241	8.598891508	CORE	24	Pd	Pd	0.0000	24
Pd	9.646822887	3.895276415	8.599334404	CORE	25	Pd	Pd	0.0000	25
Pd	11.096261310	1.383436470	8.598996838	CORE	26	Pd	Pd	0.0000	26
Pd	8.196560479	6.407055489	8.599357814	CORE	27	Pd	Pd	0.0000	27
Pd	6.745960494	8.918219637	8.599027684	CORE	28	Pd	Pd	0.0000	28
Pd	2.396365455	1.383718188	8.599138079	CORE	29	Pd	Pd	0.0000	29
Pd	12.546369931	3.894993974	8.599714782	CORE	30	Pd	Pd	0.0000	30
Pd	9.646092187	8.918242765	8.599728379	CORE	31	Pd	Pd	0.0000	31
Pd	11.096426310	6.406760277	8.599885411	CORE	32	Pd	Pd	0.0000	32
H	13.966125551	4.748953754	7.090172091	CORE	33	H	H	0.0000	33
H	11.095843995	9.720660436	7.090205342	CORE	34	H	H	0.0000	34
H	3.762469203	2.172306700	7.151879904	CORE	35	H	H	0.0000	35
H	11.088054196	4.720768041	7.106096184	CORE	36	H	H	0.0000	36
H	9.632236062	7.242354712	7.106403093	CORE	37	H	H	0.0000	37
H	9.656494872	2.239241128	7.061700226	CORE	38	H	H	0.0000	38
H	6.767328375	7.243231015	7.061730988	CORE	39	H	H	0.0000	39
H	5.362474569	4.720515917	7.163971161	CORE	40	H	H	0.0000	40
H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.203449963	4.736959293	10.926843366	CORE	45	Pd	Pd	0.0000	45
Pd	9.635228272	2.222790800	10.944073894	CORE	46	Pd	Pd	0.0000	46

Pd	6.741703687	7.234292837	10.944346328 CORE	47 Pd Pd	0.0000	47	
Pd	14.018550236	9.763368241	10.931049344 CORE	48 Pd Pd	0.0000	48	
Pd	6.746876497	2.250671500	10.938775160 CORE	49 Pd Pd	0.0000	49	
Pd	15.463766511	7.260172896	10.931099709 CORE	50 Pd Pd	0.0000	50	
Pd	5.322015816	4.718656335	10.938833120 CORE	51 Pd Pd	0.0000	51	
Pd	16.879602704	9.746255652	10.931882806 CORE	52 Pd Pd	0.0000	52	
Pd	14.011942685	4.730660217	10.930054122 CORE	53 Pd Pd	0.0000	53	
Pd	11.102437024	9.770791188	10.930031763 CORE	54 Pd Pd	0.0000	54	
Pd	3.876704592	2.239185412	10.951737695 CORE	55 Pd Pd	0.0000	55	
Pd	12.543747183	7.243005242	10.925213504 CORE	56 Pd Pd	0.0000	56	
Pd	12.539507336	2.199595515	10.914728426 CORE	57 Pd Pd	0.0000	57	
Pd	8.173861156	9.761147113	10.914956746 CORE	58 Pd Pd	0.0000	58	
Pd	11.104233321	4.735576996	10.918450520 CORE	59 Pd Pd	0.0000	59	
Pd	9.652281627	7.250102633	10.918558563 CORE	60 Pd Pd	0.0000	60	
Pd	5.278763915	3.048705141	13.318238217 CORE	61 Pd Pd	0.0000	61	
Pd	9.648199241	0.560548120	13.205171853 CORE	62 Pd Pd	0.0000	62	
Pd	5.308553474	8.076823259	13.205295245 CORE	63 Pd Pd	0.0000	63	
Pd	8.167370569	3.115210028	13.317659938 CORE	64 Pd Pd	0.0000	64	
Pd	6.780648915	5.516974344	13.317657255 CORE	65 Pd Pd	0.0000	65	
Pd	6.756179084	0.555059913	13.195131393 CORE	66 Pd Pd	0.0000	66	
Pd	3.857856372	5.574973956	13.195029287 CORE	67 Pd Pd	0.0000	67	
Pd	14.006381559	8.087627820	13.221809128 CORE	68 Pd Pd	0.0000	68	
Pd	2.373456365	3.044428278	13.200106176 CORE	69 Pd Pd	0.0000	69	
Pd	9.694282511	5.598002091	13.165194002 CORE	70 Pd Pd	0.0000	70	
Pd	3.822424625	0.534799285	13.200103222 CORE	71 Pd Pd	0.0000	71	
Pd	0.934689247	0.540738820	13.213863915 CORE	72 Pd Pd	0.0000	72	
Pd	11.102847209	3.058886634	13.197282397 CORE	73 Pd Pd	0.0000	73	
Pd	8.199530068	8.087432066	13.197614748 CORE	74 Pd Pd	0.0000	74	
Pd	12.565529176	5.574247382	13.215308006 CORE	75 Pd Pd	0.0000	75	
Pd	11.109360794	8.096509412	13.215458304 CORE	76 Pd Pd	0.0000	76	
H	2.690551914	3.223397680	9.883242654 CORE	77 H H	0.0000	77	
H	4.136822579	0.720304396	9.883844450 CORE	78 H H	0.0000	78	
H	7.039348479	0.747400052	9.920280198 CORE	79 H H	0.0000	79	
H	4.167482501	5.724520106	9.920917518 CORE	80 H H	0.0000	80	
H	7.005831269	5.732015603	9.885520958 CORE	81 H H	0.0000	81	
H	8.464972180	3.202313916	9.884993298 CORE	82 H H	0.0000	82	
H	0.705278789	0.408465923	9.729123876 CORE	83 H H	0.0000	83	
H	14.283281200	8.248236374	9.851534399 CORE	84 H H	0.0000	84	
H	11.329291167	3.174978222	9.893289685 CORE	85 H H	0.0000	85	
H	8.412580972	8.227600245	9.891992457 CORE	86 H H	0.0000	86	
H	11.167455427	7.920526007	9.800501047 CORE	87 H H	0.0000	87	
H	12.458285308	5.717841181	9.793534186 CORE	88 H H	0.0000	88	
H	5.269390321	1.310485767	13.873632574 CORE	89 H H	0.0000	89	
H	8.206222126	1.355972517	13.921059351 CORE	90 H H	0.0000	90	

H	5.276502181	6.430222513	13.920997472 CORE	91 H	H	0.0000	91
H	2.376800313	1.373218487	13.908803877 CORE	92 H	H	0.0000	92
H	15.462017712	8.928149764	13.896955143 CORE	93 H	H	0.0000	93
H	14.012832950	6.408956057	13.905056041 CORE	94 H	H	0.0000	94
H	12.555906251	8.932570361	13.905143133 CORE	95 H	H	0.0000	95
H	9.732103937	3.933232677	13.886831805 CORE	96 H	H	0.0000	96
H	8.271620577	6.463063963	13.886920936 CORE	97 H	H	0.0000	97
H	12.545183663	3.896661669	13.905541261 CORE	98 H	H	0.0000	98
H	9.646311105	8.917795066	13.905584216 CORE	99 H	H	0.0000	99
H	11.099096086	1.396689861	13.908139850 CORE	100 H	H	0.0000	100
H	6.757937500	8.915491542	13.908124661 CORE	101 H	H	0.0000	101
H	11.132153502	6.428149135	13.906035980 CORE	102 H	H	0.0000	102
H	3.768705494	3.909717730	13.873623108 CORE	103 H	H	0.0000	103
C	7.188329429	4.151074382	14.789780275 CORE	104 C	C	0.0000	104
C	6.012050308	3.471718130	15.259596645 CORE	105 C	C	0.0000	105
H	7.919685066	4.573543375	15.493230220 CORE	106 H	H	0.0000	106
H	6.167540889	2.507272019	15.758605027 CORE	107 H	H	0.0000	107
H	5.254398978	4.088669891	15.759012139 CORE	108 H	H	0.0000	108

end

end

TS from vinyl to ethene on Pd_4H_3(111). The energy from VASP is -486.213376 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	60.00000000		
Pd	6.747338531	0.544541613	6.403267290 CORE	1 Pd	Pd	0.0000	1
Pd	3.845151399	5.571142423	6.403290684 CORE	2 Pd	Pd	0.0000	2
Pd	5.298982544	3.059410650	6.403296328 CORE	3 Pd	Pd	0.0000	3
Pd	9.648025542	0.547773874	6.403201805 CORE	4 Pd	Pd	0.0000	4
Pd	5.298282266	8.081617720	6.403218683 CORE	5 Pd	Pd	0.0000	5
Pd	8.196069754	3.060087698	6.403506017 CORE	6 Pd	Pd	0.0000	6
Pd	6.748041394	5.568042339	6.403528135 CORE	7 Pd	Pd	0.0000	7
Pd	2.396203981	3.056086329	6.403974639 CORE	8 Pd	Pd	0.0000	8
Pd	3.844692371	0.547193572	6.403980644 CORE	9 Pd	Pd	0.0000	9
Pd	13.995599937	8.080432901	6.403915026 CORE	10 Pd	Pd	0.0000	10
Pd	11.097339485	3.057320193	6.404178400 CORE	11 Pd	Pd	0.0000	11
Pd	8.196252877	8.082018112	6.404201419 CORE	12 Pd	Pd	0.0000	12
Pd	12.547118135	5.570172821	6.404809441 CORE	13 Pd	Pd	0.0000	13
Pd	11.097374320	8.081197886	6.404806864 CORE	14 Pd	Pd	0.0000	14
Pd	0.947647213	0.547191260	6.404240481 CORE	15 Pd	Pd	0.0000	15
Pd	9.647863113	5.570318755	6.404626518 CORE	16 Pd	Pd	0.0000	16
Pd	5.296345229	1.383774072	8.598645002 CORE	17 Pd	Pd	0.0000	17
Pd	3.846430041	3.895121361	8.598650689 CORE	18 Pd	Pd	0.0000	18
Pd	15.446747886	8.918407968	8.598673994 CORE	19 Pd	Pd	0.0000	19
Pd	8.196524484	1.383846907	8.598440679 CORE	20 Pd	Pd	0.0000	20
Pd	5.296487130	6.406750055	8.598478119 CORE	21 Pd	Pd	0.0000	21

Pd	6.746726050	3.895397354	8.597899801	CORE	22	Pd	Pd	0.0000	22
Pd	12.546601356	8.918351911	8.598885115	CORE	23	Pd	Pd	0.0000	23
Pd	13.996646681	6.406823241	8.598891508	CORE	24	Pd	Pd	0.0000	24
Pd	9.646822887	3.895276415	8.599334404	CORE	25	Pd	Pd	0.0000	25
Pd	11.096261310	1.383436470	8.598996838	CORE	26	Pd	Pd	0.0000	26
Pd	8.196560479	6.407055489	8.599357814	CORE	27	Pd	Pd	0.0000	27
Pd	6.745960494	8.918219637	8.599027684	CORE	28	Pd	Pd	0.0000	28
Pd	2.396365455	1.383718188	8.599138079	CORE	29	Pd	Pd	0.0000	29
Pd	12.546369931	3.894993974	8.599714782	CORE	30	Pd	Pd	0.0000	30
Pd	9.646092187	8.918242765	8.599728379	CORE	31	Pd	Pd	0.0000	31
Pd	11.096426310	6.406760277	8.599885411	CORE	32	Pd	Pd	0.0000	32
H	13.966125551	4.748953754	7.090172091	CORE	33	H	H	0.0000	33
H	11.095843995	9.720660436	7.090205342	CORE	34	H	H	0.0000	34
H	3.762469203	2.172306700	7.151879904	CORE	35	H	H	0.0000	35
H	11.088054196	4.720768041	7.106096184	CORE	36	H	H	0.0000	36
H	9.632236062	7.242354712	7.106403093	CORE	37	H	H	0.0000	37
H	9.656494872	2.239241128	7.061700226	CORE	38	H	H	0.0000	38
H	6.767328375	7.243231015	7.061730988	CORE	39	H	H	0.0000	39
H	5.362474569	4.720515917	7.163971161	CORE	40	H	H	0.0000	40
H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.195003198	4.725295928	10.899897963	CORE	45	Pd	Pd	0.0000	45
Pd	9.632731644	2.219876875	10.935767804	CORE	46	Pd	Pd	0.0000	46
Pd	6.743293406	7.223735461	10.937411750	CORE	47	Pd	Pd	0.0000	47
Pd	14.006892759	9.748959062	10.919280790	CORE	48	Pd	Pd	0.0000	48
Pd	6.756780772	2.230004799	10.947428268	CORE	49	Pd	Pd	0.0000	49
Pd	15.454443514	7.238045782	10.930433786	CORE	50	Pd	Pd	0.0000	50
Pd	5.302616056	4.713302399	10.934714605	CORE	51	Pd	Pd	0.0000	51
Pd	16.878028018	9.736890298	10.932412015	CORE	52	Pd	Pd	0.0000	52
Pd	14.014363209	4.709462878	10.935215234	CORE	53	Pd	Pd	0.0000	53
Pd	11.088990990	9.777503634	10.922953927	CORE	54	Pd	Pd	0.0000	54
Pd	3.870728347	2.234190733	10.960323388	CORE	55	Pd	Pd	0.0000	55
Pd	12.524420520	7.225262827	10.933721388	CORE	56	Pd	Pd	0.0000	56
Pd	12.532358191	2.212229853	10.928121161	CORE	57	Pd	Pd	0.0000	57
Pd	8.180710618	9.755421339	10.910962790	CORE	58	Pd	Pd	0.0000	58
Pd	11.090642102	4.711781617	10.932524660	CORE	59	Pd	Pd	0.0000	59
Pd	9.637642553	7.244295172	10.932297726	CORE	60	Pd	Pd	0.0000	60
Pd	5.302552864	3.058974776	13.369296678	CORE	61	Pd	Pd	0.0000	61
Pd	9.648008793	0.528769586	13.200765597	CORE	62	Pd	Pd	0.0000	62
Pd	5.293627311	8.064276116	13.215274934	CORE	63	Pd	Pd	0.0000	63
Pd	8.254795435	3.098039542	13.277529242	CORE	64	Pd	Pd	0.0000	64
Pd	6.762318060	5.509466350	13.280006225	CORE	65	Pd	Pd	0.0000	65

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Pd      6.745222899   0.514348496   13.193114541 CORE   66 Pd Pd   0.0000   66
Pd      3.846952035   5.553083451   13.229814938 CORE   67 Pd Pd   0.0000   67
Pd      13.992874865  8.058966735   13.229405331 CORE   68 Pd Pd   0.0000   68
Pd      2.374838032   3.040874315   13.244352898 CORE   69 Pd Pd   0.0000   69
Pd      9.681214526   5.578522942   13.172581098 CORE   70 Pd Pd   0.0000   70
Pd      3.824669833   0.532723339   13.220977132 CORE   71 Pd Pd   0.0000   71
Pd      0.932127088   0.531860161   13.225013509 CORE   72 Pd Pd   0.0000   72
Pd      11.096034881  3.045790770   13.239268688 CORE   73 Pd Pd   0.0000   73
Pd      8.189428776   8.097108955   13.212110498 CORE   74 Pd Pd   0.0000   74
Pd      12.547991128  5.550822630   13.237312828 CORE   75 Pd Pd   0.0000   75
Pd      11.092507815  8.073807320   13.244444520 CORE   76 Pd Pd   0.0000   76
H       2.448780096   3.068618988   9.919216711 CORE    77 H  H    0.0000   77
H       3.888208881   0.595251489   9.901321009 CORE    78 H  H    0.0000   78
H       6.780413613   0.562748911   9.925012772 CORE    79 H  H    0.0000   79
H       3.904421698   5.537325212   9.960868803 CORE    80 H  H    0.0000   80
H       6.752616207   5.572364039   9.871266751 CORE    81 H  H    0.0000   81
H       8.180962414   3.057611608   9.930881805 CORE    82 H  H    0.0000   82
H       0.696314348   0.399666446   9.743270651 CORE    83 H  H    0.0000   83
H       14.260299166  8.206381962   9.828908256 CORE    84 H  H    0.0000   84
H       11.079723486  3.099694106   9.874163544 CORE    85 H  H    0.0000   85
H       8.213914586   7.973316045   9.904497978 CORE    86 H  H    0.0000   86
H       11.060927406  7.875564170   9.836148779 CORE    87 H  H    0.0000   87
H       12.330594703  5.652329460   9.819540275 CORE    88 H  H    0.0000   88
H       5.274500646   1.289198717   13.893240312 CORE   89 H  H    0.0000   89
H       8.198636530   1.331990109   13.871721256 CORE   90 H  H    0.0000   90
H       5.295900296   6.403934894   13.907275056 CORE   91 H  H    0.0000   91
H       2.370234940   1.362570958   13.937300356 CORE   92 H  H    0.0000   92
H       15.441066598  8.898158611   13.918959113 CORE   93 H  H    0.0000   93
H       13.997242204  6.387903084   13.936566275 CORE   94 H  H    0.0000   94
H       12.546025430  8.899726810   13.935513456 CORE   95 H  H    0.0000   95
H       8.958833389   3.732666799   14.585602010 CORE   96 H  H    0.0000   96
H       8.292961083   6.469789193   13.853476519 CORE   97 H  H    0.0000   97
H       12.519606624  3.866527175   13.951032372 CORE   98 H  H    0.0000   98
H       9.637670571   8.916213616   13.941798447 CORE   99 H  H    0.0000   99
H       11.097798073  1.391043689   13.921550183 CORE   100 H  H   0.0000   100
H       6.739812307   8.913569817   13.929544777 CORE   101 H  H   0.0000   101
H       11.096044972  6.389464299   13.936628520 CORE   102 H  H   0.0000   102
H       3.785309505   3.887689071   13.941984092 CORE   103 H  H   0.0000   103
C       7.340331283   4.161724394   14.829291863 CORE   104 C  C   0.0000   104
C       6.238193095   3.372980664   15.296348902 CORE   105 C  C   0.0000   105
H       7.718913125   4.962694424   15.477587105 CORE   106 H  H   0.0000   106
H       6.420254140   2.332016649   15.576327633 CORE   107 H  H   0.0000   107
H       5.528483163   3.890789489   15.953825348 CORE   108 H  H   0.0000   108
end
```

end

Ethene adsorbed on Pd_4H_3(111). The energy from VASP is -494.890176 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	60.00000000	
Pd	6.747338531	0.544541613	6.403267290 CORE	1 Pd Pd	0.0000	1	
Pd	3.845151399	5.571142423	6.403290684 CORE	2 Pd Pd	0.0000	2	
Pd	5.298982544	3.059410650	6.403296328 CORE	3 Pd Pd	0.0000	3	
Pd	9.648025542	0.547773874	6.403201805 CORE	4 Pd Pd	0.0000	4	
Pd	5.298282266	8.081617720	6.403218683 CORE	5 Pd Pd	0.0000	5	
Pd	8.196069754	3.060087698	6.403506017 CORE	6 Pd Pd	0.0000	6	
Pd	6.748041394	5.568042339	6.403528135 CORE	7 Pd Pd	0.0000	7	
Pd	2.396203981	3.056086329	6.403974639 CORE	8 Pd Pd	0.0000	8	
Pd	3.844692371	0.547193572	6.403980644 CORE	9 Pd Pd	0.0000	9	
Pd	13.995599937	8.080432901	6.403915026 CORE	10 Pd Pd	0.0000	10	
Pd	11.097339485	3.057320193	6.404178400 CORE	11 Pd Pd	0.0000	11	
Pd	8.196252877	8.082018112	6.404201419 CORE	12 Pd Pd	0.0000	12	
Pd	12.547118135	5.570172821	6.404809441 CORE	13 Pd Pd	0.0000	13	
Pd	11.097374320	8.081197886	6.404806864 CORE	14 Pd Pd	0.0000	14	
Pd	0.947647213	0.547191260	6.404240481 CORE	15 Pd Pd	0.0000	15	
Pd	9.647863113	5.570318755	6.404626518 CORE	16 Pd Pd	0.0000	16	
Pd	5.296345229	1.383774072	8.598645002 CORE	17 Pd Pd	0.0000	17	
Pd	3.846430041	3.895121361	8.598650689 CORE	18 Pd Pd	0.0000	18	
Pd	15.446747886	8.918407968	8.598673994 CORE	19 Pd Pd	0.0000	19	
Pd	8.196524484	1.383846907	8.598440679 CORE	20 Pd Pd	0.0000	20	
Pd	5.296487130	6.406750055	8.598478119 CORE	21 Pd Pd	0.0000	21	
Pd	6.746726050	3.895397354	8.597899801 CORE	22 Pd Pd	0.0000	22	
Pd	12.546601356	8.918351911	8.598885115 CORE	23 Pd Pd	0.0000	23	
Pd	13.996646681	6.406823241	8.598891508 CORE	24 Pd Pd	0.0000	24	
Pd	9.646822887	3.895276415	8.599334404 CORE	25 Pd Pd	0.0000	25	
Pd	11.096261310	1.383436470	8.598996838 CORE	26 Pd Pd	0.0000	26	
Pd	8.196560479	6.407055489	8.599357814 CORE	27 Pd Pd	0.0000	27	
Pd	6.745960494	8.918219637	8.599027684 CORE	28 Pd Pd	0.0000	28	
Pd	2.396365455	1.383718188	8.599138079 CORE	29 Pd Pd	0.0000	29	
Pd	12.546369931	3.894993974	8.599714782 CORE	30 Pd Pd	0.0000	30	
Pd	9.646092187	8.918242765	8.599728379 CORE	31 Pd Pd	0.0000	31	
Pd	11.096426310	6.406760277	8.599885411 CORE	32 Pd Pd	0.0000	32	
H	13.966125551	4.748953754	7.090172091 CORE	33 H H	0.0000	33	
H	11.095843995	9.720660436	7.090205342 CORE	34 H H	0.0000	34	
H	3.762469203	2.172306700	7.151879904 CORE	35 H H	0.0000	35	
H	11.088054196	4.720768041	7.106096184 CORE	36 H H	0.0000	36	
H	9.632236062	7.242354712	7.106403093 CORE	37 H H	0.0000	37	
H	9.656494872	2.239241128	7.061700226 CORE	38 H H	0.0000	38	
H	6.767328375	7.243231015	7.061730988 CORE	39 H H	0.0000	39	
H	5.362474569	4.720515917	7.163971161 CORE	40 H H	0.0000	40	

H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.203331219	4.719322644	10.960943013	CORE	45	Pd	Pd	0.0000	45
Pd	9.637822201	2.222853190	10.971249534	CORE	46	Pd	Pd	0.0000	46
Pd	6.748714997	7.252613711	10.908366793	CORE	47	Pd	Pd	0.0000	47
Pd	14.013142728	9.763983405	10.926407025	CORE	48	Pd	Pd	0.0000	48
Pd	6.775661651	2.238734500	10.974107375	CORE	49	Pd	Pd	0.0000	49
Pd	15.458775557	7.253844354	10.930713155	CORE	50	Pd	Pd	0.0000	50
Pd	5.303251062	4.724066652	10.918383141	CORE	51	Pd	Pd	0.0000	51
Pd	16.886676845	9.749124088	10.914504869	CORE	52	Pd	Pd	0.0000	52
Pd	14.009101983	4.730156163	10.929786672	CORE	53	Pd	Pd	0.0000	53
Pd	11.088708998	9.765216283	10.918695642	CORE	54	Pd	Pd	0.0000	54
Pd	3.861072668	2.213624744	10.921509775	CORE	55	Pd	Pd	0.0000	55
Pd	12.538376427	7.239291220	10.920658235	CORE	56	Pd	Pd	0.0000	56
Pd	12.544534385	2.202049823	10.909266695	CORE	57	Pd	Pd	0.0000	57
Pd	8.186043832	9.751287032	10.906896916	CORE	58	Pd	Pd	0.0000	58
Pd	11.089858123	4.726863262	10.925562264	CORE	59	Pd	Pd	0.0000	59
Pd	9.657003561	7.240555829	10.915473794	CORE	60	Pd	Pd	0.0000	60
Pd	5.271583213	3.051250005	13.183142462	CORE	61	Pd	Pd	0.0000	61
Pd	9.664838222	0.515378004	13.188171926	CORE	62	Pd	Pd	0.0000	62
Pd	5.305887697	8.081638594	13.190737482	CORE	63	Pd	Pd	0.0000	63
Pd	8.208294394	3.041665904	13.671444066	CORE	64	Pd	Pd	0.0000	64
Pd	6.738470901	5.599323931	13.191347765	CORE	65	Pd	Pd	0.0000	65
Pd	6.727312874	0.514673046	13.196890693	CORE	66	Pd	Pd	0.0000	66
Pd	3.848804310	5.568106593	13.217606437	CORE	67	Pd	Pd	0.0000	67
Pd	13.998646323	8.071604251	13.217742125	CORE	68	Pd	Pd	0.0000	68
Pd	2.401381889	3.050144796	13.204956874	CORE	69	Pd	Pd	0.0000	69
Pd	9.663881061	5.599629607	13.184324274	CORE	70	Pd	Pd	0.0000	70
Pd	3.836876712	0.538723209	13.206694192	CORE	71	Pd	Pd	0.0000	71
Pd	0.952576828	0.537349238	13.199799513	CORE	72	Pd	Pd	0.0000	72
Pd	11.130736623	3.055172977	13.193964216	CORE	73	Pd	Pd	0.0000	73
Pd	8.201159735	8.085480633	13.197158469	CORE	74	Pd	Pd	0.0000	74
Pd	12.555100789	5.566363711	13.217020146	CORE	75	Pd	Pd	0.0000	75
Pd	11.094735270	8.080407795	13.213423861	CORE	76	Pd	Pd	0.0000	76
H	2.661863099	3.198724628	9.887970101	CORE	77	H	H	0.0000	77
H	4.001204984	0.661938410	9.849722064	CORE	78	H	H	0.0000	78
H	7.006549315	0.764686608	9.909808919	CORE	79	H	H	0.0000	79
H	4.083772775	5.719127853	9.886300312	CORE	80	H	H	0.0000	80
H	6.808659538	5.307790953	9.861143487	CORE	81	H	H	0.0000	81
H	8.500283320	3.201442159	9.911281237	CORE	82	H	H	0.0000	82
H	0.739966309	0.374194452	9.739262919	CORE	83	H	H	0.0000	83
H	14.287359161	8.249851752	9.863708530	CORE	84	H	H	0.0000	84

H 11.309915196 3.121709087 9.865145759 CORE 85 H H 0.0000 85
H 8.202801536 7.819208328 9.901690348 CORE 86 H H 0.0000 86
H 11.178588236 8.145665389 9.888546103 CORE 87 H H 0.0000 87
H 12.305083460 5.691709927 9.847404063 CORE 88 H H 0.0000 88
H 5.284245803 1.367119975 13.880404244 CORE 89 H H 0.0000 89
H 8.190028794 1.231050887 13.859208375 CORE 90 H H 0.0000 90
H 5.286302220 6.421780299 13.905934720 CORE 91 H H 0.0000 91
H 2.388896067 1.381269679 13.903662845 CORE 92 H H 0.0000 92
H 15.458968820 8.896630721 13.901968758 CORE 93 H H 0.0000 93
H 13.999370550 6.399272902 13.910467306 CORE 94 H H 0.0000 94
H 12.545527062 8.898958857 13.913215956 CORE 95 H H 0.0000 95
H 8.200800772 6.417483848 13.885844821 CORE 96 H H 0.0000 96
H 12.567974857 3.889162211 13.910125026 CORE 97 H H 0.0000 97
H 9.643403009 8.916189810 13.907875036 CORE 98 H H 0.0000 98
H 11.114576228 1.377796796 13.873622358 CORE 99 H H 0.0000 99
H 6.758768418 8.910582762 13.898183102 CORE 100 H H 0.0000 100
H 11.121040130 6.416197149 13.907472935 CORE 101 H H 0.0000 101
H 3.838024660 3.897209390 13.905614524 CORE 102 H H 0.0000 102
H 9.759610646 3.972594628 13.836562241 CORE 103 H H 0.0000 103
H 6.646081311 3.960014324 13.821984887 CORE 104 H H 0.0000 104
C 8.884227231 2.832680701 15.982705877 CORE 105 C C 0.0000 105
C 7.554883903 3.156994839 15.982957784 CORE 106 C C 0.0000 106
H 9.650762740 3.595815740 16.115834722 CORE 107 H H 0.0000 107
H 6.783932887 2.387981988 16.038545462 CORE 108 H H 0.0000 108
H 7.227280120 4.187968691 16.117722651 CORE 109 H H 0.0000 109
H 9.215683425 1.795514450 16.037062059 CORE 110 H H 0.0000 110
end
end

TS from ethene to ethyl on Pd_4H_3(111). The energy from VASP is -494.388964 eV.

PBC 11.60000000 11.60000000 20.00000000 90.00000000 90.00000000 60.00000000
Pd 6.747338531 0.544541613 6.403267290 CORE 1 Pd Pd 0.0000 1
Pd 3.845151399 5.571142423 6.403290684 CORE 2 Pd Pd 0.0000 2
Pd 5.298982544 3.059410650 6.403296328 CORE 3 Pd Pd 0.0000 3
Pd 9.648025542 0.547773874 6.403201805 CORE 4 Pd Pd 0.0000 4
Pd 5.298282266 8.081617720 6.403218683 CORE 5 Pd Pd 0.0000 5
Pd 8.196069754 3.060087698 6.403506017 CORE 6 Pd Pd 0.0000 6
Pd 6.748041394 5.568042339 6.403528135 CORE 7 Pd Pd 0.0000 7
Pd 2.396203981 3.056086329 6.403974639 CORE 8 Pd Pd 0.0000 8
Pd 3.844692371 0.547193572 6.403980644 CORE 9 Pd Pd 0.0000 9
Pd 13.995599937 8.080432901 6.403915026 CORE 10 Pd Pd 0.0000 10
Pd 11.097339485 3.057320193 6.404178400 CORE 11 Pd Pd 0.0000 11
Pd 8.196252877 8.082018112 6.404201419 CORE 12 Pd Pd 0.0000 12
Pd 12.547118135 5.570172821 6.404809441 CORE 13 Pd Pd 0.0000 13

Pd	11.097374320	8.081197886	6.404806864	CORE	14	Pd	Pd	0.0000	14
Pd	0.947647213	0.547191260	6.404240481	CORE	15	Pd	Pd	0.0000	15
Pd	9.647863113	5.570318755	6.404626518	CORE	16	Pd	Pd	0.0000	16
Pd	5.296345229	1.383774072	8.598645002	CORE	17	Pd	Pd	0.0000	17
Pd	3.846430041	3.895121361	8.598650689	CORE	18	Pd	Pd	0.0000	18
Pd	15.446747886	8.918407968	8.598673994	CORE	19	Pd	Pd	0.0000	19
Pd	8.196524484	1.383846907	8.598440679	CORE	20	Pd	Pd	0.0000	20
Pd	5.296487130	6.406750055	8.598478119	CORE	21	Pd	Pd	0.0000	21
Pd	6.746726050	3.895397354	8.597899801	CORE	22	Pd	Pd	0.0000	22
Pd	12.546601356	8.918351911	8.598885115	CORE	23	Pd	Pd	0.0000	23
Pd	13.996646681	6.406823241	8.598891508	CORE	24	Pd	Pd	0.0000	24
Pd	9.646822887	3.895276415	8.599334404	CORE	25	Pd	Pd	0.0000	25
Pd	11.096261310	1.383436470	8.598996838	CORE	26	Pd	Pd	0.0000	26
Pd	8.196560479	6.407055489	8.599357814	CORE	27	Pd	Pd	0.0000	27
Pd	6.745960494	8.918219637	8.599027684	CORE	28	Pd	Pd	0.0000	28
Pd	2.396365455	1.383718188	8.599138079	CORE	29	Pd	Pd	0.0000	29
Pd	12.546369931	3.894993974	8.599714782	CORE	30	Pd	Pd	0.0000	30
Pd	9.646092187	8.918242765	8.599728379	CORE	31	Pd	Pd	0.0000	31
Pd	11.096426310	6.406760277	8.599885411	CORE	32	Pd	Pd	0.0000	32
H	13.966125551	4.748953754	7.090172091	CORE	33	H	H	0.0000	33
H	11.095843995	9.720660436	7.090205342	CORE	34	H	H	0.0000	34
H	3.762469203	2.172306700	7.151879904	CORE	35	H	H	0.0000	35
H	11.088054196	4.720768041	7.106096184	CORE	36	H	H	0.0000	36
H	9.632236062	7.242354712	7.106403093	CORE	37	H	H	0.0000	37
H	9.656494872	2.239241128	7.061700226	CORE	38	H	H	0.0000	38
H	6.767328375	7.243231015	7.061730988	CORE	39	H	H	0.0000	39
H	5.362474569	4.720515917	7.163971161	CORE	40	H	H	0.0000	40
H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.186864505	4.713497572	10.939178607	CORE	45	Pd	Pd	0.0000	45
Pd	9.626765526	2.232289078	10.965019448	CORE	46	Pd	Pd	0.0000	46
Pd	6.751051846	7.239905307	10.922694360	CORE	47	Pd	Pd	0.0000	47
Pd	14.004772315	9.755108550	10.923090416	CORE	48	Pd	Pd	0.0000	48
Pd	6.760422555	2.231450188	10.955799249	CORE	49	Pd	Pd	0.0000	49
Pd	15.451809316	7.244614144	10.931544201	CORE	50	Pd	Pd	0.0000	50
Pd	5.298632341	4.722326478	10.915112527	CORE	51	Pd	Pd	0.0000	51
Pd	16.876891299	9.738493631	10.928933006	CORE	52	Pd	Pd	0.0000	52
Pd	14.009951119	4.716560455	10.934585578	CORE	53	Pd	Pd	0.0000	53
Pd	11.088344696	9.771892242	10.919975698	CORE	54	Pd	Pd	0.0000	54
Pd	3.846381283	2.216973458	10.926280842	CORE	55	Pd	Pd	0.0000	55
Pd	12.525581786	7.230496249	10.932197534	CORE	56	Pd	Pd	0.0000	56
Pd	12.534927308	2.207359865	10.912442554	CORE	57	Pd	Pd	0.0000	57

Pd	8.181298916	9.745990779	10.920202373	CORE	58	Pd	Pd	0.0000	58
Pd	11.085901139	4.724571690	10.930247523	CORE	59	Pd	Pd	0.0000	59
Pd	9.639269400	7.250451955	10.923588385	CORE	60	Pd	Pd	0.0000	60
Pd	5.277901901	3.060329941	13.200781267	CORE	61	Pd	Pd	0.0000	61
Pd	9.659082324	0.517437978	13.200915958	CORE	62	Pd	Pd	0.0000	62
Pd	5.294565756	8.072496704	13.216776670	CORE	63	Pd	Pd	0.0000	63
Pd	8.223178390	3.062380316	13.583066139	CORE	64	Pd	Pd	0.0000	64
Pd	6.723907673	5.572494844	13.203656928	CORE	65	Pd	Pd	0.0000	65
Pd	6.727615549	0.513839704	13.199676374	CORE	66	Pd	Pd	0.0000	66
Pd	3.841796449	5.561365251	13.231854241	CORE	67	Pd	Pd	0.0000	67
Pd	13.991330323	8.067218149	13.231109384	CORE	68	Pd	Pd	0.0000	68
Pd	2.394376233	3.042860183	13.232653972	CORE	69	Pd	Pd	0.0000	69
Pd	9.657189489	5.610430090	13.174344326	CORE	70	Pd	Pd	0.0000	70
Pd	3.829387958	0.530725807	13.224718099	CORE	71	Pd	Pd	0.0000	71
Pd	0.946235598	0.528407281	13.219374800	CORE	72	Pd	Pd	0.0000	72
Pd	11.128168814	3.035925390	13.208878494	CORE	73	Pd	Pd	0.0000	73
Pd	8.189168371	8.079108848	13.234459799	CORE	74	Pd	Pd	0.0000	74
Pd	12.549223615	5.559969723	13.239721615	CORE	75	Pd	Pd	0.0000	75
Pd	11.089301275	8.081629086	13.238358950	CORE	76	Pd	Pd	0.0000	76
H	2.440396569	3.086719278	9.910134076	CORE	77	H	H	0.0000	77
H	3.863037163	0.613430548	9.895617529	CORE	78	H	H	0.0000	78
H	6.799001123	0.617929635	9.925978100	CORE	79	H	H	0.0000	79
H	3.899790234	5.569132424	9.929297194	CORE	80	H	H	0.0000	80
H	6.778235267	5.551829907	9.880743701	CORE	81	H	H	0.0000	81
H	8.222093601	3.068672726	9.959123093	CORE	82	H	H	0.0000	82
H	0.672745746	0.404851752	9.725918720	CORE	83	H	H	0.0000	83
H	14.258849249	8.210218303	9.834166367	CORE	84	H	H	0.0000	84
H	11.018550105	3.064917878	9.909259121	CORE	85	H	H	0.0000	85
H	8.164967952	7.960971728	9.880015772	CORE	86	H	H	0.0000	86
H	11.083557943	7.941320933	9.870281104	CORE	87	H	H	0.0000	87
H	12.324702998	5.657403609	9.824515165	CORE	88	H	H	0.0000	88
H	5.272089475	1.357757901	13.887928526	CORE	89	H	H	0.0000	89
H	8.193946417	1.217121875	13.890384232	CORE	90	H	H	0.0000	90
H	5.301703825	6.394733134	13.926534411	CORE	91	H	H	0.0000	91
H	2.380714617	1.367154103	13.937344613	CORE	92	H	H	0.0000	92
H	15.447111465	8.896043298	13.924714073	CORE	93	H	H	0.0000	93
H	13.995159891	6.396283874	13.939497780	CORE	94	H	H	0.0000	94
H	12.543945155	8.904028692	13.940741768	CORE	95	H	H	0.0000	95
H	8.167910708	6.393367777	13.898286282	CORE	96	H	H	0.0000	96
H	12.560572138	3.881079884	13.941960417	CORE	97	H	H	0.0000	97
H	9.631646659	8.912494601	13.944642784	CORE	98	H	H	0.0000	98
H	11.106702931	1.366202212	13.917766821	CORE	99	H	H	0.0000	99
H	6.742270502	8.906449470	13.937903250	CORE	100	H	H	0.0000	100
H	11.110172672	6.410665699	13.932822738	CORE	101	H	H	0.0000	101

H	3.838592473	3.892311351	13.934154584	CORE	102	H	H	0.0000	102
H	9.779375333	3.974771970	13.828453818	CORE	103	H	H	0.0000	103
H	6.594687081	3.623168691	14.370506729	CORE	104	H	H	0.0000	104
C	8.503909253	3.161334129	15.745905247	CORE	105	C	C	0.0000	105
C	7.111293189	3.461146095	15.734940986	CORE	106	C	C	0.0000	106
H	9.211704950	3.966412795	15.943773776	CORE	107	H	H	0.0000	107
H	6.413724481	2.668945462	16.015651629	CORE	108	H	H	0.0000	108
H	6.803759072	4.472073718	16.012030832	CORE	109	H	H	0.0000	109
H	8.843042741	2.160918440	16.012461599	CORE	110	H	H	0.0000	110

end

end

Ethyl adsorbed on Pd_4H_3(111). The energy from VASP is -498.787035 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	60.00000000		
Pd	6.747338531	0.544541613	6.403267290	CORE	1	Pd	Pd	0.0000	1
Pd	3.845151399	5.571142423	6.403290684	CORE	2	Pd	Pd	0.0000	2
Pd	5.298982544	3.059410650	6.403296328	CORE	3	Pd	Pd	0.0000	3
Pd	9.648025542	0.547773874	6.403201805	CORE	4	Pd	Pd	0.0000	4
Pd	5.298282266	8.081617720	6.403218683	CORE	5	Pd	Pd	0.0000	5
Pd	8.196069754	3.060087698	6.403506017	CORE	6	Pd	Pd	0.0000	6
Pd	6.748041394	5.568042339	6.403528135	CORE	7	Pd	Pd	0.0000	7
Pd	2.396203981	3.056086329	6.403974639	CORE	8	Pd	Pd	0.0000	8
Pd	3.844692371	0.547193572	6.403980644	CORE	9	Pd	Pd	0.0000	9
Pd	13.995599937	8.080432901	6.403915026	CORE	10	Pd	Pd	0.0000	10
Pd	11.097339485	3.057320193	6.404178400	CORE	11	Pd	Pd	0.0000	11
Pd	8.196252877	8.082018112	6.404201419	CORE	12	Pd	Pd	0.0000	12
Pd	12.547118135	5.570172821	6.404809441	CORE	13	Pd	Pd	0.0000	13
Pd	11.097374320	8.081197886	6.404806864	CORE	14	Pd	Pd	0.0000	14
Pd	0.947647213	0.547191260	6.404240481	CORE	15	Pd	Pd	0.0000	15
Pd	9.647863113	5.570318755	6.404626518	CORE	16	Pd	Pd	0.0000	16
Pd	5.296345229	1.383774072	8.598645002	CORE	17	Pd	Pd	0.0000	17
Pd	3.846430041	3.895121361	8.598650689	CORE	18	Pd	Pd	0.0000	18
Pd	15.446747886	8.918407968	8.598673994	CORE	19	Pd	Pd	0.0000	19
Pd	8.196524484	1.383846907	8.598440679	CORE	20	Pd	Pd	0.0000	20
Pd	5.296487130	6.406750055	8.598478119	CORE	21	Pd	Pd	0.0000	21
Pd	6.746726050	3.895397354	8.597899801	CORE	22	Pd	Pd	0.0000	22
Pd	12.546601356	8.918351911	8.598885115	CORE	23	Pd	Pd	0.0000	23
Pd	13.996646681	6.406823241	8.598891508	CORE	24	Pd	Pd	0.0000	24
Pd	9.646822887	3.895276415	8.599334404	CORE	25	Pd	Pd	0.0000	25
Pd	11.096261310	1.383436470	8.598996838	CORE	26	Pd	Pd	0.0000	26
Pd	8.196560479	6.407055489	8.599357814	CORE	27	Pd	Pd	0.0000	27
Pd	6.745960494	8.918219637	8.599027684	CORE	28	Pd	Pd	0.0000	28
Pd	2.396365455	1.383718188	8.599138079	CORE	29	Pd	Pd	0.0000	29
Pd	12.546369931	3.894993974	8.599714782	CORE	30	Pd	Pd	0.0000	30

Pd	9.646092187	8.918242765	8.599728379	CORE	31	Pd	Pd	0.0000	31
Pd	11.096426310	6.406760277	8.599885411	CORE	32	Pd	Pd	0.0000	32
H	13.966125551	4.748953754	7.090172091	CORE	33	H	H	0.0000	33
H	11.095843995	9.720660436	7.090205342	CORE	34	H	H	0.0000	34
H	3.762469203	2.172306700	7.151879904	CORE	35	H	H	0.0000	35
H	11.088054196	4.720768041	7.106096184	CORE	36	H	H	0.0000	36
H	9.632236062	7.242354712	7.106403093	CORE	37	H	H	0.0000	37
H	9.656494872	2.239241128	7.061700226	CORE	38	H	H	0.0000	38
H	6.767328375	7.243231015	7.061730988	CORE	39	H	H	0.0000	39
H	5.362474569	4.720515917	7.163971161	CORE	40	H	H	0.0000	40
H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.195394732	4.714510258	10.944669914	CORE	45	Pd	Pd	0.0000	45
Pd	9.626868159	2.218888979	10.950015796	CORE	46	Pd	Pd	0.0000	46
Pd	6.740361163	7.242515285	10.913905345	CORE	47	Pd	Pd	0.0000	47
Pd	14.010927770	9.751282369	10.929406214	CORE	48	Pd	Pd	0.0000	48
Pd	6.758567040	2.240323425	10.954356354	CORE	49	Pd	Pd	0.0000	49
Pd	15.451051532	7.251727852	10.933473942	CORE	50	Pd	Pd	0.0000	50
Pd	5.301460683	4.717713366	10.919218767	CORE	51	Pd	Pd	0.0000	51
Pd	16.879294800	9.740284746	10.924917820	CORE	52	Pd	Pd	0.0000	52
Pd	13.998852361	4.724583864	10.928697745	CORE	53	Pd	Pd	0.0000	53
Pd	11.096390298	9.760238215	10.920909023	CORE	54	Pd	Pd	0.0000	54
Pd	3.852145843	2.221120411	10.924425695	CORE	55	Pd	Pd	0.0000	55
Pd	12.533854720	7.233987540	10.920288460	CORE	56	Pd	Pd	0.0000	56
Pd	12.545419406	2.200753203	10.907106169	CORE	57	Pd	Pd	0.0000	57
Pd	8.184417113	9.753820450	10.911929973	CORE	58	Pd	Pd	0.0000	58
Pd	11.087994406	4.737895174	10.924168442	CORE	59	Pd	Pd	0.0000	59
Pd	9.642673977	7.242058792	10.918081219	CORE	60	Pd	Pd	0.0000	60
Pd	5.277066099	3.048043793	13.185590773	CORE	61	Pd	Pd	0.0000	61
Pd	9.656088484	0.529966428	13.192899869	CORE	62	Pd	Pd	0.0000	62
Pd	5.296461951	8.075972438	13.198503405	CORE	63	Pd	Pd	0.0000	63
Pd	8.194433319	3.049263957	13.541291516	CORE	64	Pd	Pd	0.0000	64
Pd	6.738784213	5.580243569	13.201813286	CORE	65	Pd	Pd	0.0000	65
Pd	6.733407318	0.529463319	13.196407735	CORE	66	Pd	Pd	0.0000	66
Pd	3.842219706	5.562684115	13.211506629	CORE	67	Pd	Pd	0.0000	67
Pd	13.991199296	8.070537318	13.220030457	CORE	68	Pd	Pd	0.0000	68
Pd	2.392984545	3.044958593	13.208664905	CORE	69	Pd	Pd	0.0000	69
Pd	9.647034206	5.587969809	13.184075757	CORE	70	Pd	Pd	0.0000	70
Pd	3.833575228	0.537705375	13.205587634	CORE	71	Pd	Pd	0.0000	71
Pd	0.946700348	0.531343813	13.207869549	CORE	72	Pd	Pd	0.0000	72
Pd	11.114650750	3.041742957	13.194331101	CORE	73	Pd	Pd	0.0000	73
Pd	8.192402777	8.080939643	13.208167009	CORE	74	Pd	Pd	0.0000	74

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Pd      12.545564338    5.562260515    13.219277596 CORE   75 Pd Pd    0.0000    75
Pd      11.089686326    8.077584623    13.212851118 CORE   76 Pd Pd    0.0000    76
H        2.628345740    3.196799660     9.872460835 CORE   77 H  H     0.0000    77
H        4.082295976    0.687383918     9.874749019 CORE   78 H  H     0.0000    78
H        7.024954390    0.728109716     9.930283649 CORE   79 H  H     0.0000    79
H        4.124127079    5.721264956     9.904106749 CORE   80 H  H     0.0000    80
H        6.992706088    5.674779555     9.854934958 CORE   81 H  H     0.0000    81
H        8.388890623    3.185117400     9.890134832 CORE   82 H  H     0.0000    82
H        0.669156389    0.437221245     9.725836825 CORE   83 H  H     0.0000    83
H       14.276030597    8.222805134     9.846157716 CORE   84 H  H     0.0000    84
H       11.104056767    3.054653342    10.108096372 CORE   85 H  H     0.0000    85
H        8.167997178    8.111462271    10.009235640 CORE   86 H  H     0.0000    86
H       11.081026389    7.908592419     9.868869781 CORE   87 H  H     0.0000    87
H       12.389120120    5.632237853     9.820049006 CORE   88 H  H     0.0000    88
H        5.280800367    1.367382517    13.875440489 CORE   89 H  H     0.0000    89
H        8.196272032    1.258425026    13.906926268 CORE   90 H  H     0.0000    90
H        5.280068157    6.409002640    13.900880632 CORE   91 H  H     0.0000    91
H        2.385955051    1.373319688    13.905991024 CORE   92 H  H     0.0000    92
H       15.447465175    8.904770195    13.895887634 CORE   93 H  H     0.0000    93
H       13.994538956    6.392997375    13.907252696 CORE   94 H  H     0.0000    94
H       12.537641335    8.907501724    13.902592759 CORE   95 H  H     0.0000    95
H        8.193399555    6.416232968    13.892068252 CORE   96 H  H     0.0000    96
H       12.554658217    3.884645682    13.904699051 CORE   97 H  H     0.0000    97
H        9.638620862    8.917253889    13.904076430 CORE   98 H  H     0.0000    98
H       11.108051514    1.373986826    13.891881494 CORE   99 H  H     0.0000    99
H        6.748056368    8.905660671    13.903382120 CORE  100 H  H     0.0000   100
H       11.106462838    6.409979206    13.899913801 CORE  101 H  H     0.0000   101
H        3.833177255    3.892935253    13.896705712 CORE  102 H  H     0.0000   102
H        9.747059424    3.950374063    13.855345847 CORE  103 H  H     0.0000   103
H        6.644641998    3.946568146    13.889569341 CORE  104 H  H     0.0000   104
C        8.299801490    3.128898493    15.671823974 CORE  105 C  C     0.0000   105
C        7.123250535    2.517782580    16.380840703 CORE  106 C  C     0.0000   106
H        8.407047208    4.204823971    15.848006647 CORE  107 H  H     0.0000   107
H        7.000129567    1.449261071    16.162615108 CORE  108 H  H     0.0000   108
H        7.301086400    2.614358113    17.470176392 CORE  109 H  H     0.0000   109
H        9.245943536    2.610029241    15.861333674 CORE  110 H  H     0.0000   110
H        6.178073047    3.029312218    16.157929068 CORE  111 H  H     0.0000   111
end
end
```

TS from ethyl to ethane on Pd_4H_3(111). The energy from VASP is -498.305229 eV.

```
PBC    11.60000000    11.60000000    20.00000000    90.00000000    90.00000000    60.00000000
Pd      6.747338531    0.544541613    6.403267290 CORE    1 Pd Pd    0.0000    1
Pd      3.845151399    5.571142423    6.403290684 CORE    2 Pd Pd    0.0000    2
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Pd	5.298982544	3.059410650	6.403296328	CORE	3	Pd	Pd	0.0000	3
Pd	9.648025542	0.547773874	6.403201805	CORE	4	Pd	Pd	0.0000	4
Pd	5.298282266	8.081617720	6.403218683	CORE	5	Pd	Pd	0.0000	5
Pd	8.196069754	3.060087698	6.403506017	CORE	6	Pd	Pd	0.0000	6
Pd	6.748041394	5.568042339	6.403528135	CORE	7	Pd	Pd	0.0000	7
Pd	2.396203981	3.056086329	6.403974639	CORE	8	Pd	Pd	0.0000	8
Pd	3.844692371	0.547193572	6.403980644	CORE	9	Pd	Pd	0.0000	9
Pd	13.995599937	8.080432901	6.403915026	CORE	10	Pd	Pd	0.0000	10
Pd	11.097339485	3.057320193	6.404178400	CORE	11	Pd	Pd	0.0000	11
Pd	8.196252877	8.082018112	6.404201419	CORE	12	Pd	Pd	0.0000	12
Pd	12.547118135	5.570172821	6.404809441	CORE	13	Pd	Pd	0.0000	13
Pd	11.097374320	8.081197886	6.404806864	CORE	14	Pd	Pd	0.0000	14
Pd	0.947647213	0.547191260	6.404240481	CORE	15	Pd	Pd	0.0000	15
Pd	9.647863113	5.570318755	6.404626518	CORE	16	Pd	Pd	0.0000	16
Pd	5.296345229	1.383774072	8.598645002	CORE	17	Pd	Pd	0.0000	17
Pd	3.846430041	3.895121361	8.598650689	CORE	18	Pd	Pd	0.0000	18
Pd	15.446747886	8.918407968	8.598673994	CORE	19	Pd	Pd	0.0000	19
Pd	8.196524484	1.383846907	8.598440679	CORE	20	Pd	Pd	0.0000	20
Pd	5.296487130	6.406750055	8.598478119	CORE	21	Pd	Pd	0.0000	21
Pd	6.746726050	3.895397354	8.597899801	CORE	22	Pd	Pd	0.0000	22
Pd	12.546601356	8.918351911	8.598885115	CORE	23	Pd	Pd	0.0000	23
Pd	13.996646681	6.406823241	8.598891508	CORE	24	Pd	Pd	0.0000	24
Pd	9.646822887	3.895276415	8.599334404	CORE	25	Pd	Pd	0.0000	25
Pd	11.096261310	1.383436470	8.598996838	CORE	26	Pd	Pd	0.0000	26
Pd	8.196560479	6.407055489	8.599357814	CORE	27	Pd	Pd	0.0000	27
Pd	6.745960494	8.918219637	8.599027684	CORE	28	Pd	Pd	0.0000	28
Pd	2.396365455	1.383718188	8.599138079	CORE	29	Pd	Pd	0.0000	29
Pd	12.546369931	3.894993974	8.599714782	CORE	30	Pd	Pd	0.0000	30
Pd	9.646092187	8.918242765	8.599728379	CORE	31	Pd	Pd	0.0000	31
Pd	11.096426310	6.406760277	8.599885411	CORE	32	Pd	Pd	0.0000	32
H	13.966125551	4.748953754	7.090172091	CORE	33	H	H	0.0000	33
H	11.095843995	9.720660436	7.090205342	CORE	34	H	H	0.0000	34
H	3.762469203	2.172306700	7.151879904	CORE	35	H	H	0.0000	35
H	11.088054196	4.720768041	7.106096184	CORE	36	H	H	0.0000	36
H	9.632236062	7.242354712	7.106403093	CORE	37	H	H	0.0000	37
H	9.656494872	2.239241128	7.061700226	CORE	38	H	H	0.0000	38
H	6.767328375	7.243231015	7.061730988	CORE	39	H	H	0.0000	39
H	5.362474569	4.720515917	7.163971161	CORE	40	H	H	0.0000	40
H	6.769252512	2.283876307	7.163619640	CORE	41	H	H	0.0000	41
H	13.968851986	9.732357995	7.138363957	CORE	42	H	H	0.0000	42
H	15.412790580	7.231225571	7.138471255	CORE	43	H	H	0.0000	43
H	16.946132197	9.783930798	7.152525864	CORE	44	H	H	0.0000	44
Pd	8.184045048	4.715469170	10.922169227	CORE	45	Pd	Pd	0.0000	45
Pd	9.629483909	2.224033065	10.937027614	CORE	46	Pd	Pd	0.0000	46

Pd	6.742651349	7.244547801	10.917829914 CORE	47 Pd Pd	0.0000	47	
Pd	13.993496582	9.753242002	10.925484911 CORE	48 Pd Pd	0.0000	48	
Pd	6.758793810	2.228455187	10.972350866 CORE	49 Pd Pd	0.0000	49	
Pd	15.444766072	7.244743765	10.933723805 CORE	50 Pd Pd	0.0000	50	
Pd	5.286313918	4.725861238	10.917712038 CORE	51 Pd Pd	0.0000	51	
Pd	16.873230355	9.737795921	10.932718691 CORE	52 Pd Pd	0.0000	52	
Pd	14.000841317	4.716520811	10.937448425 CORE	53 Pd Pd	0.0000	53	
Pd	11.085966154	9.766389394	10.925918250 CORE	54 Pd Pd	0.0000	54	
Pd	3.835507798	2.214433471	10.923883490 CORE	55 Pd Pd	0.0000	55	
Pd	12.515942850	7.225612689	10.934540445 CORE	56 Pd Pd	0.0000	56	
Pd	12.524778960	2.213168752	10.926933986 CORE	57 Pd Pd	0.0000	57	
Pd	8.179432297	9.743410507	10.922636953 CORE	58 Pd Pd	0.0000	58	
Pd	11.074077259	4.722711055	10.939433129 CORE	59 Pd Pd	0.0000	59	
Pd	9.635494847	7.233996421	10.941252990 CORE	60 Pd Pd	0.0000	60	
Pd	5.236615919	3.040330390	13.195084079 CORE	61 Pd Pd	0.0000	61	
Pd	9.634249313	0.519669141	13.193452159 CORE	62 Pd Pd	0.0000	62	
Pd	5.277226306	8.069360251	13.219133517 CORE	63 Pd Pd	0.0000	63	
Pd	8.186890225	3.046046400	13.439061949 CORE	64 Pd Pd	0.0000	64	
Pd	6.716602635	5.579016317	13.198871578 CORE	65 Pd Pd	0.0000	65	
Pd	6.709304791	0.508363563	13.219309081 CORE	66 Pd Pd	0.0000	66	
Pd	3.820455675	5.559465238	13.239970077 CORE	67 Pd Pd	0.0000	67	
Pd	13.971961696	8.060982979	13.231362194 CORE	68 Pd Pd	0.0000	68	
Pd	2.361761033	3.042202625	13.245309084 CORE	69 Pd Pd	0.0000	69	
Pd	9.623020109	5.551071682	13.213840510 CORE	70 Pd Pd	0.0000	70	
Pd	3.818729908	0.530702631	13.234092455 CORE	71 Pd Pd	0.0000	71	
Pd	0.929792451	0.528966743	13.226974934 CORE	72 Pd Pd	0.0000	72	
Pd	11.071620513	3.047971242	13.225354664 CORE	73 Pd Pd	0.0000	73	
Pd	8.176496809	8.077269259	13.234931099 CORE	74 Pd Pd	0.0000	74	
Pd	12.520800109	5.549751893	13.241870400 CORE	75 Pd Pd	0.0000	75	
Pd	11.066828053	8.059153928	13.250397018 CORE	76 Pd Pd	0.0000	76	
H	2.407406427	3.059286991	9.923830141 CORE	77 H H	0.0000	77	
H	3.848713171	0.598149181	9.905203442 CORE	78 H H	0.0000	78	
H	6.797704451	0.611251446	9.926958138 CORE	79 H H	0.0000	79	
H	3.880855623	5.569532246	9.948278515 CORE	80 H H	0.0000	80	
H	6.787798969	5.572174044	9.863314931 CORE	81 H H	0.0000	81	
H	8.203905093	3.072552499	9.923883838 CORE	82 H H	0.0000	82	
H	0.668719330	0.405760688	9.722242160 CORE	83 H H	0.0000	83	
H	14.260185551	8.219251519	9.837794609 CORE	84 H H	0.0000	84	
H	11.029068497	3.054273487	9.925610837 CORE	85 H H	0.0000	85	
H	8.185374709	7.982170787	9.917401421 CORE	86 H H	0.0000	86	
H	11.062400784	7.950275334	9.885981008 CORE	87 H H	0.0000	87	
H	12.310850371	5.650178326	9.817470058 CORE	88 H H	0.0000	88	
H	5.270042775	1.365215211	13.918714776 CORE	89 H H	0.0000	89	
H	8.169292296	1.249910895	13.904841406 CORE	90 H H	0.0000	90	

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H          5.267868235    6.399285526   13.932792142 CORE   91 H    H      0.0000    91
H          2.368778045    1.365967594   13.944756429 CORE   92 H    H      0.0000    92
H         15.422023290    8.897770212   13.921531940 CORE   93 H    H      0.0000    93
H         13.970403571    6.391262048   13.940651288 CORE   94 H    H      0.0000    94
H         12.520907916    8.888802978   13.942484021 CORE   95 H    H      0.0000    95
H          8.180372962    6.407611935   13.904793485 CORE   96 H    H      0.0000    96
H         12.500309297    3.866097434   13.946887214 CORE   97 H    H      0.0000    97
H          9.620774090    8.912355816   13.952669566 CORE   98 H    H      0.0000    98
H         11.090939550    1.382240317   13.899513920 CORE   99 H    H      0.0000    99
H          6.732874333    8.906325661   13.931998983 CORE  100 H    H      0.0000   100
H         11.064259199    6.375592996   13.938447527 CORE  101 H    H      0.0000   101
H          3.802986886    3.887292382   13.938624046 CORE  102 H    H      0.0000   102
H          9.374133151    3.892734048   14.295932435 CORE  103 H    H      0.0000   103
H          6.622737222    3.931365207   13.846420379 CORE  104 H    H      0.0000   104
C          8.757593170    3.371730676   15.673279387 CORE  105 C    C      0.0000   105
C          7.468568141    2.905577551   16.328599626 CORE  106 C    C      0.0000   106
H          9.008138471    4.391657200   15.988215835 CORE  107 H    H      0.0000   107
H          7.198216894    1.876186397   16.062696653 CORE  108 H    H      0.0000   108
H          7.635661964    2.937898161   17.422513953 CORE  109 H    H      0.0000   109
H          9.602660857    2.707554448   15.876196046 CORE  110 H    H      0.0000   110
H          6.613998262    3.555140141   16.109139889 CORE  111 H    H      0.0000   111
end
end
```

Initial Pd(100). The energy from VASP is -372.550587 eV.

```
PBC    11.15000000    11.15000000    20.00000000    90.00000000    90.00000000    90.00000000
Pd        10.597740511    5.052097766    6.971435851 CORE    1 Pd Pd    0.0000     1
Pd         5.016640882   10.622407807    6.972012903 CORE    2 Pd Pd    0.0000     2
Pd         2.230223226    5.049854980    6.970471652 CORE    3 Pd Pd    0.0000     3
Pd         7.800416967   10.624591683    6.969912369 CORE    4 Pd Pd    0.0000     4
Pd         5.016274142    2.253949823    6.972670109 CORE    5 Pd Pd    0.0000     5
Pd         2.229944252    2.256956188    6.972582338 CORE    6 Pd Pd    0.0000     6
Pd         2.228413734   10.624718305    6.970006299 CORE    7 Pd Pd    0.0000     7
Pd        10.597206020    2.263659019    6.970036445 CORE    8 Pd Pd    0.0000     8
Pd         7.801704797    7.837842446    6.970623655 CORE    9 Pd Pd    0.0000     9
Pd         2.230101993    7.831322293    6.970481309 CORE   10 Pd Pd    0.0000    10
Pd        10.597535023    7.837059081    6.971582148 CORE   11 Pd Pd    0.0000    11
Pd        10.596798114   10.627094906    6.970621961 CORE   12 Pd Pd    0.0000    12
Pd         7.803055937    5.045716439    6.970928879 CORE   13 Pd Pd    0.0000    13
Pd         5.020239126    5.047289691    6.971467557 CORE   14 Pd Pd    0.0000    14
Pd         7.800761438    2.262637522    6.970691684 CORE   15 Pd Pd    0.0000    15
Pd         5.020279192    7.830435235    6.972662179 CORE   16 Pd Pd    0.0000    16
Pd         0.838578788    6.443772149    8.914560183 CORE   17 Pd Pd    0.0000    17
Pd         6.411284480    0.864013686    8.916862625 CORE   18 Pd Pd    0.0000    18
```

Pd	0.833839460	3.655784084	8.918734532 CORE	19 Pd Pd	0.0000	19
Pd	6.415512658	9.227179303	8.918643034 CORE	20 Pd Pd	0.0000	20
Pd	3.622943088	0.864417525	8.916836450 CORE	21 Pd Pd	0.0000	21
Pd	0.833799274	9.231256748	8.920264273 CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540 CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432 CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921 CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165 CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244 CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202 CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905 CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344 CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620 CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449 CORE	32 Pd Pd	0.0000	32
Pd	2.228572351	10.623545165	10.893082603 CORE	33 Pd Pd	0.0000	33
Pd	2.229345590	7.834238822	10.893330686 CORE	34 Pd Pd	0.0000	34
Pd	2.228484766	2.259026087	10.891637898 CORE	35 Pd Pd	0.0000	35
Pd	10.594493994	7.836949961	10.895397497 CORE	36 Pd Pd	0.0000	36
Pd	5.018820700	7.832911058	10.893024349 CORE	37 Pd Pd	0.0000	37
Pd	7.804786242	5.049309701	10.895354300 CORE	38 Pd Pd	0.0000	38
Pd	5.018777857	2.257975997	10.891213062 CORE	39 Pd Pd	0.0000	39
Pd	7.803737577	2.261054263	10.894878280 CORE	40 Pd Pd	0.0000	40
Pd	7.804483537	7.835622021	10.896092856 CORE	41 Pd Pd	0.0000	41
Pd	10.592882136	2.262468362	10.893591067 CORE	42 Pd Pd	0.0000	42
Pd	5.019266836	5.046463569	10.891957196 CORE	43 Pd Pd	0.0000	43
Pd	10.593184140	10.625883673	10.895673422 CORE	44 Pd Pd	0.0000	44
Pd	7.803254956	10.624087768	10.896239181 CORE	45 Pd Pd	0.0000	45
Pd	5.018132383	10.621718666	10.892444357 CORE	46 Pd Pd	0.0000	46
Pd	10.594393144	5.050514639	10.893961403 CORE	47 Pd Pd	0.0000	47
Pd	2.229415298	5.047976459	10.892268531 CORE	48 Pd Pd	0.0000	48
Pd	3.623639470	9.227305476	12.960402948 CORE	49 Pd Pd	0.0000	49
Pd	0.836797950	9.230554617	12.962596031 CORE	50 Pd Pd	0.0000	50
Pd	9.198686018	9.231381060	12.963158635 CORE	51 Pd Pd	0.0000	51
Pd	6.411170319	3.653232617	12.961799081 CORE	52 Pd Pd	0.0000	52
Pd	3.624777877	6.439699567	12.960746507 CORE	53 Pd Pd	0.0000	53
Pd	3.623765130	3.652021836	12.959201562 CORE	54 Pd Pd	0.0000	54
Pd	9.198881811	3.656403708	12.962330513 CORE	55 Pd Pd	0.0000	55
Pd	0.837486441	6.442859886	12.962733675 CORE	56 Pd Pd	0.0000	56
Pd	0.837079238	3.655354784	12.961256248 CORE	57 Pd Pd	0.0000	57
Pd	6.409980027	0.866197963	12.962455935 CORE	58 Pd Pd	0.0000	58
Pd	9.199939466	6.443979730	12.962998392 CORE	59 Pd Pd	0.0000	59
Pd	6.410633044	9.228264896	12.962790947 CORE	60 Pd Pd	0.0000	60
Pd	0.835995036	0.868524359	12.962310950 CORE	61 Pd Pd	0.0000	61
Pd	9.198218787	0.869542270	12.962799607 CORE	62 Pd Pd	0.0000	62

Pd 6.411461431 6.440729584 12.962705543 CORE 63 Pd Pd 0.0000 63
Pd 3.623262226 0.865223751 12.960342894 CORE 64 Pd Pd 0.0000 64
H 2.230572982 5.048251989 13.164358695 CORE 65 H H 0.0000 65
H 10.592619144 5.048889189 13.165582108 CORE 66 H H 0.0000 66
H 10.592779420 7.836943519 13.165757173 CORE 67 H H 0.0000 67
H 7.805005704 10.623174000 13.164348502 CORE 68 H H 0.0000 68
H 10.592168285 10.624204518 13.165160590 CORE 69 H H 0.0000 69
H 2.230184710 7.835424767 13.164882378 CORE 70 H H 0.0000 70
H 5.017210093 10.622447137 13.165455208 CORE 71 H H 0.0000 71
H 7.805110550 2.261552139 13.164854187 CORE 72 H H 0.0000 72
H 5.017600378 7.835074437 13.165598990 CORE 73 H H 0.0000 73
H 7.805530994 5.048486093 13.164547104 CORE 74 H H 0.0000 74
H 5.017674135 5.047665352 13.165264756 CORE 75 H H 0.0000 75
H 5.017332822 2.259978916 13.165671343 CORE 76 H H 0.0000 76
H 2.230000932 10.623456222 13.164393292 CORE 77 H H 0.0000 77
H 10.592026365 2.262096105 13.165894030 CORE 78 H H 0.0000 78
H 7.805552332 7.836567660 13.164773255 CORE 79 H H 0.0000 79
H 2.230251824 2.260390464 13.164658618 CORE 80 H H 0.0000 80
end
end

Acetylene adsorbed on Pd(100). The energy from VASP is -393.594171 eV.

PBC 11.15000000 11.15000000 20.00000000 90.00000000 90.00000000 90.00000000
Pd 10.597740511 5.052097766 6.971435851 CORE 1 Pd Pd 0.0000 1
Pd 5.016640882 10.622407807 6.972012903 CORE 2 Pd Pd 0.0000 2
Pd 2.230223226 5.049854980 6.970471652 CORE 3 Pd Pd 0.0000 3
Pd 7.800416967 10.624591683 6.969912369 CORE 4 Pd Pd 0.0000 4
Pd 5.016274142 2.253949823 6.972670109 CORE 5 Pd Pd 0.0000 5
Pd 2.229944252 2.256956188 6.972582338 CORE 6 Pd Pd 0.0000 6
Pd 2.228413734 10.624718305 6.970006299 CORE 7 Pd Pd 0.0000 7
Pd 10.597206020 2.263659019 6.970036445 CORE 8 Pd Pd 0.0000 8
Pd 7.801704797 7.837842446 6.970623655 CORE 9 Pd Pd 0.0000 9
Pd 2.230101993 7.831322293 6.970481309 CORE 10 Pd Pd 0.0000 10
Pd 10.597535023 7.837059081 6.971582148 CORE 11 Pd Pd 0.0000 11
Pd 10.596798114 10.627094906 6.970621961 CORE 12 Pd Pd 0.0000 12
Pd 7.803055937 5.045716439 6.970928879 CORE 13 Pd Pd 0.0000 13
Pd 5.020239126 5.047289691 6.971467557 CORE 14 Pd Pd 0.0000 14
Pd 7.800761438 2.262637522 6.970691684 CORE 15 Pd Pd 0.0000 15
Pd 5.020279192 7.830435235 6.972662179 CORE 16 Pd Pd 0.0000 16
Pd 0.838578788 6.443772149 8.914560183 CORE 17 Pd Pd 0.0000 17
Pd 6.411284480 0.864013686 8.916862625 CORE 18 Pd Pd 0.0000 18
Pd 0.833839460 3.655784084 8.918734532 CORE 19 Pd Pd 0.0000 19
Pd 6.415512658 9.227179303 8.918643034 CORE 20 Pd Pd 0.0000 20
Pd 3.622943088 0.864417525 8.916836450 CORE 21 Pd Pd 0.0000 21

Pd	0.833799274	9.231256748	8.920264273	CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540	CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432	CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921	CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165	CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244	CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202	CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905	CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344	CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620	CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449	CORE	32 Pd Pd	0.0000	32
Pd	2.229911412	10.623760941	10.888719035	CORE	33 Pd Pd	0.0000	33
Pd	2.245533813	7.820810852	10.910455636	CORE	34 Pd Pd	0.0000	34
Pd	2.244686376	2.272705185	10.909201640	CORE	35 Pd Pd	0.0000	35
Pd	10.594646912	7.844679419	10.879091651	CORE	36 Pd Pd	0.0000	36
Pd	5.018682738	7.832955419	10.884197069	CORE	37 Pd Pd	0.0000	37
Pd	7.793214276	5.049067571	10.906964369	CORE	38 Pd Pd	0.0000	38
Pd	5.018547810	2.258417398	10.882518386	CORE	39 Pd Pd	0.0000	39
Pd	7.788354222	2.274824636	10.912252474	CORE	40 Pd Pd	0.0000	40
Pd	7.788959996	7.821996575	10.913105852	CORE	41 Pd Pd	0.0000	41
Pd	10.592967666	2.254890517	10.877374662	CORE	42 Pd Pd	0.0000	42
Pd	5.019115183	5.046316175	10.892156395	CORE	43 Pd Pd	0.0000	43
Pd	10.593222026	10.625627872	10.892478239	CORE	44 Pd Pd	0.0000	44
Pd	7.802397525	10.624089825	10.891483540	CORE	45 Pd Pd	0.0000	45
Pd	5.017814534	10.621773301	10.893352404	CORE	46 Pd Pd	0.0000	46
Pd	10.594533386	5.050170022	10.877285743	CORE	47 Pd Pd	0.0000	47
Pd	2.241873535	5.047891761	10.904389568	CORE	48 Pd Pd	0.0000	48
Pd	3.622482846	9.223468240	12.958919817	CORE	49 Pd Pd	0.0000	49
Pd	0.834536768	9.235305150	12.960732576	CORE	50 Pd Pd	0.0000	50
Pd	9.201487874	9.236159671	12.960735744	CORE	51 Pd Pd	0.0000	51
Pd	6.397524957	3.660455635	13.006593139	CORE	52 Pd Pd	0.0000	52
Pd	3.638471599	6.433094671	13.004917711	CORE	53 Pd Pd	0.0000	53
Pd	3.638809141	3.659769421	13.004321917	CORE	54 Pd Pd	0.0000	54
Pd	9.214911456	3.642842648	12.946708759	CORE	55 Pd Pd	0.0000	55
Pd	0.822863819	6.456221075	12.947459908	CORE	56 Pd Pd	0.0000	56
Pd	0.822565866	3.641524321	12.946118747	CORE	57 Pd Pd	0.0000	57
Pd	6.411095633	0.870603032	12.960902456	CORE	58 Pd Pd	0.0000	58
Pd	9.215014553	6.457225328	12.947347997	CORE	59 Pd Pd	0.0000	59
Pd	6.412172935	9.224000799	12.960993116	CORE	60 Pd Pd	0.0000	60
Pd	0.833246895	0.863159061	12.960817909	CORE	61 Pd Pd	0.0000	61
Pd	9.200736300	0.864280336	12.960686638	CORE	62 Pd Pd	0.0000	62
Pd	6.397863095	6.433673195	13.007044123	CORE	63 Pd Pd	0.0000	63
Pd	3.621716249	0.869946026	12.959006411	CORE	64 Pd Pd	0.0000	64
H	1.977814446	5.049055115	12.979662076	CORE	65 H H	0.0000	65

H	10.592229547	5.048291470	13.180501669	CORE	66 H	H	0.0000	66
H	10.592734765	7.899747816	13.216242176	CORE	67 H	H	0.0000	67
H	7.864231460	10.623461588	13.179350218	CORE	68 H	H	0.0000	68
H	10.592110068	10.624352693	13.179639612	CORE	69 H	H	0.0000	69
H	2.145292765	7.936424054	13.163830009	CORE	70 H	H	0.0000	70
H	5.017320964	10.622869904	13.146246078	CORE	71 H	H	0.0000	71
H	7.888964760	2.162100774	13.161251373	CORE	72 H	H	0.0000	72
H	5.017389638	8.011144008	13.163793600	CORE	73 H	H	0.0000	73
H	8.058979504	5.050103010	12.981637017	CORE	74 H	H	0.0000	74
H	5.016401898	2.083746613	13.164020117	CORE	75 H	H	0.0000	75
H	2.171341708	10.623853576	13.179727793	CORE	76 H	H	0.0000	76
H	10.592055019	2.198874062	13.216969365	CORE	77 H	H	0.0000	77
H	7.890240374	7.937262517	13.161579749	CORE	78 H	H	0.0000	78
H	2.145679757	2.160264675	13.163426652	CORE	79 H	H	0.0000	79
C	5.710171182	5.046871105	14.368735850	CORE	80 C	C	0.0000	80
C	4.323722111	5.046263744	14.367560025	CORE	81 C	C	0.0000	81
H	6.316845028	5.047196395	15.286226552	CORE	82 H	H	0.0000	82
H	3.715583425	5.045827174	15.284398722	CORE	83 H	H	0.0000	83

end

end

TS from acetylene to vinyl on Pd(100). The energy from VASP is -392.737484 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	90.00000000		
Pd	10.597740511	5.052097766	6.971435851	CORE	1 Pd	Pd	0.0000	1
Pd	5.016640882	10.622407807	6.972012903	CORE	2 Pd	Pd	0.0000	2
Pd	2.230223226	5.049854980	6.970471652	CORE	3 Pd	Pd	0.0000	3
Pd	7.800416967	10.624591683	6.969912369	CORE	4 Pd	Pd	0.0000	4
Pd	5.016274142	2.253949823	6.972670109	CORE	5 Pd	Pd	0.0000	5
Pd	2.229944252	2.256956188	6.972582338	CORE	6 Pd	Pd	0.0000	6
Pd	2.228413734	10.624718305	6.970006299	CORE	7 Pd	Pd	0.0000	7
Pd	10.597206020	2.263659019	6.970036445	CORE	8 Pd	Pd	0.0000	8
Pd	7.801704797	7.837842446	6.970623655	CORE	9 Pd	Pd	0.0000	9
Pd	2.230101993	7.831322293	6.970481309	CORE	10 Pd	Pd	0.0000	10
Pd	10.597535023	7.837059081	6.971582148	CORE	11 Pd	Pd	0.0000	11
Pd	10.596798114	10.627094906	6.970621961	CORE	12 Pd	Pd	0.0000	12
Pd	7.803055937	5.045716439	6.970928879	CORE	13 Pd	Pd	0.0000	13
Pd	5.020239126	5.047289691	6.971467557	CORE	14 Pd	Pd	0.0000	14
Pd	7.800761438	2.262637522	6.970691684	CORE	15 Pd	Pd	0.0000	15
Pd	5.020279192	7.830435235	6.972662179	CORE	16 Pd	Pd	0.0000	16
Pd	0.838578788	6.443772149	8.914560183	CORE	17 Pd	Pd	0.0000	17
Pd	6.411284480	0.864013686	8.916862625	CORE	18 Pd	Pd	0.0000	18
Pd	0.833839460	3.655784084	8.918734532	CORE	19 Pd	Pd	0.0000	19
Pd	6.415512658	9.227179303	8.918643034	CORE	20 Pd	Pd	0.0000	20
Pd	3.622943088	0.864417525	8.916836450	CORE	21 Pd	Pd	0.0000	21

Pd	0.833799274	9.231256748	8.920264273	CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540	CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432	CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921	CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165	CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244	CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202	CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905	CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344	CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620	CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449	CORE	32 Pd Pd	0.0000	32
Pd	2.226884390	10.625000571	10.890097257	CORE	33 Pd Pd	0.0000	33
Pd	2.239733784	7.821873925	10.912157330	CORE	34 Pd Pd	0.0000	34
Pd	2.239953561	2.274666435	10.915111054	CORE	35 Pd Pd	0.0000	35
Pd	10.587215616	7.849526428	10.880270003	CORE	36 Pd Pd	0.0000	36
Pd	5.020000752	7.834041293	10.885409613	CORE	37 Pd Pd	0.0000	37
Pd	7.787374663	5.046132035	10.924355364	CORE	38 Pd Pd	0.0000	38
Pd	5.009111828	2.265713350	10.909961549	CORE	39 Pd Pd	0.0000	39
Pd	7.788434184	2.270835421	10.927277952	CORE	40 Pd Pd	0.0000	40
Pd	7.783752916	7.818266507	10.925049237	CORE	41 Pd Pd	0.0000	41
Pd	10.599851468	2.259990269	10.887249303	CORE	42 Pd Pd	0.0000	42
Pd	5.009577605	5.048652362	10.893750777	CORE	43 Pd Pd	0.0000	43
Pd	10.593470605	10.628938803	10.894053287	CORE	44 Pd Pd	0.0000	44
Pd	7.807833971	10.618849738	10.899212313	CORE	45 Pd Pd	0.0000	45
Pd	5.023554996	10.620933314	10.886899650	CORE	46 Pd Pd	0.0000	46
Pd	10.604471434	5.051807937	10.892545929	CORE	47 Pd Pd	0.0000	47
Pd	2.232183325	5.051863850	10.907243078	CORE	48 Pd Pd	0.0000	48
Pd	3.631848006	9.232358922	12.963026071	CORE	49 Pd Pd	0.0000	49
Pd	0.839127730	9.247665441	12.968727373	CORE	50 Pd Pd	0.0000	50
Pd	9.210618378	9.237245304	12.972426696	CORE	51 Pd Pd	0.0000	51
Pd	6.376307609	3.657278115	13.037411113	CORE	52 Pd Pd	0.0000	52
Pd	3.595708188	6.480939155	12.973791382	CORE	53 Pd Pd	0.0000	53
Pd	3.623258726	3.609925791	12.999125138	CORE	54 Pd Pd	0.0000	54
Pd	9.229240271	3.643697966	12.956329488	CORE	55 Pd Pd	0.0000	55
Pd	0.811700412	6.465466981	12.933428985	CORE	56 Pd Pd	0.0000	56
Pd	0.846676848	3.673030185	12.969352099	CORE	57 Pd Pd	0.0000	57
Pd	6.426126962	0.852148624	12.969745623	CORE	58 Pd Pd	0.0000	58
Pd	9.200088301	6.459662499	12.958720219	CORE	59 Pd Pd	0.0000	59
Pd	6.415810992	9.211919743	12.968799952	CORE	60 Pd Pd	0.0000	60
Pd	0.840254480	0.872371608	12.971252532	CORE	61 Pd Pd	0.0000	61
Pd	9.219066056	0.861342573	12.972738202	CORE	62 Pd Pd	0.0000	62
Pd	6.345582397	6.402008080	13.042159863	CORE	63 Pd Pd	0.0000	63
Pd	3.635048615	0.835308616	12.962664508	CORE	64 Pd Pd	0.0000	64
H	2.843096793	4.567627705	14.054360760	CORE	65 H H	0.0000	65

H 10.661813671 5.045011353 13.187918596 CORE 66 H H 0.0000 66
H 10.603892760 7.875026908 13.217147300 CORE 67 H H 0.0000 67
H 7.860548099 10.628054148 13.185418651 CORE 68 H H 0.0000 68
H 10.606407905 10.626184962 13.224194521 CORE 69 H H 0.0000 69
H 2.114204811 7.887626764 13.159144119 CORE 70 H H 0.0000 70
H 5.005338383 10.613150918 13.207631921 CORE 71 H H 0.0000 71
H 7.903567744 2.171035998 13.097202215 CORE 72 H H 0.0000 72
H 5.040376831 7.998757234 13.148159677 CORE 73 H H 0.0000 73
H 8.007189117 5.056587486 12.914011320 CORE 74 H H 0.0000 74
H 5.063151567 2.072585776 13.128774282 CORE 75 H H 0.0000 75
H 2.208215166 10.631630012 13.182771151 CORE 76 H H 0.0000 76
H 10.616454187 2.245949980 13.213921955 CORE 77 H H 0.0000 77
H 7.888460182 7.909720329 13.112937203 CORE 78 H H 0.0000 78
H 2.146094418 2.199795934 13.112062699 CORE 79 H H 0.0000 79
C 5.554860454 4.985590117 14.362499159 CORE 80 C C 0.0000 80
C 4.166544765 5.174835849 14.477358952 CORE 81 C C 0.0000 81
H 6.166255317 4.972812470 15.281637987 CORE 82 H H 0.0000 82
H 3.750607759 5.379117636 15.472782957 CORE 83 H H 0.0000 83
end
end

Vinyl adsorbed on Pd(100). The energy from VASP is -396.958681 eV.

PBC 11.15000000 11.15000000 20.00000000 90.00000000 90.00000000 90.00000000
Pd 10.597740511 5.052097766 6.971435851 CORE 1 Pd Pd 0.0000 1
Pd 5.016640882 10.622407807 6.972012903 CORE 2 Pd Pd 0.0000 2
Pd 2.230223226 5.049854980 6.970471652 CORE 3 Pd Pd 0.0000 3
Pd 7.800416967 10.624591683 6.969912369 CORE 4 Pd Pd 0.0000 4
Pd 5.016274142 2.253949823 6.972670109 CORE 5 Pd Pd 0.0000 5
Pd 2.229944252 2.256956188 6.972582338 CORE 6 Pd Pd 0.0000 6
Pd 2.228413734 10.624718305 6.970006299 CORE 7 Pd Pd 0.0000 7
Pd 10.597206020 2.263659019 6.970036445 CORE 8 Pd Pd 0.0000 8
Pd 7.801704797 7.837842446 6.970623655 CORE 9 Pd Pd 0.0000 9
Pd 2.230101993 7.831322293 6.970481309 CORE 10 Pd Pd 0.0000 10
Pd 10.597535023 7.837059081 6.971582148 CORE 11 Pd Pd 0.0000 11
Pd 10.596798114 10.627094906 6.970621961 CORE 12 Pd Pd 0.0000 12
Pd 7.803055937 5.045716439 6.970928879 CORE 13 Pd Pd 0.0000 13
Pd 5.020239126 5.047289691 6.971467557 CORE 14 Pd Pd 0.0000 14
Pd 7.800761438 2.262637522 6.970691684 CORE 15 Pd Pd 0.0000 15
Pd 5.020279192 7.830435235 6.972662179 CORE 16 Pd Pd 0.0000 16
Pd 0.838578788 6.443772149 8.914560183 CORE 17 Pd Pd 0.0000 17
Pd 6.411284480 0.864013686 8.916862625 CORE 18 Pd Pd 0.0000 18
Pd 0.833839460 3.655784084 8.918734532 CORE 19 Pd Pd 0.0000 19
Pd 6.415512658 9.227179303 8.918643034 CORE 20 Pd Pd 0.0000 20
Pd 3.622943088 0.864417525 8.916836450 CORE 21 Pd Pd 0.0000 21

Pd	0.833799274	9.231256748	8.920264273	CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540	CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432	CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921	CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165	CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244	CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202	CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905	CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344	CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620	CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449	CORE	32 Pd Pd	0.0000	32
Pd	2.233030604	10.609861492	10.889728583	CORE	33 Pd Pd	0.0000	33
Pd	2.259616581	7.810000312	10.917156630	CORE	34 Pd Pd	0.0000	34
Pd	2.221782945	2.244467589	10.872563348	CORE	35 Pd Pd	0.0000	35
Pd	10.608302627	7.849431310	10.878278268	CORE	36 Pd Pd	0.0000	36
Pd	5.017896087	7.825763837	10.888890959	CORE	37 Pd Pd	0.0000	37
Pd	7.784838687	5.050665925	10.914453905	CORE	38 Pd Pd	0.0000	38
Pd	5.023756414	2.260543463	10.890351783	CORE	39 Pd Pd	0.0000	39
Pd	7.783807193	2.283045879	10.913013810	CORE	40 Pd Pd	0.0000	40
Pd	7.795448319	7.833544034	10.905318473	CORE	41 Pd Pd	0.0000	41
Pd	10.583623132	2.258406118	10.881162258	CORE	42 Pd Pd	0.0000	42
Pd	5.009287108	5.044548871	10.904430421	CORE	43 Pd Pd	0.0000	43
Pd	10.595946416	10.630797415	10.899839519	CORE	44 Pd Pd	0.0000	44
Pd	7.806701765	10.637448234	10.902302036	CORE	45 Pd Pd	0.0000	45
Pd	5.026740011	10.621009145	10.895938918	CORE	46 Pd Pd	0.0000	46
Pd	10.591936711	5.051061344	10.885138173	CORE	47 Pd Pd	0.0000	47
Pd	2.238339782	5.046582790	10.904510992	CORE	48 Pd Pd	0.0000	48
Pd	3.623398206	9.181414584	12.963551042	CORE	49 Pd Pd	0.0000	49
Pd	0.837997869	9.254952271	12.966638792	CORE	50 Pd Pd	0.0000	50
Pd	9.203431030	9.225382922	12.959538523	CORE	51 Pd Pd	0.0000	51
Pd	6.327607608	3.721243945	13.063588449	CORE	52 Pd Pd	0.0000	52
Pd	3.671099274	6.374624737	13.053012581	CORE	53 Pd Pd	0.0000	53
Pd	3.580828298	3.559711634	12.911273682	CORE	54 Pd Pd	0.0000	54
Pd	9.172989570	3.626658486	12.957084400	CORE	55 Pd Pd	0.0000	55
Pd	0.862236442	6.474488477	12.955198789	CORE	56 Pd Pd	0.0000	56
Pd	0.794488944	3.669531218	12.948873198	CORE	57 Pd Pd	0.0000	57
Pd	6.429020264	0.932656832	12.975988554	CORE	58 Pd Pd	0.0000	58
Pd	9.243497917	6.456416187	12.942116333	CORE	59 Pd Pd	0.0000	59
Pd	6.415072736	9.257028689	12.961070194	CORE	60 Pd Pd	0.0000	60
Pd	0.858524602	0.895174153	12.961016624	CORE	61 Pd Pd	0.0000	61
Pd	9.221339639	0.857545433	12.969771033	CORE	62 Pd Pd	0.0000	62
Pd	6.403163968	6.466440173	12.992892939	CORE	63 Pd Pd	0.0000	63
Pd	3.641330738	0.804451064	12.960879973	CORE	64 Pd Pd	0.0000	64
H	10.588234804	5.041204987	13.162806099	CORE	65 H H	0.0000	65

H	10.613374969	7.905414742	13.219035646	CORE	66	H	0.0000	66
H	7.856889067	10.648777041	13.153858268	CORE	67	H	0.0000	67
H	10.624360895	10.638175078	13.164015686	CORE	68	H	0.0000	68
H	2.128667254	7.920272974	13.197203740	CORE	69	H	0.0000	69
H	4.980975751	10.589811365	13.154661575	CORE	70	H	0.0000	70
H	7.911381872	2.122578503	13.246738269	CORE	71	H	0.0000	71
H	5.046825017	8.007036659	13.172157277	CORE	72	H	0.0000	72
H	8.064799026	5.070800917	12.886687105	CORE	73	H	0.0000	73
H	4.943263928	2.138907656	13.208986619	CORE	74	H	0.0000	74
H	2.201787649	10.626061244	13.183182864	CORE	75	H	0.0000	75
H	10.605868585	2.216608040	13.219541593	CORE	76	H	0.0000	76
H	7.889268639	7.956858275	13.188058666	CORE	77	H	0.0000	77
H	2.202519473	2.237594314	13.202857586	CORE	78	H	0.0000	78
H	2.076973306	5.048040190	12.983840087	CORE	79	H	0.0000	79
C	5.837116361	5.123476480	14.430840654	CORE	80	C	0.0000	80
C	4.460403548	5.365857067	14.766085148	CORE	81	C	0.0000	81
H	6.619140404	5.223326697	15.203500107	CORE	82	H	0.0000	82
H	4.284868582	6.108519933	15.561765138	CORE	83	H	0.0000	83
H	3.809749658	4.476044334	14.921531926	CORE	84	H	0.0000	84

end

end

TS from vinyl to ethene on Pd(100). The energy from VASP is -396.313335 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	90.00000000		
Pd	10.597740511	5.052097766	6.971435851	CORE	1	Pd	0.0000	1
Pd	5.016640882	10.622407807	6.972012903	CORE	2	Pd	0.0000	2
Pd	2.230223226	5.049854980	6.970471652	CORE	3	Pd	0.0000	3
Pd	7.800416967	10.624591683	6.969912369	CORE	4	Pd	0.0000	4
Pd	5.016274142	2.253949823	6.972670109	CORE	5	Pd	0.0000	5
Pd	2.229944252	2.256956188	6.972582338	CORE	6	Pd	0.0000	6
Pd	2.228413734	10.624718305	6.970006299	CORE	7	Pd	0.0000	7
Pd	10.597206020	2.263659019	6.970036445	CORE	8	Pd	0.0000	8
Pd	7.801704797	7.837842446	6.970623655	CORE	9	Pd	0.0000	9
Pd	2.230101993	7.831322293	6.970481309	CORE	10	Pd	0.0000	10
Pd	10.597535023	7.837059081	6.971582148	CORE	11	Pd	0.0000	11
Pd	10.596798114	10.627094906	6.970621961	CORE	12	Pd	0.0000	12
Pd	7.803055937	5.045716439	6.970928879	CORE	13	Pd	0.0000	13
Pd	5.020239126	5.047289691	6.971467557	CORE	14	Pd	0.0000	14
Pd	7.800761438	2.262637522	6.970691684	CORE	15	Pd	0.0000	15
Pd	5.020279192	7.830435235	6.972662179	CORE	16	Pd	0.0000	16
Pd	0.838578788	6.443772149	8.914560183	CORE	17	Pd	0.0000	17
Pd	6.411284480	0.864013686	8.916862625	CORE	18	Pd	0.0000	18
Pd	0.833839460	3.655784084	8.918734532	CORE	19	Pd	0.0000	19
Pd	6.415512658	9.227179303	8.918643034	CORE	20	Pd	0.0000	20

Pd	3.622943088	0.864417525	8.916836450 CORE	21 Pd Pd	0.0000	21
Pd	0.833799274	9.231256748	8.920264273 CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540 CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432 CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921 CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165 CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244 CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202 CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905 CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344 CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620 CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449 CORE	32 Pd Pd	0.0000	32
Pd	2.225201915	10.601859369	10.887641118 CORE	33 Pd Pd	0.0000	33
Pd	2.264224017	7.807514859	10.929415176 CORE	34 Pd Pd	0.0000	34
Pd	2.219773132	2.237440960	10.868078201 CORE	35 Pd Pd	0.0000	35
Pd	10.620779474	7.847698492	10.876789089 CORE	36 Pd Pd	0.0000	36
Pd	5.008736811	7.820141977	10.886861913 CORE	37 Pd Pd	0.0000	37
Pd	7.800656848	5.044979537	10.919773435 CORE	38 Pd Pd	0.0000	38
Pd	5.037175001	2.268643126	10.906618737 CORE	39 Pd Pd	0.0000	39
Pd	7.784102081	2.302907740	10.947482526 CORE	40 Pd Pd	0.0000	40
Pd	7.807020203	7.825818388	10.904841921 CORE	41 Pd Pd	0.0000	41
Pd	10.586061134	2.255394281	10.878068828 CORE	42 Pd Pd	0.0000	42
Pd	5.046819754	5.032218820	10.930320418 CORE	43 Pd Pd	0.0000	43
Pd	10.596682191	10.625660045	10.884386637 CORE	44 Pd Pd	0.0000	44
Pd	7.804083935	10.638322924	10.889972140 CORE	45 Pd Pd	0.0000	45
Pd	5.012980508	10.620234658	10.879852452 CORE	46 Pd Pd	0.0000	46
Pd	10.598288452	5.050955427	10.877262772 CORE	47 Pd Pd	0.0000	47
Pd	2.258517234	5.055602904	10.903255313 CORE	48 Pd Pd	0.0000	48
Pd	3.616661894	9.183355320	12.963942819 CORE	49 Pd Pd	0.0000	49
Pd	0.822179422	9.247701493	12.971619832 CORE	50 Pd Pd	0.0000	50
Pd	9.197282757	9.230621902	12.953019527 CORE	51 Pd Pd	0.0000	51
Pd	6.419262711	3.717981848	13.181670066 CORE	52 Pd Pd	0.0000	52
Pd	3.725359444	6.349513651	13.124703054 CORE	53 Pd Pd	0.0000	53
Pd	3.590404096	3.574526745	12.884751338 CORE	54 Pd Pd	0.0000	54
Pd	9.222077304	3.658868227	12.940635712 CORE	55 Pd Pd	0.0000	55
Pd	0.888151627	6.453037243	12.954800997 CORE	56 Pd Pd	0.0000	56
Pd	0.819038605	3.658630722	12.941019828 CORE	57 Pd Pd	0.0000	57
Pd	6.401699484	0.891677110	12.970645753 CORE	58 Pd Pd	0.0000	58
Pd	9.265491171	6.445540864	12.913930460 CORE	59 Pd Pd	0.0000	59
Pd	6.397209030	9.262815031	12.944021801 CORE	60 Pd Pd	0.0000	60
Pd	0.838913046	0.878889584	12.959449850 CORE	61 Pd Pd	0.0000	61
Pd	9.221214800	0.842161826	12.960792935 CORE	62 Pd Pd	0.0000	62
Pd	6.441816857	6.486885382	12.934963427 CORE	63 Pd Pd	0.0000	63
Pd	3.616948443	0.800386459	12.954714625 CORE	64 Pd Pd	0.0000	64

H 10.517877895 5.005927816 13.237125209 CORE 65 H H 0.0000 65
H 10.601249675 7.854271575 13.191816409 CORE 66 H H 0.0000 66
H 7.809182112 10.644599021 13.164054101 CORE 67 H H 0.0000 67
H 10.585756946 10.612907004 13.254158591 CORE 68 H H 0.0000 68
H 2.148473540 7.900874432 13.095970230 CORE 69 H H 0.0000 69
H 5.052475543 10.621172996 13.229696640 CORE 70 H H 0.0000 70
H 7.913560587 2.158247092 12.933142031 CORE 71 H H 0.0000 71
H 5.007354641 7.966433057 13.119479818 CORE 72 H H 0.0000 72
H 6.600310097 3.433448347 14.717136020 CORE 73 H H 0.0000 73
H 4.888539993 2.141319078 13.061186494 CORE 74 H H 0.0000 74
H 2.200605811 10.612080960 13.206152846 CORE 75 H H 0.0000 75
H 10.599133236 2.262952256 13.188808431 CORE 76 H H 0.0000 76
H 7.929452941 7.861555319 13.058235877 CORE 77 H H 0.0000 77
H 2.209986492 2.224767808 13.156453724 CORE 78 H H 0.0000 78
H 2.157540347 5.025802855 13.007115048 CORE 79 H H 0.0000 79
C 6.011025027 5.226695196 14.518244044 CORE 80 C C 0.0000 80
C 4.640317417 5.467419636 14.890614052 CORE 81 C C 0.0000 81
H 6.792704866 5.579786128 15.208823248 CORE 82 H H 0.0000 82
H 4.484480194 6.239925478 15.658733683 CORE 83 H H 0.0000 83
H 3.980618525 4.595416041 15.031995085 CORE 84 H H 0.0000 84
end
end

Ethene adsorbed on Pd(100). The energy from VASP is -404.975219 eV.

PBC 11.15000000 11.15000000 20.00000000 90.00000000 90.00000000 90.00000000
Pd 10.597740511 5.052097766 6.971435851 CORE 1 Pd Pd 0.0000 1
Pd 5.016640882 10.622407807 6.972012903 CORE 2 Pd Pd 0.0000 2
Pd 2.230223226 5.049854980 6.970471652 CORE 3 Pd Pd 0.0000 3
Pd 7.800416967 10.624591683 6.969912369 CORE 4 Pd Pd 0.0000 4
Pd 5.016274142 2.253949823 6.972670109 CORE 5 Pd Pd 0.0000 5
Pd 2.229944252 2.256956188 6.972582338 CORE 6 Pd Pd 0.0000 6
Pd 2.228413734 10.624718305 6.970006299 CORE 7 Pd Pd 0.0000 7
Pd 10.597206020 2.263659019 6.970036445 CORE 8 Pd Pd 0.0000 8
Pd 7.801704797 7.837842446 6.970623655 CORE 9 Pd Pd 0.0000 9
Pd 2.230101993 7.831322293 6.970481309 CORE 10 Pd Pd 0.0000 10
Pd 10.597535023 7.837059081 6.971582148 CORE 11 Pd Pd 0.0000 11
Pd 10.596798114 10.627094906 6.970621961 CORE 12 Pd Pd 0.0000 12
Pd 7.803055937 5.045716439 6.970928879 CORE 13 Pd Pd 0.0000 13
Pd 5.020239126 5.047289691 6.971467557 CORE 14 Pd Pd 0.0000 14
Pd 7.800761438 2.262637522 6.970691684 CORE 15 Pd Pd 0.0000 15
Pd 5.020279192 7.830435235 6.972662179 CORE 16 Pd Pd 0.0000 16
Pd 0.838578788 6.443772149 8.914560183 CORE 17 Pd Pd 0.0000 17
Pd 6.411284480 0.864013686 8.916862625 CORE 18 Pd Pd 0.0000 18
Pd 0.833839460 3.655784084 8.918734532 CORE 19 Pd Pd 0.0000 19

Pd	6.415512658	9.227179303	8.918643034 CORE	20 Pd Pd	0.0000	20
Pd	3.622943088	0.864417525	8.916836450 CORE	21 Pd Pd	0.0000	21
Pd	0.833799274	9.231256748	8.920264273 CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540 CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432 CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921 CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165 CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244 CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202 CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905 CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344 CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620 CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449 CORE	32 Pd Pd	0.0000	32
Pd	2.222003387	10.630226820	10.887768798 CORE	33 Pd Pd	0.0000	33
Pd	2.229030176	7.839207658	10.879853691 CORE	34 Pd Pd	0.0000	34
Pd	2.224069483	2.254429046	10.889477400 CORE	35 Pd Pd	0.0000	35
Pd	10.595749441	7.844125946	10.882249869 CORE	36 Pd Pd	0.0000	36
Pd	5.041091450	7.811095395	10.935455725 CORE	37 Pd Pd	0.0000	37
Pd	7.782660324	5.072139385	10.938043173 CORE	38 Pd Pd	0.0000	38
Pd	5.011598196	2.257134045	10.878280186 CORE	39 Pd Pd	0.0000	39
Pd	7.808908397	2.261228296	10.881514738 CORE	40 Pd Pd	0.0000	40
Pd	7.789689467	7.820951689	10.926658596 CORE	41 Pd Pd	0.0000	41
Pd	10.599212342	2.256294462	10.888628279 CORE	42 Pd Pd	0.0000	42
Pd	5.034027672	5.061560073	10.922486926 CORE	43 Pd Pd	0.0000	43
Pd	10.597511925	10.630537844	10.893422502 CORE	44 Pd Pd	0.0000	44
Pd	7.810378032	10.626044828	10.882901960 CORE	45 Pd Pd	0.0000	45
Pd	5.012740619	10.622557002	10.878931123 CORE	46 Pd Pd	0.0000	46
Pd	10.594640226	5.045339412	10.880675848 CORE	47 Pd Pd	0.0000	47
Pd	2.228301368	5.040881223	10.879080438 CORE	48 Pd Pd	0.0000	48
Pd	3.606205845	9.243739574	12.945883553 CORE	49 Pd Pd	0.0000	49
Pd	0.835460240	9.228596268	12.960993932 CORE	50 Pd Pd	0.0000	50
Pd	9.211644984	9.244678025	12.956332562 CORE	51 Pd Pd	0.0000	51
Pd	6.404537749	3.618891412	12.943748200 CORE	52 Pd Pd	0.0000	52
Pd	3.588808134	6.432151392	12.942253645 CORE	53 Pd Pd	0.0000	53
Pd	3.610724036	3.638072892	12.952797573 CORE	54 Pd Pd	0.0000	54
Pd	9.215724787	3.639484352	12.948606039 CORE	55 Pd Pd	0.0000	55
Pd	0.838409679	6.443407560	12.954890285 CORE	56 Pd Pd	0.0000	56
Pd	0.837496373	3.658658938	12.959870013 CORE	57 Pd Pd	0.0000	57
Pd	6.409774186	0.868197474	12.954714694 CORE	58 Pd Pd	0.0000	58
Pd	9.237688635	6.449714640	12.944795812 CORE	59 Pd Pd	0.0000	59
Pd	6.416448219	9.267518273	12.944058459 CORE	60 Pd Pd	0.0000	60
Pd	0.835856681	0.868958851	12.971952535 CORE	61 Pd Pd	0.0000	61
Pd	9.195373591	0.868403203	12.961251144 CORE	62 Pd Pd	0.0000	62
Pd	6.412946408	6.443407983	13.266848739 CORE	63 Pd Pd	0.0000	63

Pd	3.625570103	0.865020715	12.958798555	CORE	64	Pd	Pd	0.0000	64
H	10.603207468	5.049278961	13.182100795	CORE	65	H	H	0.0000	65
H	10.598158358	7.830115680	13.193277686	CORE	66	H	H	0.0000	66
H	7.797839205	10.628798010	13.192856529	CORE	67	H	H	0.0000	67
H	10.613911251	10.645483629	13.189824529	CORE	68	H	H	0.0000	68
H	2.219447434	7.834807167	13.180938617	CORE	69	H	H	0.0000	69
H	5.018002354	10.634517890	13.181914142	CORE	70	H	H	0.0000	70
H	7.805469129	2.251601337	13.181771869	CORE	71	H	H	0.0000	71
H	4.929898903	7.921109080	12.880442456	CORE	72	H	H	0.0000	72
H	5.023985047	2.255321285	13.193092292	CORE	73	H	H	0.0000	73
H	2.212781446	10.640735871	13.194812982	CORE	74	H	H	0.0000	74
H	10.608722745	2.244843390	13.195308939	CORE	75	H	H	0.0000	75
H	7.899685022	7.931378187	12.981421328	CORE	76	H	H	0.0000	76
H	2.208446402	2.238972654	13.189610822	CORE	77	H	H	0.0000	77
H	2.224759342	5.055133186	13.192981285	CORE	78	H	H	0.0000	78
H	7.890596478	4.962272177	12.886585149	CORE	79	H	H	0.0000	79
H	4.922682232	4.951308380	12.985104477	CORE	80	H	H	0.0000	80
C	6.910053012	5.973297524	15.417944195	CORE	81	C	C	0.0000	81
C	5.912813210	6.933780850	15.413594314	CORE	82	C	C	0.0000	82
H	7.956156903	6.251465746	15.559296383	CORE	83	H	H	0.0000	83
H	6.150624983	7.990513192	15.550771614	CORE	84	H	H	0.0000	84
H	4.866216916	6.657324516	15.555713567	CORE	85	H	H	0.0000	85
H	6.672086586	4.917751817	15.563493643	CORE	86	H	H	0.0000	86

end

end

TS from ethene to ethyl on Pd(100). The energy from VASP is -404.345694 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	90.00000000		
Pd	10.597740511	5.052097766	6.971435851	CORE	1	Pd	Pd	0.0000	1
Pd	5.016640882	10.622407807	6.972012903	CORE	2	Pd	Pd	0.0000	2
Pd	2.230223226	5.049854980	6.970471652	CORE	3	Pd	Pd	0.0000	3
Pd	7.800416967	10.624591683	6.969912369	CORE	4	Pd	Pd	0.0000	4
Pd	5.016274142	2.253949823	6.972670109	CORE	5	Pd	Pd	0.0000	5
Pd	2.229944252	2.256956188	6.972582338	CORE	6	Pd	Pd	0.0000	6
Pd	2.228413734	10.624718305	6.970006299	CORE	7	Pd	Pd	0.0000	7
Pd	10.597206020	2.263659019	6.970036445	CORE	8	Pd	Pd	0.0000	8
Pd	7.801704797	7.837842446	6.970623655	CORE	9	Pd	Pd	0.0000	9
Pd	2.230101993	7.831322293	6.970481309	CORE	10	Pd	Pd	0.0000	10
Pd	10.597535023	7.837059081	6.971582148	CORE	11	Pd	Pd	0.0000	11
Pd	10.596798114	10.627094906	6.970621961	CORE	12	Pd	Pd	0.0000	12
Pd	7.803055937	5.045716439	6.970928879	CORE	13	Pd	Pd	0.0000	13
Pd	5.020239126	5.047289691	6.971467557	CORE	14	Pd	Pd	0.0000	14
Pd	7.800761438	2.262637522	6.970691684	CORE	15	Pd	Pd	0.0000	15
Pd	5.020279192	7.830435235	6.972662179	CORE	16	Pd	Pd	0.0000	16

Pd	0.838578788	6.443772149	8.914560183 CORE	17 Pd Pd	0.0000	17
Pd	6.411284480	0.864013686	8.916862625 CORE	18 Pd Pd	0.0000	18
Pd	0.833839460	3.655784084	8.918734532 CORE	19 Pd Pd	0.0000	19
Pd	6.415512658	9.227179303	8.918643034 CORE	20 Pd Pd	0.0000	20
Pd	3.622943088	0.864417525	8.916836450 CORE	21 Pd Pd	0.0000	21
Pd	0.833799274	9.231256748	8.920264273 CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540 CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432 CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921 CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165 CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244 CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202 CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905 CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344 CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620 CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449 CORE	32 Pd Pd	0.0000	32
Pd	2.226466274	10.631412170	10.895304636 CORE	33 Pd Pd	0.0000	33
Pd	2.241751911	7.844859322	10.882057006 CORE	34 Pd Pd	0.0000	34
Pd	2.219385961	2.255114753	10.890725721 CORE	35 Pd Pd	0.0000	35
Pd	10.602648951	7.842282544	10.889189234 CORE	36 Pd Pd	0.0000	36
Pd	5.047660671	7.811969072	10.930269091 CORE	37 Pd Pd	0.0000	37
Pd	7.786040404	5.060784458	10.940550269 CORE	38 Pd Pd	0.0000	38
Pd	5.002818470	2.247037530	10.868603783 CORE	39 Pd Pd	0.0000	39
Pd	7.804807385	2.265803364	10.885851233 CORE	40 Pd Pd	0.0000	40
Pd	7.794652475	7.796447725	10.944479853 CORE	41 Pd Pd	0.0000	41
Pd	10.598449060	2.259222489	10.882543242 CORE	42 Pd Pd	0.0000	42
Pd	5.049864007	5.059827757	10.929555473 CORE	43 Pd Pd	0.0000	43
Pd	10.604553499	10.633696147	10.886267426 CORE	44 Pd Pd	0.0000	44
Pd	7.809354877	10.621034750	10.883255495 CORE	45 Pd Pd	0.0000	45
Pd	5.011269540	10.616978105	10.876175750 CORE	46 Pd Pd	0.0000	46
Pd	10.586793267	5.048273032	10.886717272 CORE	47 Pd Pd	0.0000	47
Pd	2.234252679	5.046806233	10.883522498 CORE	48 Pd Pd	0.0000	48
Pd	3.618038984	9.246951159	12.955360703 CORE	49 Pd Pd	0.0000	49
Pd	0.843893706	9.241276320	12.965399896 CORE	50 Pd Pd	0.0000	50
Pd	9.229056683	9.258497821	12.948309776 CORE	51 Pd Pd	0.0000	51
Pd	6.386592885	3.581226886	12.914400494 CORE	52 Pd Pd	0.0000	52
Pd	3.638763050	6.443646709	12.944660743 CORE	53 Pd Pd	0.0000	53
Pd	3.591633814	3.639971260	12.948795051 CORE	54 Pd Pd	0.0000	54
Pd	9.195151218	3.642803265	12.929205191 CORE	55 Pd Pd	0.0000	55
Pd	0.875497277	6.458786428	12.950705236 CORE	56 Pd Pd	0.0000	56
Pd	0.819759819	3.672069692	12.959785431 CORE	57 Pd Pd	0.0000	57
Pd	6.408792406	0.842838335	12.953772674 CORE	58 Pd Pd	0.0000	58
Pd	9.265169827	6.426936206	12.955870457 CORE	59 Pd Pd	0.0000	59
Pd	6.412216144	9.248902752	12.943257637 CORE	60 Pd Pd	0.0000	60

Pd	0.833851207	0.880123226	12.971680102	CORE	61	Pd	Pd	0.0000	61
Pd	9.196588100	0.875603518	12.954483710	CORE	62	Pd	Pd	0.0000	62
Pd	6.410778238	6.390526204	13.309284499	CORE	63	Pd	Pd	0.0000	63
Pd	3.629006547	0.868895162	12.963057075	CORE	64	Pd	Pd	0.0000	64
H	10.545818844	5.005685672	13.201428188	CORE	65	H	H	0.0000	65
H	10.666095796	7.889465588	13.183857299	CORE	66	H	H	0.0000	66
H	7.803363932	10.626620751	13.184386339	CORE	67	H	H	0.0000	67
H	10.617979429	10.663661269	13.215133453	CORE	68	H	H	0.0000	68
H	2.224313300	7.837919142	13.184769503	CORE	69	H	H	0.0000	69
H	5.011944769	10.641323273	13.218786393	CORE	70	H	H	0.0000	70
H	7.811026412	2.299359390	13.177176079	CORE	71	H	H	0.0000	71
H	4.930286822	7.910307244	12.990487073	CORE	72	H	H	0.0000	72
H	5.014781087	2.243268561	13.206548207	CORE	73	H	H	0.0000	73
H	2.228976763	10.642496789	13.197864537	CORE	74	H	H	0.0000	74
H	10.586572750	2.268200498	13.180750895	CORE	75	H	H	0.0000	75
H	7.879256281	8.029518785	12.842558247	CORE	76	H	H	0.0000	76
H	2.205768752	2.256920873	13.182547752	CORE	77	H	H	0.0000	77
H	2.220489828	5.047068477	13.176230994	CORE	78	H	H	0.0000	78
H	7.971160681	5.974955323	14.165485114	CORE	79	H	H	0.0000	79
H	4.943003575	4.922054553	12.990648687	CORE	80	H	H	0.0000	80
C	7.311213331	6.113100718	15.470336025	CORE	81	C	C	0.0000	81
C	5.949719287	6.545050358	15.396746050	CORE	82	C	C	0.0000	82
H	8.053523836	6.834890533	15.819886151	CORE	83	H	H	0.0000	83
H	5.712278381	7.588476712	15.611505788	CORE	84	H	H	0.0000	84
H	5.151521621	5.829310609	15.600618134	CORE	85	H	H	0.0000	85
H	7.506572873	5.077652728	15.760466514	CORE	86	H	H	0.0000	86

end

end

Ethyl adsorbed on Pd(100). The energy from VASP is -408.714986 eV.

PBC	11.15000000	11.15000000	20.00000000	90.00000000	90.00000000	90.00000000
Pd	10.597740511	5.052097766	6.971435851	CORE	1 Pd	Pd 0.0000 1
Pd	5.016640882	10.622407807	6.972012903	CORE	2 Pd	Pd 0.0000 2
Pd	2.230223226	5.049854980	6.970471652	CORE	3 Pd	Pd 0.0000 3
Pd	7.800416967	10.624591683	6.969912369	CORE	4 Pd	Pd 0.0000 4
Pd	5.016274142	2.253949823	6.972670109	CORE	5 Pd	Pd 0.0000 5
Pd	2.229944252	2.256956188	6.972582338	CORE	6 Pd	Pd 0.0000 6
Pd	2.228413734	10.624718305	6.970006299	CORE	7 Pd	Pd 0.0000 7
Pd	10.597206020	2.263659019	6.970036445	CORE	8 Pd	Pd 0.0000 8
Pd	7.801704797	7.837842446	6.970623655	CORE	9 Pd	Pd 0.0000 9
Pd	2.230101993	7.831322293	6.970481309	CORE	10 Pd	Pd 0.0000 10
Pd	10.597535023	7.837059081	6.971582148	CORE	11 Pd	Pd 0.0000 11
Pd	10.596798114	10.627094906	6.970621961	CORE	12 Pd	Pd 0.0000 12
Pd	7.803055937	5.045716439	6.970928879	CORE	13 Pd	Pd 0.0000 13

Pd	5.020239126	5.047289691	6.971467557 CORE	14 Pd Pd	0.0000	14
Pd	7.800761438	2.262637522	6.970691684 CORE	15 Pd Pd	0.0000	15
Pd	5.020279192	7.830435235	6.972662179 CORE	16 Pd Pd	0.0000	16
Pd	0.838578788	6.443772149	8.914560183 CORE	17 Pd Pd	0.0000	17
Pd	6.411284480	0.864013686	8.916862625 CORE	18 Pd Pd	0.0000	18
Pd	0.833839460	3.655784084	8.918734532 CORE	19 Pd Pd	0.0000	19
Pd	6.415512658	9.227179303	8.918643034 CORE	20 Pd Pd	0.0000	20
Pd	3.622943088	0.864417525	8.916836450 CORE	21 Pd Pd	0.0000	21
Pd	0.833799274	9.231256748	8.920264273 CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540 CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432 CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921 CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165 CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244 CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202 CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905 CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344 CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620 CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449 CORE	32 Pd Pd	0.0000	32
Pd	2.227918771	10.624059013	10.889521289 CORE	33 Pd Pd	0.0000	33
Pd	2.234517434	7.834737877	10.888110603 CORE	34 Pd Pd	0.0000	34
Pd	2.228312970	2.257297263	10.888119797 CORE	35 Pd Pd	0.0000	35
Pd	10.595228520	7.839935865	10.888123155 CORE	36 Pd Pd	0.0000	36
Pd	5.035412721	7.816929932	10.910074149 CORE	37 Pd Pd	0.0000	37
Pd	7.788706563	5.066574476	10.922485152 CORE	38 Pd Pd	0.0000	38
Pd	5.015608728	2.257952592	10.884338626 CORE	39 Pd Pd	0.0000	39
Pd	7.803902239	2.262178387	10.888270361 CORE	40 Pd Pd	0.0000	40
Pd	7.791577022	7.820379423	10.913376806 CORE	41 Pd Pd	0.0000	41
Pd	10.595668707	2.259358338	10.886525641 CORE	42 Pd Pd	0.0000	42
Pd	5.034808806	5.059861352	10.909209160 CORE	43 Pd Pd	0.0000	43
Pd	10.594250905	10.626002734	10.892317512 CORE	44 Pd Pd	0.0000	44
Pd	7.804960073	10.620125925	10.890422700 CORE	45 Pd Pd	0.0000	45
Pd	5.016930229	10.617252598	10.887508237 CORE	46 Pd Pd	0.0000	46
Pd	10.593751796	5.049889671	10.887808373 CORE	47 Pd Pd	0.0000	47
Pd	2.234340223	5.046010189	10.886743868 CORE	48 Pd Pd	0.0000	48
Pd	3.616799052	9.232538206	12.953744495 CORE	49 Pd Pd	0.0000	49
Pd	0.837015062	9.228308179	12.957876652 CORE	50 Pd Pd	0.0000	50
Pd	9.206091568	9.239641004	12.958002246 CORE	51 Pd Pd	0.0000	51
Pd	6.403985361	3.649628122	12.949603698 CORE	52 Pd Pd	0.0000	52
Pd	3.639007905	6.436389237	12.947262343 CORE	53 Pd Pd	0.0000	53
Pd	3.615063599	3.643020526	12.954374291 CORE	54 Pd Pd	0.0000	54
Pd	9.209500878	3.644513163	12.948814638 CORE	55 Pd Pd	0.0000	55
Pd	0.847252230	6.442227425	12.955358726 CORE	56 Pd Pd	0.0000	56
Pd	0.837039145	3.655372986	12.955046041 CORE	57 Pd Pd	0.0000	57

Pd 6.410231932 0.860598043 12.955266626 CORE 58 Pd Pd 0.0000 58
Pd 9.208109032 6.450243192 12.950871331 CORE 59 Pd Pd 0.0000 59
Pd 6.412014796 9.218584698 12.949128033 CORE 60 Pd Pd 0.0000 60
Pd 0.836426836 0.867730308 12.963482487 CORE 61 Pd Pd 0.0000 61
Pd 9.197773103 0.868088465 12.956564554 CORE 62 Pd Pd 0.0000 62
Pd 6.419628012 6.439007025 13.198883589 CORE 63 Pd Pd 0.0000 63
Pd 3.625168904 0.863088812 12.955823046 CORE 64 Pd Pd 0.0000 64
H 10.608349017 5.032961229 13.155250694 CORE 65 H H 0.0000 65
H 10.601547069 7.841082450 13.170628325 CORE 66 H H 0.0000 66
H 7.814427150 10.627425205 13.162966952 CORE 67 H H 0.0000 67
H 10.616696158 10.643497145 13.178001330 CORE 68 H H 0.0000 68
H 2.224117494 7.841502041 13.161151763 CORE 69 H H 0.0000 69
H 5.011584065 10.628982878 13.161146627 CORE 70 H H 0.0000 70
H 7.821951953 2.247085597 13.157852237 CORE 71 H H 0.0000 71
H 4.922452071 7.925045153 13.133710666 CORE 72 H H 0.0000 72
H 5.011025462 2.250312015 13.171469844 CORE 73 H H 0.0000 73
H 2.208481332 10.644533278 13.177520542 CORE 74 H H 0.0000 74
H 10.610264721 2.243151911 13.182640532 CORE 75 H H 0.0000 75
H 7.915896050 7.923421650 13.154827695 CORE 76 H H 0.0000 76
H 2.209370130 2.234942761 13.178509929 CORE 77 H H 0.0000 77
H 2.226529298 5.037788172 13.163041416 CORE 78 H H 0.0000 78
H 8.407300309 5.925317030 15.719641619 CORE 79 H H 0.0000 79
H 4.929873840 4.934184851 13.153396621 CORE 80 H H 0.0000 80
H 7.886278475 4.960276789 13.045721947 CORE 81 H H 0.0000 81
C 7.374725235 5.641066100 15.969656154 CORE 82 C C 0.0000 82
C 6.351837510 6.512001106 15.289129586 CORE 83 C C 0.0000 83
H 7.261031195 5.756537182 17.065717500 CORE 84 H H 0.0000 84
H 6.489878051 7.583138456 15.486704193 CORE 85 H H 0.0000 85
H 5.315844231 6.214814711 15.497429036 CORE 86 H H 0.0000 86
H 7.244779090 4.574598696 15.739033038 CORE 87 H H 0.0000 87
end
end

TS from ethyl to ethane on Pd(100). The energy from VASP is -408.127524 eV.

PBC 11.15000000 11.15000000 20.00000000 90.00000000 90.00000000 90.00000000
Pd 10.597740511 5.052097766 6.971435851 CORE 1 Pd Pd 0.0000 1
Pd 5.016640882 10.622407807 6.972012903 CORE 2 Pd Pd 0.0000 2
Pd 2.230223226 5.049854980 6.970471652 CORE 3 Pd Pd 0.0000 3
Pd 7.800416967 10.624591683 6.969912369 CORE 4 Pd Pd 0.0000 4
Pd 5.016274142 2.253949823 6.972670109 CORE 5 Pd Pd 0.0000 5
Pd 2.229944252 2.256956188 6.972582338 CORE 6 Pd Pd 0.0000 6
Pd 2.228413734 10.624718305 6.970006299 CORE 7 Pd Pd 0.0000 7
Pd 10.597206020 2.263659019 6.970036445 CORE 8 Pd Pd 0.0000 8
Pd 7.801704797 7.837842446 6.970623655 CORE 9 Pd Pd 0.0000 9
Pd 2.230101993 7.831322293 6.970481309 CORE 10 Pd Pd 0.0000 10

Pd	10.597535023	7.837059081	6.971582148 CORE	11 Pd Pd	0.0000	11
Pd	10.596798114	10.627094906	6.970621961 CORE	12 Pd Pd	0.0000	12
Pd	7.803055937	5.045716439	6.970928879 CORE	13 Pd Pd	0.0000	13
Pd	5.020239126	5.047289691	6.971467557 CORE	14 Pd Pd	0.0000	14
Pd	7.800761438	2.262637522	6.970691684 CORE	15 Pd Pd	0.0000	15
Pd	5.020279192	7.830435235	6.972662179 CORE	16 Pd Pd	0.0000	16
Pd	0.838578788	6.443772149	8.914560183 CORE	17 Pd Pd	0.0000	17
Pd	6.411284480	0.864013686	8.916862625 CORE	18 Pd Pd	0.0000	18
Pd	0.833839460	3.655784084	8.918734532 CORE	19 Pd Pd	0.0000	19
Pd	6.415512658	9.227179303	8.918643034 CORE	20 Pd Pd	0.0000	20
Pd	3.622943088	0.864417525	8.916836450 CORE	21 Pd Pd	0.0000	21
Pd	0.833799274	9.231256748	8.920264273 CORE	22 Pd Pd	0.0000	22
Pd	0.835023409	0.866698032	8.915039540 CORE	23 Pd Pd	0.0000	23
Pd	6.417179426	3.654547459	8.917452432 CORE	24 Pd Pd	0.0000	24
Pd	9.197941661	0.868301073	8.924963921 CORE	25 Pd Pd	0.0000	25
Pd	9.200992917	6.444440101	8.925476165 CORE	26 Pd Pd	0.0000	26
Pd	6.411374866	6.441253388	8.917431244 CORE	27 Pd Pd	0.0000	27
Pd	3.623006947	9.227316503	8.925778202 CORE	28 Pd Pd	0.0000	28
Pd	3.623901043	3.651372649	8.923714905 CORE	29 Pd Pd	0.0000	29
Pd	3.623446846	6.439213918	8.918210344 CORE	30 Pd Pd	0.0000	30
Pd	9.196391064	3.657368059	8.921895620 CORE	31 Pd Pd	0.0000	31
Pd	9.197731635	9.232208688	8.926076449 CORE	32 Pd Pd	0.0000	32
Pd	2.227395621	10.628797350	10.885026864 CORE	33 Pd Pd	0.0000	33
Pd	2.234292755	7.834783127	10.888155726 CORE	34 Pd Pd	0.0000	34
Pd	2.226946091	2.253416974	10.893019575 CORE	35 Pd Pd	0.0000	35
Pd	10.598577039	7.840171367	10.882255410 CORE	36 Pd Pd	0.0000	36
Pd	5.021871247	7.829473597	10.909846162 CORE	37 Pd Pd	0.0000	37
Pd	7.775958556	5.079622901	10.945160405 CORE	38 Pd Pd	0.0000	38
Pd	5.015727141	2.260612735	10.882138964 CORE	39 Pd Pd	0.0000	39
Pd	7.811803991	2.269598945	10.887026090 CORE	40 Pd Pd	0.0000	40
Pd	7.780655457	7.830320866	10.926109829 CORE	41 Pd Pd	0.0000	41
Pd	10.599123175	2.258287043	10.893013443 CORE	42 Pd Pd	0.0000	42
Pd	5.030550443	5.072604085	10.918562901 CORE	43 Pd Pd	0.0000	43
Pd	10.599706180	10.632291373	10.887887124 CORE	44 Pd Pd	0.0000	44
Pd	7.809236857	10.631497458	10.890960177 CORE	45 Pd Pd	0.0000	45
Pd	5.019073602	10.620123647	10.885398850 CORE	46 Pd Pd	0.0000	46
Pd	10.589490324	5.041776544	10.880995910 CORE	47 Pd Pd	0.0000	47
Pd	2.222916087	5.035115758	10.876524450 CORE	48 Pd Pd	0.0000	48
Pd	3.620195177	9.226309384	12.930072142 CORE	49 Pd Pd	0.0000	49
Pd	0.847433544	9.231131155	12.957946900 CORE	50 Pd Pd	0.0000	50
Pd	9.229294353	9.240965329	12.950284163 CORE	51 Pd Pd	0.0000	51
Pd	6.408298650	3.658743410	12.946460230 CORE	52 Pd Pd	0.0000	52
Pd	3.579396710	6.415143874	12.915513276 CORE	53 Pd Pd	0.0000	53
Pd	3.621292331	3.625784822	12.957441800 CORE	54 Pd Pd	0.0000	54

Pd	9.219002962	3.635842691	12.961516252	CORE	55	Pd	Pd	0.0000	55
Pd	0.826205186	6.443164221	12.956050439	CORE	56	Pd	Pd	0.0000	56
Pd	0.843477491	3.659585787	12.965308332	CORE	57	Pd	Pd	0.0000	57
Pd	6.418800158	0.889445935	12.955747475	CORE	58	Pd	Pd	0.0000	58
Pd	9.219451916	6.436781681	12.942612189	CORE	59	Pd	Pd	0.0000	59
Pd	6.406842751	9.275529024	12.944620633	CORE	60	Pd	Pd	0.0000	60
Pd	0.842077039	0.869486573	12.971593771	CORE	61	Pd	Pd	0.0000	61
Pd	9.206375910	0.861646232	12.966978164	CORE	62	Pd	Pd	0.0000	62
Pd	6.345780642	6.489238121	13.189365439	CORE	63	Pd	Pd	0.0000	63
Pd	3.633985943	0.851926877	12.961122956	CORE	64	Pd	Pd	0.0000	64
H	10.618631137	5.030384210	13.203944755	CORE	65	H	H	0.0000	65
H	10.594225808	7.830714785	13.190778575	CORE	66	H	H	0.0000	66
H	7.837502624	10.673179620	13.162391641	CORE	67	H	H	0.0000	67
H	10.631265304	10.635381956	13.210482086	CORE	68	H	H	0.0000	68
H	2.278828516	7.831660284	13.156449384	CORE	69	H	H	0.0000	69
H	5.001353734	10.590314636	13.189425586	CORE	70	H	H	0.0000	70
H	7.823232853	2.253470050	13.181773892	CORE	71	H	H	0.0000	71
H	5.894169116	7.864477169	14.037588406	CORE	72	H	H	0.0000	72
H	5.012424302	2.258598935	13.197804106	CORE	73	H	H	0.0000	73
H	2.246553393	10.603358894	13.169783892	CORE	74	H	H	0.0000	74
H	10.611841337	2.252565614	13.217386231	CORE	75	H	H	0.0000	75
H	7.973811909	7.877347173	12.913903905	CORE	76	H	H	0.0000	76
H	2.232026645	2.233766583	13.184190647	CORE	77	H	H	0.0000	77
H	2.221688928	5.045116589	13.186955849	CORE	78	H	H	0.0000	78
H	8.032692309	6.136030240	15.723874306	CORE	79	H	H	0.0000	79
H	4.941153299	4.965698500	13.090118929	CORE	80	H	H	0.0000	80
H	7.884444698	4.941415340	12.983610655	CORE	81	H	H	0.0000	81
C	6.983325939	5.955042838	15.994874953	CORE	82	C	C	0.0000	82
C	6.033220002	6.962983192	15.374271369	CORE	83	C	C	0.0000	83
H	6.910669921	6.051958176	17.094943785	CORE	84	H	H	0.0000	84
H	6.239623034	7.971651811	15.756968029	CORE	85	H	H	0.0000	85
H	4.974084720	6.738445800	15.541354231	CORE	86	H	H	0.0000	86
H	6.731458344	4.919727152	15.730386119	CORE	87	H	H	0.0000	87

end

end

Initial Pd_4H_3(100). The energy from VASP is -493.313966 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	90.00000000		
Pd	10.782813856	5.016247660	7.193226476	CORE	1	Pd	Pd	0.0000	1
Pd	4.983148483	10.816790048	7.193170144	CORE	2	Pd	Pd	0.0000	2
Pd	2.085019604	5.016620832	7.193299683	CORE	3	Pd	Pd	0.0000	3
Pd	7.884901240	10.816521313	7.193479525	CORE	4	Pd	Pd	0.0000	4
Pd	4.983416221	2.117754835	7.193565625	CORE	5	Pd	Pd	0.0000	5
Pd	2.083689210	2.116303795	7.193523055	CORE	6	Pd	Pd	0.0000	6

Pd	2.083337101	10.816628396	7.193560017	CORE	7	Pd	Pd	0.0000	7
Pd	10.783357174	2.116005107	7.193717507	CORE	8	Pd	Pd	0.0000	8
Pd	7.884314250	7.916229331	7.194179624	CORE	9	Pd	Pd	0.0000	9
Pd	2.084485458	7.917186866	7.193893349	CORE	10	Pd	Pd	0.0000	10
Pd	10.783518995	7.917095999	7.193878528	CORE	11	Pd	Pd	0.0000	11
Pd	10.784183220	10.816439879	7.193774103	CORE	12	Pd	Pd	0.0000	12
Pd	7.883464201	5.016721878	7.194093710	CORE	13	Pd	Pd	0.0000	13
Pd	4.984519188	5.017098245	7.194084067	CORE	14	Pd	Pd	0.0000	14
Pd	7.884069627	2.117381531	7.193905540	CORE	15	Pd	Pd	0.0000	15
Pd	4.984015372	7.916443018	7.194219365	CORE	16	Pd	Pd	0.0000	16
Pd	0.634013228	6.466332063	9.009721539	CORE	17	Pd	Pd	0.0000	17
Pd	6.433640859	0.666804909	9.009776069	CORE	18	Pd	Pd	0.0000	18
Pd	0.633707465	3.566812798	9.009902151	CORE	19	Pd	Pd	0.0000	19
Pd	6.434087100	9.367309174	9.010160968	CORE	20	Pd	Pd	0.0000	20
Pd	3.533869947	0.666899228	9.010240576	CORE	21	Pd	Pd	0.0000	21
Pd	0.633969081	9.366447775	9.010826567	CORE	22	Pd	Pd	0.0000	22
Pd	0.633676922	0.666672598	9.010533542	CORE	23	Pd	Pd	0.0000	23
Pd	6.433782001	3.566623726	9.011031260	CORE	24	Pd	Pd	0.0000	24
Pd	9.333604600	0.666638656	9.010546436	CORE	25	Pd	Pd	0.0000	25
Pd	9.334234437	6.466445910	9.010863765	CORE	26	Pd	Pd	0.0000	26
Pd	6.434155127	6.466929211	9.011104041	CORE	27	Pd	Pd	0.0000	27
Pd	3.534124022	9.367105408	9.010616024	CORE	28	Pd	Pd	0.0000	28
Pd	3.533628327	3.566955412	9.010687856	CORE	29	Pd	Pd	0.0000	29
Pd	3.533991674	6.466788159	9.010808806	CORE	30	Pd	Pd	0.0000	30
Pd	9.333852689	3.566664034	9.010894518	CORE	31	Pd	Pd	0.0000	31
Pd	9.333931906	9.366801997	9.011053461	CORE	32	Pd	Pd	0.0000	32
H	9.580275272	3.552800903	6.954668839	CORE	33	H	H	0.0000	33
H	3.295746757	3.547762072	6.962678283	CORE	34	H	H	0.0000	34
H	9.086881997	9.341519786	6.949637981	CORE	35	H	H	0.0000	35
H	0.584442804	9.413295161	7.028496754	CORE	36	H	H	0.0000	36
H	3.745807373	9.375081903	6.966885887	CORE	37	H	H	0.0000	37
H	6.434765974	3.610391075	7.040123954	CORE	38	H	H	0.0000	38
H	9.579247705	6.450013154	6.934030077	CORE	39	H	H	0.0000	39
H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48
H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50

H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.069885345	10.841788349	11.098649443	CORE	57	Pd	Pd	0.0000	57
Pd	2.110649190	7.919817862	11.104961337	CORE	58	Pd	Pd	0.0000	58
Pd	2.065878178	2.103961912	11.152815662	CORE	59	Pd	Pd	0.0000	59
Pd	10.793770409	7.930902252	11.115434035	CORE	60	Pd	Pd	0.0000	60
Pd	5.012809656	7.910225094	11.112336238	CORE	61	Pd	Pd	0.0000	61
Pd	7.893508778	5.066857551	11.105184114	CORE	62	Pd	Pd	0.0000	62
Pd	4.943714069	2.138682709	11.104843396	CORE	63	Pd	Pd	0.0000	63
Pd	7.873267610	2.154304033	11.101208540	CORE	64	Pd	Pd	0.0000	64
Pd	7.912276342	7.936244816	11.158535763	CORE	65	Pd	Pd	0.0000	65
Pd	10.761228465	2.111863510	11.153872136	CORE	66	Pd	Pd	0.0000	66
Pd	5.000386777	5.040730439	11.099540609	CORE	67	Pd	Pd	0.0000	67
Pd	10.765637137	10.848383564	11.094567332	CORE	68	Pd	Pd	0.0000	68
Pd	7.887923176	10.845510924	11.104886670	CORE	69	Pd	Pd	0.0000	69
Pd	4.949650128	10.830215819	11.109909018	CORE	70	Pd	Pd	0.0000	70
Pd	10.778784198	5.036211349	11.116316222	CORE	71	Pd	Pd	0.0000	71
Pd	2.112048867	5.014187034	11.115734096	CORE	72	Pd	Pd	0.0000	72
Pd	3.567816304	9.343002951	13.134740705	CORE	73	Pd	Pd	0.0000	73
Pd	0.658497796	9.357324175	13.115115773	CORE	74	Pd	Pd	0.0000	74
Pd	9.343777866	9.387121351	13.146297091	CORE	75	Pd	Pd	0.0000	75
Pd	6.428617829	3.618633186	13.128822638	CORE	76	Pd	Pd	0.0000	76
Pd	3.587061317	6.438171341	13.134621266	CORE	77	Pd	Pd	0.0000	77
Pd	3.526693804	3.528060979	13.152488837	CORE	78	Pd	Pd	0.0000	78
Pd	9.322266336	3.552023360	13.141137075	CORE	79	Pd	Pd	0.0000	79
Pd	0.642405665	6.506132490	13.097170451	CORE	80	Pd	Pd	0.0000	80
Pd	0.634003386	3.635562803	13.137956460	CORE	81	Pd	Pd	0.0000	81
Pd	6.361556779	0.752016769	13.113470210	CORE	82	Pd	Pd	0.0000	82
Pd	9.357984012	6.464099573	13.128952541	CORE	83	Pd	Pd	0.0000	83
Pd	6.450076899	9.453360684	13.146673979	CORE	84	Pd	Pd	0.0000	84
Pd	0.584172917	0.629393268	13.126499738	CORE	85	Pd	Pd	0.0000	85
Pd	9.311132256	0.656775589	13.131181434	CORE	86	Pd	Pd	0.0000	86
Pd	6.475610377	6.483784928	13.137189215	CORE	87	Pd	Pd	0.0000	87
Pd	3.464653930	0.624023234	13.133276921	CORE	88	Pd	Pd	0.0000	88
H	0.616605575	9.802957321	10.812443681	CORE	89	H	H	0.0000	89
H	9.292363902	3.944922645	10.827830345	CORE	90	H	H	0.0000	90
H	3.464245339	9.719049653	10.827371283	CORE	91	H	H	0.0000	91
H	9.669845065	9.406953086	10.841044385	CORE	92	H	H	0.0000	92
H	3.833155018	3.637013647	10.836076418	CORE	93	H	H	0.0000	93
H	3.264085415	6.465676707	10.876507418	CORE	94	H	H	0.0000	94

H 6.468560091 3.990187620 10.795280112 CORE 95 H H 0.0000 95
H 6.736156386 0.698246167 11.340812296 CORE 96 H H 0.0000 96
H 0.608131466 3.235204054 11.353178890 CORE 97 H H 0.0000 97
H 6.446548536 9.055169570 11.366124060 CORE 98 H H 0.0000 98
H 2.123953528 4.854352229 13.243832049 CORE 99 H H 0.0000 99
H 10.867529361 5.183829516 13.244143919 CORE 100 H H 0.0000 100
H 11.047794847 7.919352540 13.281445188 CORE 101 H H 0.0000 101
H 8.039519389 10.660114822 13.293737049 CORE 102 H H 0.0000 102
H 10.704883291 11.044467018 13.286790873 CORE 103 H H 0.0000 103
H 1.966974715 8.025108039 13.236390983 CORE 104 H H 0.0000 104
H 4.916518170 10.658644319 13.269848465 CORE 105 H H 0.0000 105
H 7.854085459 2.433486374 13.308517196 CORE 106 H H 0.0000 106
H 4.703971683 7.889146205 13.312542434 CORE 107 H H 0.0000 107
H 7.894676240 5.262760405 13.253445716 CORE 108 H H 0.0000 108
H 5.069731103 5.272762993 13.282301252 CORE 109 H H 0.0000 109
H 5.115800003 2.286550503 13.278559675 CORE 110 H H 0.0000 110
H 2.009828899 11.057309108 13.275004062 CORE 111 H H 0.0000 111
H 10.471248712 2.097185418 13.294380003 CORE 112 H H 0.0000 112
H 8.155131806 7.909318986 13.273751146 CORE 113 H H 0.0000 113
H 2.374537929 2.092239555 13.307072794 CORE 114 H H 0.0000 114
end
end

Acetylene adsorbed on Pd_4H_3(100). The energy from VASP is -514.517507 eV.

PBC 11.60000000 11.60000000 20.00000000 90.00000000 90.00000000 90.00000000
Pd 10.782813856 5.016247660 7.193226476 CORE 1 Pd Pd 0.0000 1
Pd 4.983148483 10.816790048 7.193170144 CORE 2 Pd Pd 0.0000 2
Pd 2.085019604 5.016620832 7.193299683 CORE 3 Pd Pd 0.0000 3
Pd 7.884901240 10.816521313 7.193479525 CORE 4 Pd Pd 0.0000 4
Pd 4.983416221 2.117754835 7.193565625 CORE 5 Pd Pd 0.0000 5
Pd 2.083689210 2.116303795 7.193523055 CORE 6 Pd Pd 0.0000 6
Pd 2.083337101 10.816628396 7.193560017 CORE 7 Pd Pd 0.0000 7
Pd 10.783357174 2.116005107 7.193717507 CORE 8 Pd Pd 0.0000 8
Pd 7.884314250 7.916229331 7.194179624 CORE 9 Pd Pd 0.0000 9
Pd 2.084485458 7.917186866 7.193893349 CORE 10 Pd Pd 0.0000 10
Pd 10.783518995 7.917095999 7.193878528 CORE 11 Pd Pd 0.0000 11
Pd 10.784183220 10.816439879 7.193774103 CORE 12 Pd Pd 0.0000 12
Pd 7.883464201 5.016721878 7.194093710 CORE 13 Pd Pd 0.0000 13
Pd 4.984519188 5.017098245 7.194084067 CORE 14 Pd Pd 0.0000 14
Pd 7.884069627 2.117381531 7.193905540 CORE 15 Pd Pd 0.0000 15
Pd 4.984015372 7.916443018 7.194219365 CORE 16 Pd Pd 0.0000 16
Pd 0.634013228 6.466332063 9.009721539 CORE 17 Pd Pd 0.0000 17
Pd 6.433640859 0.666804909 9.009776069 CORE 18 Pd Pd 0.0000 18
Pd 0.633707465 3.566812798 9.009902151 CORE 19 Pd Pd 0.0000 19

Pd	6.434087100	9.367309174	9.010160968	CORE	20	Pd	Pd	0.0000	20
Pd	3.533869947	0.666899228	9.010240576	CORE	21	Pd	Pd	0.0000	21
Pd	0.633969081	9.366447775	9.010826567	CORE	22	Pd	Pd	0.0000	22
Pd	0.633676922	0.666672598	9.010533542	CORE	23	Pd	Pd	0.0000	23
Pd	6.433782001	3.566623726	9.011031260	CORE	24	Pd	Pd	0.0000	24
Pd	9.333604600	0.666638656	9.010546436	CORE	25	Pd	Pd	0.0000	25
Pd	9.334234437	6.466445910	9.010863765	CORE	26	Pd	Pd	0.0000	26
Pd	6.434155127	6.466929211	9.011104041	CORE	27	Pd	Pd	0.0000	27
Pd	3.534124022	9.367105408	9.010616024	CORE	28	Pd	Pd	0.0000	28
Pd	3.533628327	3.566955412	9.010687856	CORE	29	Pd	Pd	0.0000	29
Pd	3.533991674	6.466788159	9.010808806	CORE	30	Pd	Pd	0.0000	30
Pd	9.333852689	3.566664034	9.010894518	CORE	31	Pd	Pd	0.0000	31
Pd	9.333931906	9.366801997	9.011053461	CORE	32	Pd	Pd	0.0000	32
H	9.580275272	3.552800903	6.954668839	CORE	33	H	H	0.0000	33
H	3.295746757	3.547762072	6.962678283	CORE	34	H	H	0.0000	34
H	9.086881997	9.341519786	6.949637981	CORE	35	H	H	0.0000	35
H	0.584442804	9.413295161	7.028496754	CORE	36	H	H	0.0000	36
H	3.745807373	9.375081903	6.966885887	CORE	37	H	H	0.0000	37
H	6.434765974	3.610391075	7.040123954	CORE	38	H	H	0.0000	38
H	9.579247705	6.450013154	6.934030077	CORE	39	H	H	0.0000	39
H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48
H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50
H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.081134813	10.863419900	11.102302902	CORE	57	Pd	Pd	0.0000	57
Pd	2.107594086	7.927834198	11.126669663	CORE	58	Pd	Pd	0.0000	58
Pd	2.090783376	2.139435107	11.171160122	CORE	59	Pd	Pd	0.0000	59
Pd	10.773011036	7.955360469	11.108512282	CORE	60	Pd	Pd	0.0000	60
Pd	4.990625939	7.894663636	11.093065093	CORE	61	Pd	Pd	0.0000	61
Pd	7.871403915	5.050283580	11.113765057	CORE	62	Pd	Pd	0.0000	62
Pd	4.961076933	2.126181366	11.097625081	CORE	63	Pd	Pd	0.0000	63

Pd	7.880421824	2.144916212	11.120833906 CORE	64 Pd Pd	0.0000	64	
Pd	7.881736598	7.906102994	11.171518796 CORE	65 Pd Pd	0.0000	65	
Pd	10.788343734	2.134125998	11.142457103 CORE	66 Pd Pd	0.0000	66	
Pd	4.984756055	5.028517343	11.064009396 CORE	67 Pd Pd	0.0000	67	
Pd	10.767183116	10.878839111	11.093422032 CORE	68 Pd Pd	0.0000	68	
Pd	7.885357055	10.831292996	11.113202754 CORE	69 Pd Pd	0.0000	69	
Pd	4.961152098	10.812756417	11.114550629 CORE	70 Pd Pd	0.0000	70	
Pd	10.769625045	5.055881149	11.106842739 CORE	71 Pd Pd	0.0000	71	
Pd	2.116713962	5.037106280	11.119026148 CORE	72 Pd Pd	0.0000	72	
Pd	3.539338081	9.337383021	13.145526632 CORE	73 Pd Pd	0.0000	73	
Pd	0.629570992	9.421177346	13.111036962 CORE	74 Pd Pd	0.0000	74	
Pd	9.338784288	9.401478289	13.143130096 CORE	75 Pd Pd	0.0000	75	
Pd	6.418152936	3.611130591	13.171769094 CORE	76 Pd Pd	0.0000	76	
Pd	3.558248228	6.409293501	13.191413293 CORE	77 Pd Pd	0.0000	77	
Pd	3.592759616	3.553377433	13.215815366 CORE	78 Pd Pd	0.0000	78	
Pd	9.330202307	3.560784615	13.134275669 CORE	79 Pd Pd	0.0000	79	
Pd	0.607672432	6.540339584	13.091972046 CORE	80 Pd Pd	0.0000	80	
Pd	0.633900068	3.642330898	13.124484549 CORE	81 Pd Pd	0.0000	81	
Pd	6.390846205	0.699351029	13.112808095 CORE	82 Pd Pd	0.0000	82	
Pd	9.351404138	6.488191373	13.121539680 CORE	83 Pd Pd	0.0000	83	
Pd	6.413018022	9.327653227	13.149020971 CORE	84 Pd Pd	0.0000	84	
Pd	0.619480361	0.694416887	13.129870268 CORE	85 Pd Pd	0.0000	85	
Pd	9.336996221	0.682217237	13.130396436 CORE	86 Pd Pd	0.0000	86	
Pd	6.395426018	6.428229334	13.156900663 CORE	87 Pd Pd	0.0000	87	
Pd	3.512304991	0.648233086	13.136634327 CORE	88 Pd Pd	0.0000	88	
H	0.625048745	9.851049108	10.772376512 CORE	89 H H	0.0000	89	
H	9.295292850	3.961933725	10.811562862 CORE	90 H H	0.0000	90	
H	3.460645903	9.725066312	10.809976984 CORE	91 H H	0.0000	91	
H	9.679591142	9.453030771	10.805383629 CORE	92 H H	0.0000	92	
H	3.815008211	3.623722656	10.841846327 CORE	93 H H	0.0000	93	
H	3.319058160	6.500518991	10.866179397 CORE	94 H H	0.0000	94	
H	6.432559942	3.954663796	10.805345563 CORE	95 H H	0.0000	95	
H	6.688021067	0.714513581	11.281106842 CORE	96 H H	0.0000	96	
H	0.636627044	3.320845968	11.285796129 CORE	97 H H	0.0000	97	
H	6.427315931	9.062253528	11.310618755 CORE	98 H H	0.0000	98	
H	1.702650079	5.117281135	13.201429470 CORE	99 H H	0.0000	99	
H	10.819812905	5.274085329	13.265797175 CORE	100 H H	0.0000	100	
H	10.837780854	8.037315368	13.239994013 CORE	101 H H	0.0000	101	
H	8.112658839	10.808715285	13.242624496 CORE	102 H H	0.0000	102	
H	10.745108452	10.896491080	13.247335474 CORE	103 H H	0.0000	103	
H	1.938436233	8.106581801	13.198885533 CORE	104 H H	0.0000	104	
H	4.826791889	10.771356440	13.234895261 CORE	105 H H	0.0000	105	
H	8.141698894	2.122615435	13.254547785 CORE	106 H H	0.0000	106	
H	4.924129379	8.214551792	13.340894002 CORE	107 H H	0.0000	107	

H	8.286905692	5.054901765	13.197087697	CORE	108 H	H	0.0000	108
H	4.906432721	1.808965441	13.296477654	CORE	109 H	H	0.0000	109
H	1.864202111	10.892829045	13.227146005	CORE	110 H	H	0.0000	110
H	10.672031424	2.017440642	13.259515808	CORE	111 H	H	0.0000	111
H	8.082047483	8.055463544	13.242837262	CORE	112 H	H	0.0000	112
H	2.086857321	1.866028890	13.236226586	CORE	113 H	H	0.0000	113
C	5.703068172	5.024592150	14.481312719	CORE	114 C	C	0.0000	114
C	4.315540532	5.000834705	14.489094307	CORE	115 C	C	0.0000	115
H	6.308475889	5.034613882	15.401345274	CORE	116 H	H	0.0000	116
H	3.727999304	4.993157787	15.422027416	CORE	117 H	H	0.0000	117

end

end

TS from acetylene to vinyl on Pd_4H_3(100). The energy from VASP is -513.783855 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	90.00000000		
Pd	10.782813856	5.016247660	7.193226476	CORE	1 Pd	Pd	0.0000	1
Pd	4.983148483	10.816790048	7.193170144	CORE	2 Pd	Pd	0.0000	2
Pd	2.085019604	5.016620832	7.193299683	CORE	3 Pd	Pd	0.0000	3
Pd	7.884901240	10.816521313	7.193479525	CORE	4 Pd	Pd	0.0000	4
Pd	4.983416221	2.117754835	7.193565625	CORE	5 Pd	Pd	0.0000	5
Pd	2.083689210	2.116303795	7.193523055	CORE	6 Pd	Pd	0.0000	6
Pd	2.083337101	10.816628396	7.193560017	CORE	7 Pd	Pd	0.0000	7
Pd	10.783357174	2.116005107	7.193717507	CORE	8 Pd	Pd	0.0000	8
Pd	7.884314250	7.916229331	7.194179624	CORE	9 Pd	Pd	0.0000	9
Pd	2.084485458	7.917186866	7.193893349	CORE	10 Pd	Pd	0.0000	10
Pd	10.783518995	7.917095999	7.193878528	CORE	11 Pd	Pd	0.0000	11
Pd	10.784183220	10.816439879	7.193774103	CORE	12 Pd	Pd	0.0000	12
Pd	7.883464201	5.016721878	7.194093710	CORE	13 Pd	Pd	0.0000	13
Pd	4.984519188	5.017098245	7.194084067	CORE	14 Pd	Pd	0.0000	14
Pd	7.884069627	2.117381531	7.193905540	CORE	15 Pd	Pd	0.0000	15
Pd	4.984015372	7.916443018	7.194219365	CORE	16 Pd	Pd	0.0000	16
Pd	0.634013228	6.466332063	9.009721539	CORE	17 Pd	Pd	0.0000	17
Pd	6.433640859	0.666804909	9.009776069	CORE	18 Pd	Pd	0.0000	18
Pd	0.633707465	3.566812798	9.009902151	CORE	19 Pd	Pd	0.0000	19
Pd	6.434087100	9.367309174	9.010160968	CORE	20 Pd	Pd	0.0000	20
Pd	3.533869947	0.666899228	9.010240576	CORE	21 Pd	Pd	0.0000	21
Pd	0.633969081	9.366447775	9.010826567	CORE	22 Pd	Pd	0.0000	22
Pd	0.633676922	0.666672598	9.010533542	CORE	23 Pd	Pd	0.0000	23
Pd	6.433782001	3.566623726	9.011031260	CORE	24 Pd	Pd	0.0000	24
Pd	9.333604600	0.666638656	9.010546436	CORE	25 Pd	Pd	0.0000	25
Pd	9.334234437	6.466445910	9.010863765	CORE	26 Pd	Pd	0.0000	26
Pd	6.434155127	6.466929211	9.011104041	CORE	27 Pd	Pd	0.0000	27
Pd	3.534124022	9.367105408	9.010616024	CORE	28 Pd	Pd	0.0000	28
Pd	3.533628327	3.566955412	9.010687856	CORE	29 Pd	Pd	0.0000	29

Pd	3.533991674	6.466788159	9.010808806	CORE	30	Pd	Pd	0.0000	30
Pd	9.333852689	3.566664034	9.010894518	CORE	31	Pd	Pd	0.0000	31
Pd	9.333931906	9.366801997	9.011053461	CORE	32	Pd	Pd	0.0000	32
H	9.580275272	3.552800903	6.954668839	CORE	33	H	H	0.0000	33
H	3.295746757	3.547762072	6.962678283	CORE	34	H	H	0.0000	34
H	9.086881997	9.341519786	6.949637981	CORE	35	H	H	0.0000	35
H	0.584442804	9.413295161	7.028496754	CORE	36	H	H	0.0000	36
H	3.745807373	9.375081903	6.966885887	CORE	37	H	H	0.0000	37
H	6.434765974	3.610391075	7.040123954	CORE	38	H	H	0.0000	38
H	9.579247705	6.450013154	6.934030077	CORE	39	H	H	0.0000	39
H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48
H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50
H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.071361921	10.847639268	11.098178291	CORE	57	Pd	Pd	0.0000	57
Pd	2.117774851	7.924359365	11.120999564	CORE	58	Pd	Pd	0.0000	58
Pd	2.078837040	2.130788330	11.171694318	CORE	59	Pd	Pd	0.0000	59
Pd	10.776199367	7.953131497	11.106704544	CORE	60	Pd	Pd	0.0000	60
Pd	5.004513626	7.914532311	11.098475474	CORE	61	Pd	Pd	0.0000	61
Pd	7.874526687	5.029264242	11.126986686	CORE	62	Pd	Pd	0.0000	62
Pd	4.953793851	2.122865484	11.102753964	CORE	63	Pd	Pd	0.0000	63
Pd	7.868849190	2.133797146	11.123229659	CORE	64	Pd	Pd	0.0000	64
Pd	7.888523873	7.891655900	11.176833588	CORE	65	Pd	Pd	0.0000	65
Pd	10.780426665	2.126104524	11.137728268	CORE	66	Pd	Pd	0.0000	66
Pd	4.979168692	5.023380023	11.064651464	CORE	67	Pd	Pd	0.0000	67
Pd	10.775212760	10.858994213	11.097733814	CORE	68	Pd	Pd	0.0000	68
Pd	7.891560944	10.817488682	11.116099758	CORE	69	Pd	Pd	0.0000	69
Pd	4.955601742	10.818230770	11.103331199	CORE	70	Pd	Pd	0.0000	70
Pd	10.780435456	5.041252577	11.120866293	CORE	71	Pd	Pd	0.0000	71
Pd	2.130527754	5.029367615	11.131649472	CORE	72	Pd	Pd	0.0000	72
Pd	3.545578787	9.402871721	13.152061332	CORE	73	Pd	Pd	0.0000	73

Pd	0.642370269	9.398285668	13.120576152	CORE	74	Pd	Pd	0.0000	74
Pd	9.346064978	9.396517534	13.155477546	CORE	75	Pd	Pd	0.0000	75
Pd	6.359227474	3.594839505	13.187211220	CORE	76	Pd	Pd	0.0000	76
Pd	3.570633753	6.549376779	13.187193798	CORE	77	Pd	Pd	0.0000	77
Pd	3.541778505	3.477995311	13.242900863	CORE	78	Pd	Pd	0.0000	78
Pd	9.312881986	3.548028215	13.142323241	CORE	79	Pd	Pd	0.0000	79
Pd	0.627929395	6.539331966	13.072781768	CORE	80	Pd	Pd	0.0000	80
Pd	0.619162098	3.614505213	13.134261492	CORE	81	Pd	Pd	0.0000	81
Pd	6.395871377	0.678903898	13.111473348	CORE	82	Pd	Pd	0.0000	82
Pd	9.374482699	6.494359427	13.124657005	CORE	83	Pd	Pd	0.0000	83
Pd	6.426873760	9.326542636	13.153395575	CORE	84	Pd	Pd	0.0000	84
Pd	0.623788935	0.664513434	13.130126685	CORE	85	Pd	Pd	0.0000	85
Pd	9.337117886	0.680559058	13.135122038	CORE	86	Pd	Pd	0.0000	86
Pd	6.392852414	6.386849041	13.166462002	CORE	87	Pd	Pd	0.0000	87
Pd	3.506414522	0.640086899	13.142420437	CORE	88	Pd	Pd	0.0000	88
H	0.622673330	9.765489364	10.810550442	CORE	89	H	H	0.0000	89
H	9.295156885	3.886660984	10.820263947	CORE	90	H	H	0.0000	90
H	3.443627925	9.688046217	10.811493800	CORE	91	H	H	0.0000	91
H	9.614923077	9.465933135	10.822187513	CORE	92	H	H	0.0000	92
H	3.713336969	3.676652412	10.847698512	CORE	93	H	H	0.0000	93
H	3.381652192	6.459882684	10.875712554	CORE	94	H	H	0.0000	94
H	6.421252255	3.922643369	10.808598388	CORE	95	H	H	0.0000	95
H	6.642857108	0.705864228	11.277428340	CORE	96	H	H	0.0000	96
H	0.630584190	3.398343121	11.360949802	CORE	97	H	H	0.0000	97
H	6.471872906	9.106720541	11.338672518	CORE	98	H	H	0.0000	98
H	2.936698774	5.027638974	13.798514440	CORE	99	H	H	0.0000	99
H	10.944647338	5.136709050	13.233009965	CORE	100	H	H	0.0000	100
H	10.922264823	7.987987650	13.284776915	CORE	101	H	H	0.0000	101
H	8.082038513	10.787038670	13.242627940	CORE	102	H	H	0.0000	102
H	10.807272090	10.942914200	13.249000926	CORE	103	H	H	0.0000	103
H	1.871932207	7.994118215	13.231314249	CORE	104	H	H	0.0000	104
H	4.740560962	10.832484834	13.339493878	CORE	105	H	H	0.0000	105
H	8.129646282	2.125650026	13.261858923	CORE	106	H	H	0.0000	106
H	4.929533565	8.256354893	13.310498615	CORE	107	H	H	0.0000	107
H	8.204978215	5.129771515	13.096063608	CORE	108	H	H	0.0000	108
H	4.935759645	1.803365183	13.266187008	CORE	109	H	H	0.0000	109
H	1.966141420	10.901933017	13.263297357	CORE	110	H	H	0.0000	110
H	10.553523172	2.057539005	13.308639401	CORE	111	H	H	0.0000	111
H	8.212792059	7.965927940	13.281283852	CORE	112	H	H	0.0000	112
H	2.024419569	1.974617572	13.229326700	CORE	113	H	H	0.0000	113
C	5.586282545	5.007956736	14.470342474	CORE	114	C	C	0.0000	114
C	4.200741053	5.041805761	14.606355170	CORE	115	C	C	0.0000	115
H	6.197543645	4.996657094	15.391170670	CORE	116	H	H	0.0000	116
H	3.739561002	5.067426737	15.600332571	CORE	117	H	H	0.0000	117

end

end

Vinyl adsorbed on Pd_4H_3(100). The energy from VASP is -517.876385 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	90.00000000	
Pd	10.782813856	5.016247660	7.193226476 CORE	1 Pd Pd	0.0000	1	
Pd	4.983148483	10.816790048	7.193170144 CORE	2 Pd Pd	0.0000	2	
Pd	2.085019604	5.016620832	7.193299683 CORE	3 Pd Pd	0.0000	3	
Pd	7.884901240	10.816521313	7.193479525 CORE	4 Pd Pd	0.0000	4	
Pd	4.983416221	2.117754835	7.193565625 CORE	5 Pd Pd	0.0000	5	
Pd	2.083689210	2.116303795	7.193523055 CORE	6 Pd Pd	0.0000	6	
Pd	2.083337101	10.816628396	7.193560017 CORE	7 Pd Pd	0.0000	7	
Pd	10.783357174	2.116005107	7.193717507 CORE	8 Pd Pd	0.0000	8	
Pd	7.884314250	7.916229331	7.194179624 CORE	9 Pd Pd	0.0000	9	
Pd	2.084485458	7.917186866	7.193893349 CORE	10 Pd Pd	0.0000	10	
Pd	10.783518995	7.917095999	7.193878528 CORE	11 Pd Pd	0.0000	11	
Pd	10.784183220	10.816439879	7.193774103 CORE	12 Pd Pd	0.0000	12	
Pd	7.883464201	5.016721878	7.194093710 CORE	13 Pd Pd	0.0000	13	
Pd	4.984519188	5.017098245	7.194084067 CORE	14 Pd Pd	0.0000	14	
Pd	7.884069627	2.117381531	7.193905540 CORE	15 Pd Pd	0.0000	15	
Pd	4.984015372	7.916443018	7.194219365 CORE	16 Pd Pd	0.0000	16	
Pd	0.634013228	6.466332063	9.009721539 CORE	17 Pd Pd	0.0000	17	
Pd	6.433640859	0.666804909	9.009776069 CORE	18 Pd Pd	0.0000	18	
Pd	0.633707465	3.566812798	9.009902151 CORE	19 Pd Pd	0.0000	19	
Pd	6.434087100	9.367309174	9.010160968 CORE	20 Pd Pd	0.0000	20	
Pd	3.533869947	0.666899228	9.010240576 CORE	21 Pd Pd	0.0000	21	
Pd	0.633969081	9.366447775	9.010826567 CORE	22 Pd Pd	0.0000	22	
Pd	0.633676922	0.666672598	9.010533542 CORE	23 Pd Pd	0.0000	23	
Pd	6.433782001	3.566623726	9.011031260 CORE	24 Pd Pd	0.0000	24	
Pd	9.333604600	0.666638656	9.010546436 CORE	25 Pd Pd	0.0000	25	
Pd	9.334234437	6.466445910	9.010863765 CORE	26 Pd Pd	0.0000	26	
Pd	6.434155127	6.466929211	9.011104041 CORE	27 Pd Pd	0.0000	27	
Pd	3.534124022	9.367105408	9.010616024 CORE	28 Pd Pd	0.0000	28	
Pd	3.533628327	3.566955412	9.010687856 CORE	29 Pd Pd	0.0000	29	
Pd	3.533991674	6.466788159	9.010808806 CORE	30 Pd Pd	0.0000	30	
Pd	9.333852689	3.566664034	9.010894518 CORE	31 Pd Pd	0.0000	31	
Pd	9.333931906	9.366801997	9.011053461 CORE	32 Pd Pd	0.0000	32	
H	9.580275272	3.552800903	6.954668839 CORE	33 H H	0.0000	33	
H	3.295746757	3.547762072	6.962678283 CORE	34 H H	0.0000	34	
H	9.086881997	9.341519786	6.949637981 CORE	35 H H	0.0000	35	
H	0.584442804	9.413295161	7.028496754 CORE	36 H H	0.0000	36	
H	3.745807373	9.375081903	6.966885887 CORE	37 H H	0.0000	37	
H	6.434765974	3.610391075	7.040123954 CORE	38 H H	0.0000	38	
H	9.579247705	6.450013154	6.934030077 CORE	39 H H	0.0000	39	

H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48
H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50
H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.082803537	10.846898669	11.102539606	CORE	57	Pd	Pd	0.0000	57
Pd	2.116597757	7.913748458	11.134696882	CORE	58	Pd	Pd	0.0000	58
Pd	2.084295154	2.114446711	11.150113735	CORE	59	Pd	Pd	0.0000	59
Pd	10.783622423	7.955484626	11.108682659	CORE	60	Pd	Pd	0.0000	60
Pd	4.990117830	7.913248840	11.091594558	CORE	61	Pd	Pd	0.0000	61
Pd	7.858951778	5.052566303	11.125651290	CORE	62	Pd	Pd	0.0000	62
Pd	4.964262725	2.137584967	11.102376397	CORE	63	Pd	Pd	0.0000	63
Pd	7.876997548	2.156164659	11.110136000	CORE	64	Pd	Pd	0.0000	64
Pd	7.886604851	7.914601826	11.168003987	CORE	65	Pd	Pd	0.0000	65
Pd	10.782232043	2.127440616	11.147188470	CORE	66	Pd	Pd	0.0000	66
Pd	4.973168123	5.038154202	11.089919381	CORE	67	Pd	Pd	0.0000	67
Pd	10.776928096	10.875105449	11.097613247	CORE	68	Pd	Pd	0.0000	68
Pd	7.889062237	10.846838306	11.121740260	CORE	69	Pd	Pd	0.0000	69
Pd	4.969592104	10.830550206	11.116241492	CORE	70	Pd	Pd	0.0000	70
Pd	10.757854922	5.047695615	11.110651974	CORE	71	Pd	Pd	0.0000	71
Pd	2.107977257	5.026265525	11.121483699	CORE	72	Pd	Pd	0.0000	72
Pd	3.555244254	9.323521781	13.152082924	CORE	73	Pd	Pd	0.0000	73
Pd	0.646839588	9.429465376	13.123689582	CORE	74	Pd	Pd	0.0000	74
Pd	9.352014622	9.374966086	13.142752458	CORE	75	Pd	Pd	0.0000	75
Pd	6.346684195	3.701676176	13.234711265	CORE	76	Pd	Pd	0.0000	76
Pd	3.565978972	6.384846944	13.205838129	CORE	77	Pd	Pd	0.0000	77
Pd	3.524120574	3.436169564	13.155679528	CORE	78	Pd	Pd	0.0000	78
Pd	9.288383599	3.527154509	13.140447464	CORE	79	Pd	Pd	0.0000	79
Pd	0.624951130	6.546026677	13.099649228	CORE	80	Pd	Pd	0.0000	80
Pd	0.607607974	3.662571107	13.129647691	CORE	81	Pd	Pd	0.0000	81
Pd	6.429338067	0.795376512	13.122720648	CORE	82	Pd	Pd	0.0000	82
Pd	9.359763633	6.478815919	13.117237399	CORE	83	Pd	Pd	0.0000	83

Pd 6.426374806 9.388643644 13.142416187 CORE 84 Pd Pd 0.0000 84
Pd 0.628715370 0.698807167 13.141158862 CORE 85 Pd Pd 0.0000 85
Pd 9.355299251 0.659878328 13.135610373 CORE 86 Pd Pd 0.0000 86
Pd 6.363750456 6.485038839 13.152392571 CORE 87 Pd Pd 0.0000 87
Pd 3.521842183 0.593363605 13.140408968 CORE 88 Pd Pd 0.0000 88
H 0.625341362 9.827041512 10.782955770 CORE 89 H H 0.0000 89
H 9.280137302 3.942095056 10.809780835 CORE 90 H H 0.0000 90
H 3.473523800 9.734580256 10.806740066 CORE 91 H H 0.0000 91
H 9.679720045 9.461657970 10.808589037 CORE 92 H H 0.0000 92
H 3.785424709 3.668809082 10.861657261 CORE 93 H H 0.0000 93
H 3.312800313 6.485528794 10.885701554 CORE 94 H H 0.0000 94
H 6.423721037 3.972274830 10.783535920 CORE 95 H H 0.0000 95
H 6.640806494 0.747732396 11.279255574 CORE 96 H H 0.0000 96
H 0.635831503 3.273389040 11.303220467 CORE 97 H H 0.0000 97
H 6.440038973 9.069571388 11.301524966 CORE 98 H H 0.0000 98
H 10.888814332 5.221957384 13.257341836 CORE 99 H H 0.0000 99
H 10.855981064 8.084934401 13.266060260 CORE 100 H H 0.0000 100
H 8.109468877 10.775125618 13.230278356 CORE 101 H H 0.0000 101
H 10.859509321 10.979550533 13.272184321 CORE 102 H H 0.0000 102
H 1.907588680 8.083660660 13.215417974 CORE 103 H H 0.0000 103
H 4.766560858 10.722247436 13.288271628 CORE 104 H H 0.0000 104
H 8.110474831 2.022285761 13.286730502 CORE 105 H H 0.0000 105
H 4.997592074 8.264045316 13.369480509 CORE 106 H H 0.0000 106
H 8.291565481 5.046950358 13.129216031 CORE 107 H H 0.0000 107
H 4.847054932 1.855634669 13.299675254 CORE 108 H H 0.0000 108
H 1.902810795 10.919113185 13.262444210 CORE 109 H H 0.0000 109
H 10.657259409 2.010314147 13.276018305 CORE 110 H H 0.0000 110
H 8.170642052 7.987958383 13.263992191 CORE 111 H H 0.0000 111
H 2.273783471 2.005291669 13.290128668 CORE 112 H H 0.0000 112
H 1.741450452 5.121908630 13.207520308 CORE 113 H H 0.0000 113
C 5.773420359 5.122378801 14.540115519 CORE 114 C C 0.0000 114
C 4.373782054 5.277544044 14.824772714 CORE 115 C C 0.0000 115
H 6.516041431 5.244123458 15.349820194 CORE 116 H H 0.0000 116
H 4.122421919 5.948029640 15.664997876 CORE 117 H H 0.0000 117
H 3.770871101 4.329557883 14.950148793 CORE 118 H H 0.0000 118
end
end

TS from vinyl to ethene on Pd_4H_3(100). The energy from VASP is -517.215276 eV.

PBC 11.60000000 11.60000000 20.00000000 90.00000000 90.00000000 90.00000000
Pd 10.782813856 5.016247660 7.193226476 CORE 1 Pd Pd 0.0000 1
Pd 4.983148483 10.816790048 7.193170144 CORE 2 Pd Pd 0.0000 2
Pd 2.085019604 5.016620832 7.193299683 CORE 3 Pd Pd 0.0000 3
Pd 7.884901240 10.816521313 7.193479525 CORE 4 Pd Pd 0.0000 4

Pd	4.983416221	2.117754835	7.193565625	CORE	5	Pd	Pd	0.0000	5
Pd	2.083689210	2.116303795	7.193523055	CORE	6	Pd	Pd	0.0000	6
Pd	2.083337101	10.816628396	7.193560017	CORE	7	Pd	Pd	0.0000	7
Pd	10.783357174	2.116005107	7.193717507	CORE	8	Pd	Pd	0.0000	8
Pd	7.884314250	7.916229331	7.194179624	CORE	9	Pd	Pd	0.0000	9
Pd	2.084485458	7.917186866	7.193893349	CORE	10	Pd	Pd	0.0000	10
Pd	10.783518995	7.917095999	7.193878528	CORE	11	Pd	Pd	0.0000	11
Pd	10.784183220	10.816439879	7.193774103	CORE	12	Pd	Pd	0.0000	12
Pd	7.883464201	5.016721878	7.194093710	CORE	13	Pd	Pd	0.0000	13
Pd	4.984519188	5.017098245	7.194084067	CORE	14	Pd	Pd	0.0000	14
Pd	7.884069627	2.117381531	7.193905540	CORE	15	Pd	Pd	0.0000	15
Pd	4.984015372	7.916443018	7.194219365	CORE	16	Pd	Pd	0.0000	16
Pd	0.634013228	6.466332063	9.009721539	CORE	17	Pd	Pd	0.0000	17
Pd	6.433640859	0.666804909	9.009776069	CORE	18	Pd	Pd	0.0000	18
Pd	0.633707465	3.566812798	9.009902151	CORE	19	Pd	Pd	0.0000	19
Pd	6.434087100	9.367309174	9.010160968	CORE	20	Pd	Pd	0.0000	20
Pd	3.533869947	0.666899228	9.010240576	CORE	21	Pd	Pd	0.0000	21
Pd	0.633969081	9.366447775	9.010826567	CORE	22	Pd	Pd	0.0000	22
Pd	0.633676922	0.666672598	9.010533542	CORE	23	Pd	Pd	0.0000	23
Pd	6.433782001	3.566623726	9.011031260	CORE	24	Pd	Pd	0.0000	24
Pd	9.333604600	0.666638656	9.010546436	CORE	25	Pd	Pd	0.0000	25
Pd	9.334234437	6.466445910	9.010863765	CORE	26	Pd	Pd	0.0000	26
Pd	6.434155127	6.466929211	9.011104041	CORE	27	Pd	Pd	0.0000	27
Pd	3.534124022	9.367105408	9.010616024	CORE	28	Pd	Pd	0.0000	28
Pd	3.533628327	3.566955412	9.010687856	CORE	29	Pd	Pd	0.0000	29
Pd	3.533991674	6.466788159	9.010808806	CORE	30	Pd	Pd	0.0000	30
Pd	9.333852689	3.566664034	9.010894518	CORE	31	Pd	Pd	0.0000	31
Pd	9.333931906	9.366801997	9.011053461	CORE	32	Pd	Pd	0.0000	32
H	9.580275272	3.552800903	6.954668839	CORE	33	H	H	0.0000	33
H	3.295746757	3.547762072	6.962678283	CORE	34	H	H	0.0000	34
H	9.086881997	9.341519786	6.949637981	CORE	35	H	H	0.0000	35
H	0.584442804	9.413295161	7.028496754	CORE	36	H	H	0.0000	36
H	3.745807373	9.375081903	6.966885887	CORE	37	H	H	0.0000	37
H	6.434765974	3.610391075	7.040123954	CORE	38	H	H	0.0000	38
H	9.579247705	6.450013154	6.934030077	CORE	39	H	H	0.0000	39
H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48

H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50
H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.070329196	10.808739463	11.106076730	CORE	57	Pd	Pd	0.0000	57
Pd	2.124321743	7.889405536	11.145439103	CORE	58	Pd	Pd	0.0000	58
Pd	2.090816835	2.086597604	11.140017181	CORE	59	Pd	Pd	0.0000	59
Pd	10.787997339	7.950893190	11.107585795	CORE	60	Pd	Pd	0.0000	60
Pd	4.986831429	7.900963347	11.089557462	CORE	61	Pd	Pd	0.0000	61
Pd	7.894989428	5.057521220	11.091724835	CORE	62	Pd	Pd	0.0000	62
Pd	4.982897536	2.114805752	11.114955553	CORE	63	Pd	Pd	0.0000	63
Pd	7.889279143	2.162235158	11.137096215	CORE	64	Pd	Pd	0.0000	64
Pd	7.899012883	7.923377689	11.163753468	CORE	65	Pd	Pd	0.0000	65
Pd	10.799116970	2.118828654	11.144723990	CORE	66	Pd	Pd	0.0000	66
Pd	5.023019771	5.005291852	11.110086405	CORE	67	Pd	Pd	0.0000	67
Pd	10.793983035	10.853250931	11.096324719	CORE	68	Pd	Pd	0.0000	68
Pd	7.898667505	10.833438526	11.121910418	CORE	69	Pd	Pd	0.0000	69
Pd	4.955259509	10.810372047	11.112354138	CORE	70	Pd	Pd	0.0000	70
Pd	10.777281007	5.045117921	11.119959063	CORE	71	Pd	Pd	0.0000	71
Pd	2.150564259	5.019490900	11.140026663	CORE	72	Pd	Pd	0.0000	72
Pd	3.522485738	9.311789302	13.176130314	CORE	73	Pd	Pd	0.0000	73
Pd	0.623396466	9.381565560	13.150419614	CORE	74	Pd	Pd	0.0000	74
Pd	9.340461955	9.393935486	13.166463440	CORE	75	Pd	Pd	0.0000	75
Pd	6.461037278	3.680323906	13.298639034	CORE	76	Pd	Pd	0.0000	76
Pd	3.665716542	6.341454998	13.268330343	CORE	77	Pd	Pd	0.0000	77
Pd	3.527231518	3.405074045	13.138025086	CORE	78	Pd	Pd	0.0000	78
Pd	9.350033374	3.577320213	13.133391856	CORE	79	Pd	Pd	0.0000	79
Pd	0.658048322	6.501362553	13.106611672	CORE	80	Pd	Pd	0.0000	80
Pd	0.647563456	3.600137764	13.126285620	CORE	81	Pd	Pd	0.0000	81
Pd	6.435430306	0.716006919	13.131715353	CORE	82	Pd	Pd	0.0000	82
Pd	9.384654655	6.507526005	13.096989269	CORE	83	Pd	Pd	0.0000	83
Pd	6.382709393	9.379261887	13.137105242	CORE	84	Pd	Pd	0.0000	84
Pd	0.662186238	0.658336802	13.150945941	CORE	85	Pd	Pd	0.0000	85
Pd	9.391746893	0.652330209	13.135124845	CORE	86	Pd	Pd	0.0000	86
Pd	6.441164018	6.509990773	13.086094460	CORE	87	Pd	Pd	0.0000	87
Pd	3.520701840	0.568110625	13.147838474	CORE	88	Pd	Pd	0.0000	88
H	0.609702362	9.724181021	10.819368894	CORE	89	H	H	0.0000	89
H	9.268316527	3.857318304	11.302144312	CORE	90	H	H	0.0000	90
H	3.450011843	9.670122521	10.809502809	CORE	91	H	H	0.0000	91
H	9.562122745	9.558326932	10.810909693	CORE	92	H	H	0.0000	92

H	3.751066904	3.701782924	10.849928032 CORE	93 H	H	0.0000	93
H	3.383186147	6.490268087	10.862576635 CORE	94 H	H	0.0000	94
H	6.489511181	3.924644689	10.848532110 CORE	95 H	H	0.0000	95
H	6.502138269	0.844575882	11.348752554 CORE	96 H	H	0.0000	96
H	0.646556901	3.304521311	11.314289965 CORE	97 H	H	0.0000	97
H	6.452095009	9.143017025	11.310447992 CORE	98 H	H	0.0000	98
H	10.773678248	5.222886754	13.264656701 CORE	99 H	H	0.0000	99
H	10.896716594	8.061212738	13.301995369 CORE	100 H	H	0.0000	100
H	8.087457669	10.836721187	13.238353955 CORE	101 H	H	0.0000	101
H	10.694238087	10.780690269	13.342161577 CORE	102 H	H	0.0000	102
H	1.856923035	8.016689599	13.250221412 CORE	103 H	H	0.0000	103
H	4.818276861	10.632922684	13.336386867 CORE	104 H	H	0.0000	104
H	8.264687416	2.095506876	13.193354973 CORE	105 H	H	0.0000	105
H	4.930528370	8.191281040	13.333123491 CORE	106 H	H	0.0000	106
H	6.545483741	3.454877493	14.853991549 CORE	107 H	H	0.0000	107
H	4.701883949	1.946239146	13.278713636 CORE	108 H	H	0.0000	108
H	2.026904845	10.842980314	13.291618515 CORE	109 H	H	0.0000	109
H	10.877649963	1.877637506	13.292658726 CORE	110 H	H	0.0000	110
H	8.175750212	7.913110623	13.283102950 CORE	111 H	H	0.0000	111
H	2.199976833	1.919830493	13.310528502 CORE	112 H	H	0.0000	112
H	1.810387031	5.056593142	13.197839572 CORE	113 H	H	0.0000	113
C	6.026721946	5.200739177	14.620809683 CORE	114 C	C	0.0000	114
C	4.646095426	5.449464212	14.969009710 CORE	115 C	C	0.0000	115
H	6.794365965	5.551454652	15.328836637 CORE	116 H	H	0.0000	116
H	4.482939260	6.213181858	15.743749013 CORE	117 H	H	0.0000	117
H	3.990915858	4.568381038	15.105813788 CORE	118 H	H	0.0000	118

end

end

Ethene adsorbed on Pd_4H_3(100). The Energy from VASP is -525.817539 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	90.00000000		
Pd	10.782813856	5.016247660	7.193226476 CORE	1 Pd	Pd	0.0000	1
Pd	4.983148483	10.816790048	7.193170144 CORE	2 Pd	Pd	0.0000	2
Pd	2.085019604	5.016620832	7.193299683 CORE	3 Pd	Pd	0.0000	3
Pd	7.884901240	10.816521313	7.193479525 CORE	4 Pd	Pd	0.0000	4
Pd	4.983416221	2.117754835	7.193565625 CORE	5 Pd	Pd	0.0000	5
Pd	2.083689210	2.116303795	7.193523055 CORE	6 Pd	Pd	0.0000	6
Pd	2.083337101	10.816628396	7.193560017 CORE	7 Pd	Pd	0.0000	7
Pd	10.783357174	2.116005107	7.193717507 CORE	8 Pd	Pd	0.0000	8
Pd	7.884314250	7.916229331	7.194179624 CORE	9 Pd	Pd	0.0000	9
Pd	2.084485458	7.917186866	7.193893349 CORE	10 Pd	Pd	0.0000	10
Pd	10.783518995	7.917095999	7.193878528 CORE	11 Pd	Pd	0.0000	11
Pd	10.784183220	10.816439879	7.193774103 CORE	12 Pd	Pd	0.0000	12
Pd	7.883464201	5.016721878	7.194093710 CORE	13 Pd	Pd	0.0000	13

Pd	4.984519188	5.017098245	7.194084067	CORE	14	Pd	Pd	0.0000	14
Pd	7.884069627	2.117381531	7.193905540	CORE	15	Pd	Pd	0.0000	15
Pd	4.984015372	7.916443018	7.194219365	CORE	16	Pd	Pd	0.0000	16
Pd	0.634013228	6.466332063	9.009721539	CORE	17	Pd	Pd	0.0000	17
Pd	6.433640859	0.666804909	9.009776069	CORE	18	Pd	Pd	0.0000	18
Pd	0.633707465	3.566812798	9.009902151	CORE	19	Pd	Pd	0.0000	19
Pd	6.434087100	9.367309174	9.010160968	CORE	20	Pd	Pd	0.0000	20
Pd	3.533869947	0.666899228	9.010240576	CORE	21	Pd	Pd	0.0000	21
Pd	0.633969081	9.366447775	9.010826567	CORE	22	Pd	Pd	0.0000	22
Pd	0.633676922	0.666672598	9.010533542	CORE	23	Pd	Pd	0.0000	23
Pd	6.433782001	3.566623726	9.011031260	CORE	24	Pd	Pd	0.0000	24
Pd	9.333604600	0.666638656	9.010546436	CORE	25	Pd	Pd	0.0000	25
Pd	9.334234437	6.466445910	9.010863765	CORE	26	Pd	Pd	0.0000	26
Pd	6.434155127	6.466929211	9.011104041	CORE	27	Pd	Pd	0.0000	27
Pd	3.534124022	9.367105408	9.010616024	CORE	28	Pd	Pd	0.0000	28
Pd	3.533628327	3.566955412	9.010687856	CORE	29	Pd	Pd	0.0000	29
Pd	3.533991674	6.466788159	9.010808806	CORE	30	Pd	Pd	0.0000	30
Pd	9.333852689	3.566664034	9.010894518	CORE	31	Pd	Pd	0.0000	31
Pd	9.333931906	9.366801997	9.011053461	CORE	32	Pd	Pd	0.0000	32
H	9.580275272	3.552800903	6.954668839	CORE	33	H	H	0.0000	33
H	3.295746757	3.547762072	6.962678283	CORE	34	H	H	0.0000	34
H	9.086881997	9.341519786	6.949637981	CORE	35	H	H	0.0000	35
H	0.584442804	9.413295161	7.028496754	CORE	36	H	H	0.0000	36
H	3.745807373	9.375081903	6.966885887	CORE	37	H	H	0.0000	37
H	6.434765974	3.610391075	7.040123954	CORE	38	H	H	0.0000	38
H	9.579247705	6.450013154	6.934030077	CORE	39	H	H	0.0000	39
H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48
H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50
H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.067894678	10.866201467	11.093481603	CORE	57	Pd	Pd	0.0000	57

Pd	2.113646388	7.942654757	11.094795908	CORE	58	Pd	Pd	0.0000	58
Pd	2.063727719	2.121841637	11.149572050	CORE	59	Pd	Pd	0.0000	59
Pd	10.785977335	7.948446849	11.112689297	CORE	60	Pd	Pd	0.0000	60
Pd	5.026378912	7.870382073	11.141672557	CORE	61	Pd	Pd	0.0000	61
Pd	7.872332727	5.069188795	11.136635663	CORE	62	Pd	Pd	0.0000	62
Pd	4.942168962	2.126006863	11.097153863	CORE	63	Pd	Pd	0.0000	63
Pd	7.870623956	2.137117764	11.096471066	CORE	64	Pd	Pd	0.0000	64
Pd	7.896913861	7.893594539	11.173344811	CORE	65	Pd	Pd	0.0000	65
Pd	10.768391060	2.127299445	11.148894328	CORE	66	Pd	Pd	0.0000	66
Pd	5.010981834	5.035245814	11.119961924	CORE	67	Pd	Pd	0.0000	67
Pd	10.770092435	10.871453183	11.098998047	CORE	68	Pd	Pd	0.0000	68
Pd	7.895779029	10.827487863	11.100799657	CORE	69	Pd	Pd	0.0000	69
Pd	4.951951328	10.809611063	11.109074836	CORE	70	Pd	Pd	0.0000	70
Pd	10.770157991	5.050068897	11.105186205	CORE	71	Pd	Pd	0.0000	71
Pd	2.110184392	5.028250877	11.105670995	CORE	72	Pd	Pd	0.0000	72
Pd	3.548021427	9.356228189	13.120303234	CORE	73	Pd	Pd	0.0000	73
Pd	0.648846017	9.402451555	13.109639918	CORE	74	Pd	Pd	0.0000	74
Pd	9.347467275	9.390081018	13.139495684	CORE	75	Pd	Pd	0.0000	75
Pd	6.417206587	3.536832554	13.124973624	CORE	76	Pd	Pd	0.0000	76
Pd	3.542360825	6.436426739	13.132326374	CORE	77	Pd	Pd	0.0000	77
Pd	3.547588104	3.521306496	13.148136991	CORE	78	Pd	Pd	0.0000	78
Pd	9.303138243	3.545671431	13.127832444	CORE	79	Pd	Pd	0.0000	79
Pd	0.653688270	6.534386464	13.089109625	CORE	80	Pd	Pd	0.0000	80
Pd	0.633801866	3.667192387	13.132792312	CORE	81	Pd	Pd	0.0000	81
Pd	6.356047409	0.686541882	13.104902766	CORE	82	Pd	Pd	0.0000	82
Pd	9.409876727	6.467611576	13.132609633	CORE	83	Pd	Pd	0.0000	83
Pd	6.478738156	9.409687093	13.145024519	CORE	84	Pd	Pd	0.0000	84
Pd	0.602128504	0.696462643	13.136760132	CORE	85	Pd	Pd	0.0000	85
Pd	9.318246424	0.668557007	13.132953466	CORE	86	Pd	Pd	0.0000	86
Pd	6.490851931	6.439482593	13.378305689	CORE	87	Pd	Pd	0.0000	87
Pd	3.467354708	0.631526561	13.133010691	CORE	88	Pd	Pd	0.0000	88
H	0.621595430	9.824006474	10.803133301	CORE	89	H	H	0.0000	89
H	9.313980347	3.945568894	10.811463004	CORE	90	H	H	0.0000	90
H	3.450194803	9.731405501	10.810898674	CORE	91	H	H	0.0000	91
H	9.677274362	9.440744716	10.817163663	CORE	92	H	H	0.0000	92
H	3.825819113	3.616409780	10.822982895	CORE	93	H	H	0.0000	93
H	3.270035904	6.483822318	10.864443761	CORE	94	H	H	0.0000	94
H	6.461014659	3.968837152	10.820796644	CORE	95	H	H	0.0000	95
H	6.742869080	0.683143429	11.315145001	CORE	96	H	H	0.0000	96
H	0.608186891	3.285380220	11.344777120	CORE	97	H	H	0.0000	97
H	6.443001684	9.007936144	11.340297927	CORE	98	H	H	0.0000	98
H	10.879146555	5.284090095	13.280480360	CORE	99	H	H	0.0000	99
H	10.955045562	7.947441400	13.258691788	CORE	100	H	H	0.0000	100
H	8.036305057	10.687449539	13.290105863	CORE	101	H	H	0.0000	101

H	10.751961967	11.070137700	13.260248949	CORE	102 H	H	0.0000	102
H	2.017378595	8.138112344	13.257029621	CORE	103 H	H	0.0000	103
H	4.909502223	10.865483177	13.239833584	CORE	104 H	H	0.0000	104
H	7.861001092	2.373317520	13.318240426	CORE	105 H	H	0.0000	105
H	4.639731837	7.943209619	13.177581531	CORE	106 H	H	0.0000	106
H	5.073326900	2.274538409	13.311384947	CORE	107 H	H	0.0000	107
H	1.980048852	11.030364019	13.258655406	CORE	108 H	H	0.0000	108
H	10.553229341	2.036815953	13.287988873	CORE	109 H	H	0.0000	109
H	7.979749761	8.225190279	13.267148242	CORE	110 H	H	0.0000	110
H	2.175972198	1.952182429	13.277461872	CORE	111 H	H	0.0000	111
H	1.960662899	5.083895594	13.240410538	CORE	112 H	H	0.0000	112
H	8.176796048	5.064933023	13.093235383	CORE	113 H	H	0.0000	113
H	4.706816446	4.914605214	13.171756756	CORE	114 H	H	0.0000	114
C	7.041818257	6.056742062	15.519115227	CORE	115 C	C	0.0000	115
C	5.865830895	6.788698122	15.513636825	CORE	116 C	C	0.0000	116
H	8.004923760	6.545131541	15.681178144	CORE	117 H	H	0.0000	117
H	5.873656651	7.869392181	15.666506783	CORE	118 H	H	0.0000	118
H	4.900373427	6.295303152	15.643923203	CORE	119 H	H	0.0000	119
H	7.027247260	4.973318758	15.651173339	CORE	120 H	H	0.0000	120

end

end

TS from ethene to ethyl on Pd_4H_3(100). The energy from VASP is -525.212566 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	90.00000000		
Pd	10.782813856	5.016247660	7.193226476	CORE	1 Pd	Pd	0.0000	1
Pd	4.983148483	10.816790048	7.193170144	CORE	2 Pd	Pd	0.0000	2
Pd	2.085019604	5.016620832	7.193299683	CORE	3 Pd	Pd	0.0000	3
Pd	7.884901240	10.816521313	7.193479525	CORE	4 Pd	Pd	0.0000	4
Pd	4.983416221	2.117754835	7.193565625	CORE	5 Pd	Pd	0.0000	5
Pd	2.083689210	2.116303795	7.193523055	CORE	6 Pd	Pd	0.0000	6
Pd	2.083337101	10.816628396	7.193560017	CORE	7 Pd	Pd	0.0000	7
Pd	10.783357174	2.116005107	7.193717507	CORE	8 Pd	Pd	0.0000	8
Pd	7.884314250	7.916229331	7.194179624	CORE	9 Pd	Pd	0.0000	9
Pd	2.084485458	7.917186866	7.193893349	CORE	10 Pd	Pd	0.0000	10
Pd	10.783518995	7.917095999	7.193878528	CORE	11 Pd	Pd	0.0000	11
Pd	10.784183220	10.816439879	7.193774103	CORE	12 Pd	Pd	0.0000	12
Pd	7.883464201	5.016721878	7.194093710	CORE	13 Pd	Pd	0.0000	13
Pd	4.984519188	5.017098245	7.194084067	CORE	14 Pd	Pd	0.0000	14
Pd	7.884069627	2.117381531	7.193905540	CORE	15 Pd	Pd	0.0000	15
Pd	4.984015372	7.916443018	7.194219365	CORE	16 Pd	Pd	0.0000	16
Pd	0.634013228	6.466332063	9.009721539	CORE	17 Pd	Pd	0.0000	17
Pd	6.433640859	0.666804909	9.009776069	CORE	18 Pd	Pd	0.0000	18
Pd	0.633707465	3.566812798	9.009902151	CORE	19 Pd	Pd	0.0000	19
Pd	6.434087100	9.367309174	9.010160968	CORE	20 Pd	Pd	0.0000	20

Pd	3.533869947	0.666899228	9.010240576	CORE	21	Pd	Pd	0.0000	21
Pd	0.633969081	9.366447775	9.010826567	CORE	22	Pd	Pd	0.0000	22
Pd	0.633676922	0.666672598	9.010533542	CORE	23	Pd	Pd	0.0000	23
Pd	6.433782001	3.566623726	9.011031260	CORE	24	Pd	Pd	0.0000	24
Pd	9.333604600	0.666638656	9.010546436	CORE	25	Pd	Pd	0.0000	25
Pd	9.334234437	6.466445910	9.010863765	CORE	26	Pd	Pd	0.0000	26
Pd	6.434155127	6.466929211	9.011104041	CORE	27	Pd	Pd	0.0000	27
Pd	3.534124022	9.367105408	9.010616024	CORE	28	Pd	Pd	0.0000	28
Pd	3.533628327	3.566955412	9.010687856	CORE	29	Pd	Pd	0.0000	29
Pd	3.533991674	6.466788159	9.010808806	CORE	30	Pd	Pd	0.0000	30
Pd	9.333852689	3.566664034	9.010894518	CORE	31	Pd	Pd	0.0000	31
Pd	9.333931906	9.366801997	9.011053461	CORE	32	Pd	Pd	0.0000	32
H	9.580275272	3.552800903	6.954668839	CORE	33	H	H	0.0000	33
H	3.295746757	3.547762072	6.962678283	CORE	34	H	H	0.0000	34
H	9.086881997	9.341519786	6.949637981	CORE	35	H	H	0.0000	35
H	0.584442804	9.413295161	7.028496754	CORE	36	H	H	0.0000	36
H	3.745807373	9.375081903	6.966885887	CORE	37	H	H	0.0000	37
H	6.434765974	3.610391075	7.040123954	CORE	38	H	H	0.0000	38
H	9.579247705	6.450013154	6.934030077	CORE	39	H	H	0.0000	39
H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48
H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50
H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.079078040	10.853872502	11.096801398	CORE	57	Pd	Pd	0.0000	57
Pd	2.124662850	7.930168338	11.096296336	CORE	58	Pd	Pd	0.0000	58
Pd	2.067158877	2.112908803	11.151490726	CORE	59	Pd	Pd	0.0000	59
Pd	10.797291337	7.953784853	11.108288600	CORE	60	Pd	Pd	0.0000	60
Pd	5.040951056	7.852108465	11.153932694	CORE	61	Pd	Pd	0.0000	61
Pd	7.872575623	5.063414770	11.121182899	CORE	62	Pd	Pd	0.0000	62
Pd	4.939222132	2.107450062	11.090587321	CORE	63	Pd	Pd	0.0000	63
Pd	7.877873612	2.128919238	11.098694422	CORE	64	Pd	Pd	0.0000	64

Pd	7.899798390	7.892246813	11.176514964 CORE	65 Pd	Pd	0.0000	65
Pd	10.784153796	2.129275881	11.140348652 CORE	66 Pd	Pd	0.0000	66
Pd	5.004718763	5.015546173	11.123120329 CORE	67 Pd	Pd	0.0000	67
Pd	10.795153502	10.871283678	11.086455616 CORE	68 Pd	Pd	0.0000	68
Pd	7.903585356	10.830222887	11.101734864 CORE	69 Pd	Pd	0.0000	69
Pd	4.954393528	10.794778031	11.102444321 CORE	70 Pd	Pd	0.0000	70
Pd	10.759920652	5.053234130	11.114833985 CORE	71 Pd	Pd	0.0000	71
Pd	2.108429658	5.028724933	11.108439973 CORE	72 Pd	Pd	0.0000	72
Pd	3.572892103	9.357276922	13.133033446 CORE	73 Pd	Pd	0.0000	73
Pd	0.683439103	9.388920338	13.118975125 CORE	74 Pd	Pd	0.0000	74
Pd	9.389329928	9.424715449	13.129659615 CORE	75 Pd	Pd	0.0000	75
Pd	6.403700012	3.485320976	13.093261487 CORE	76 Pd	Pd	0.0000	76
Pd	3.539636409	6.432943700	13.143816524 CORE	77 Pd	Pd	0.0000	77
Pd	3.539087866	3.499997616	13.150807435 CORE	78 Pd	Pd	0.0000	78
Pd	9.327079768	3.553361751	13.104124752 CORE	79 Pd	Pd	0.0000	79
Pd	0.643626535	6.534082882	13.098191020 CORE	80 Pd	Pd	0.0000	80
Pd	0.639422084	3.660815006	13.132370888 CORE	81 Pd	Pd	0.0000	81
Pd	6.372511677	0.652028172	13.102123144 CORE	82 Pd	Pd	0.0000	82
Pd	9.376066118	6.486183294	13.125057820 CORE	83 Pd	Pd	0.0000	83
Pd	6.493647144	9.399167351	13.139103288 CORE	84 Pd	Pd	0.0000	84
Pd	0.612981230	0.684875085	13.147411288 CORE	85 Pd	Pd	0.0000	85
Pd	9.349037390	0.673065606	13.125200847 CORE	86 Pd	Pd	0.0000	86
Pd	6.412536480	6.401959848	13.398077983 CORE	87 Pd	Pd	0.0000	87
Pd	3.482125056	0.624330882	13.140537248 CORE	88 Pd	Pd	0.0000	88
H	0.633562406	9.781443195	10.825704496 CORE	89 H	H	0.0000	89
H	9.273127929	3.871958973	11.235389540 CORE	90 H	H	0.0000	90
H	3.440192288	9.683312500	10.824989755 CORE	91 H	H	0.0000	91
H	9.648272095	9.488442548	10.819711477 CORE	92 H	H	0.0000	92
H	3.756758451	3.590815571	10.837738195 CORE	93 H	H	0.0000	93
H	3.360539492	6.457977403	10.852867175 CORE	94 H	H	0.0000	94
H	6.485682764	3.958236451	10.840493158 CORE	95 H	H	0.0000	95
H	6.669526872	0.685835551	11.316620474 CORE	96 H	H	0.0000	96
H	0.628793201	3.313284744	11.335426494 CORE	97 H	H	0.0000	97
H	6.441430656	9.064525925	11.350923781 CORE	98 H	H	0.0000	98
H	10.848359866	5.196454220	13.244754326 CORE	99 H	H	0.0000	99
H	11.030612112	8.024309481	13.293979533 CORE	100 H	H	0.0000	100
H	8.014842394	10.695065042	13.273153642 CORE	101 H	H	0.0000	101
H	10.734771325	11.053185734	13.323227703 CORE	102 H	H	0.0000	102
H	1.964513577	8.008581338	13.271747730 CORE	103 H	H	0.0000	103
H	4.842227362	10.826955664	13.282990798 CORE	104 H	H	0.0000	104
H	7.872925660	2.399243578	13.305469708 CORE	105 H	H	0.0000	105
H	4.714977865	7.930127280	13.198318745 CORE	106 H	H	0.0000	106
H	5.007781185	2.255780834	13.335183959 CORE	107 H	H	0.0000	107
H	2.066905666	10.965339926	13.262839154 CORE	108 H	H	0.0000	108

H	10.684929498	1.937986007	13.282479955 CORE	109 H	H	0.0000	109
H	8.196830058	8.109244022	13.154058647 CORE	110 H	H	0.0000	110
H	2.150354119	1.949554527	13.284235527 CORE	111 H	H	0.0000	111
H	1.970929414	5.147669782	13.255996003 CORE	112 H	H	0.0000	112
H	7.973709342	5.939051924	14.204314699 CORE	113 H	H	0.0000	113
H	4.694860916	4.917014875	13.157523041 CORE	114 H	H	0.0000	114
C	7.324638732	5.971895892	15.520665051 CORE	115 C	C	0.0000	115
C	5.989791292	6.484276013	15.490091215 CORE	116 C	C	0.0000	116
H	8.108938119	6.619255412	15.923017612 CORE	117 H	H	0.0000	117
H	5.814283444	7.526329831	15.761104205 CORE	118 H	H	0.0000	118
H	5.155528415	5.804210825	15.669849294 CORE	119 H	H	0.0000	119
H	7.461391192	4.907485466	15.731106623 CORE	120 H	H	0.0000	120

end

end

Ethyl adsorbd on Pd_4H_3(100). The energy from VASP is -529.534376 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	90.00000000	
Pd	10.782813856	5.016247660	7.193226476 CORE	1 Pd	Pd	0.0000	1
Pd	4.983148483	10.816790048	7.193170144 CORE	2 Pd	Pd	0.0000	2
Pd	2.085019604	5.016620832	7.193299683 CORE	3 Pd	Pd	0.0000	3
Pd	7.884901240	10.816521313	7.193479525 CORE	4 Pd	Pd	0.0000	4
Pd	4.983416221	2.117754835	7.193565625 CORE	5 Pd	Pd	0.0000	5
Pd	2.083689210	2.116303795	7.193523055 CORE	6 Pd	Pd	0.0000	6
Pd	2.083337101	10.816628396	7.193560017 CORE	7 Pd	Pd	0.0000	7
Pd	10.783357174	2.116005107	7.193717507 CORE	8 Pd	Pd	0.0000	8
Pd	7.884314250	7.916229331	7.194179624 CORE	9 Pd	Pd	0.0000	9
Pd	2.084485458	7.917186866	7.193893349 CORE	10 Pd	Pd	0.0000	10
Pd	10.783518995	7.917095999	7.193878528 CORE	11 Pd	Pd	0.0000	11
Pd	10.784183220	10.816439879	7.193774103 CORE	12 Pd	Pd	0.0000	12
Pd	7.883464201	5.016721878	7.194093710 CORE	13 Pd	Pd	0.0000	13
Pd	4.984519188	5.017098245	7.194084067 CORE	14 Pd	Pd	0.0000	14
Pd	7.884069627	2.117381531	7.193905540 CORE	15 Pd	Pd	0.0000	15
Pd	4.984015372	7.916443018	7.194219365 CORE	16 Pd	Pd	0.0000	16
Pd	0.634013228	6.466332063	9.009721539 CORE	17 Pd	Pd	0.0000	17
Pd	6.433640859	0.666804909	9.009776069 CORE	18 Pd	Pd	0.0000	18
Pd	0.633707465	3.566812798	9.009902151 CORE	19 Pd	Pd	0.0000	19
Pd	6.434087100	9.367309174	9.010160968 CORE	20 Pd	Pd	0.0000	20
Pd	3.533869947	0.666899228	9.010240576 CORE	21 Pd	Pd	0.0000	21
Pd	0.633969081	9.366447775	9.010826567 CORE	22 Pd	Pd	0.0000	22
Pd	0.633676922	0.666672598	9.010533542 CORE	23 Pd	Pd	0.0000	23
Pd	6.433782001	3.566623726	9.011031260 CORE	24 Pd	Pd	0.0000	24
Pd	9.333604600	0.666638656	9.010546436 CORE	25 Pd	Pd	0.0000	25
Pd	9.334234437	6.466445910	9.010863765 CORE	26 Pd	Pd	0.0000	26
Pd	6.434155127	6.466929211	9.011104041 CORE	27 Pd	Pd	0.0000	27

Pd	3.534124022	9.367105408	9.010616024	CORE	28	Pd	Pd	0.0000	28
Pd	3.533628327	3.566955412	9.010687856	CORE	29	Pd	Pd	0.0000	29
Pd	3.533991674	6.466788159	9.010808806	CORE	30	Pd	Pd	0.0000	30
Pd	9.333852689	3.566664034	9.010894518	CORE	31	Pd	Pd	0.0000	31
Pd	9.333931906	9.366801997	9.011053461	CORE	32	Pd	Pd	0.0000	32
H	9.580275272	3.552800903	6.954668839	CORE	33	H	H	0.0000	33
H	3.295746757	3.547762072	6.962678283	CORE	34	H	H	0.0000	34
H	9.086881997	9.341519786	6.949637981	CORE	35	H	H	0.0000	35
H	0.584442804	9.413295161	7.028496754	CORE	36	H	H	0.0000	36
H	3.745807373	9.375081903	6.966885887	CORE	37	H	H	0.0000	37
H	6.434765974	3.610391075	7.040123954	CORE	38	H	H	0.0000	38
H	9.579247705	6.450013154	6.934030077	CORE	39	H	H	0.0000	39
H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48
H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50
H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.077226653	10.854625006	11.094898360	CORE	57	Pd	Pd	0.0000	57
Pd	2.105575949	7.930204662	11.102031807	CORE	58	Pd	Pd	0.0000	58
Pd	2.076788353	2.116104549	11.148380940	CORE	59	Pd	Pd	0.0000	59
Pd	10.780113087	7.949497833	11.115647336	CORE	60	Pd	Pd	0.0000	60
Pd	5.012770092	7.876782937	11.113889824	CORE	61	Pd	Pd	0.0000	61
Pd	7.866842853	5.079201507	11.117364973	CORE	62	Pd	Pd	0.0000	62
Pd	4.952379333	2.128555210	11.102693309	CORE	63	Pd	Pd	0.0000	63
Pd	7.877372812	2.151671829	11.099986356	CORE	64	Pd	Pd	0.0000	64
Pd	7.890137416	7.911050916	11.163112891	CORE	65	Pd	Pd	0.0000	65
Pd	10.776293252	2.132421343	11.148136515	CORE	66	Pd	Pd	0.0000	66
Pd	4.994214742	5.035366017	11.103965927	CORE	67	Pd	Pd	0.0000	67
Pd	10.779591194	10.871328509	11.095357680	CORE	68	Pd	Pd	0.0000	68
Pd	7.901293152	10.840302589	11.103563938	CORE	69	Pd	Pd	0.0000	69
Pd	4.960369476	10.814034764	11.113253565	CORE	70	Pd	Pd	0.0000	70
Pd	10.760714268	5.054866603	11.112300343	CORE	71	Pd	Pd	0.0000	71

Pd	2.099964840	5.022965168	11.117479057 CORE	72	Pd	Pd	0.0000	72
Pd	3.546830539	9.342904828	13.128612364 CORE	73	Pd	Pd	0.0000	73
Pd	0.648498494	9.390985597	13.109521754 CORE	74	Pd	Pd	0.0000	74
Pd	9.345838985	9.414630472	13.139453472 CORE	75	Pd	Pd	0.0000	75
Pd	6.417313303	3.598544322	13.126490799 CORE	76	Pd	Pd	0.0000	76
Pd	3.570223249	6.435300077	13.129637464 CORE	77	Pd	Pd	0.0000	77
Pd	3.545190016	3.512694289	13.155959864 CORE	78	Pd	Pd	0.0000	78
Pd	9.301388211	3.575070870	13.130945384 CORE	79	Pd	Pd	0.0000	79
Pd	0.622966137	6.519847412	13.096083435 CORE	80	Pd	Pd	0.0000	80
Pd	0.624953395	3.642946003	13.132762063 CORE	81	Pd	Pd	0.0000	81
Pd	6.391391002	0.706880866	13.105825138 CORE	82	Pd	Pd	0.0000	82
Pd	9.334104850	6.490469863	13.129791768 CORE	83	Pd	Pd	0.0000	83
Pd	6.451124225	9.385050928	13.132137386 CORE	84	Pd	Pd	0.0000	84
Pd	0.626456161	0.683393663	13.127496193 CORE	85	Pd	Pd	0.0000	85
Pd	9.342464180	0.688617715	13.126100600 CORE	86	Pd	Pd	0.0000	86
Pd	6.442475756	6.479577448	13.306741390 CORE	87	Pd	Pd	0.0000	87
Pd	3.492388576	0.623052132	13.131587579 CORE	88	Pd	Pd	0.0000	88
H	0.627478576	9.810573486	10.805083672 CORE	89	H	H	0.0000	89
H	9.298679001	3.952759157	10.810987995 CORE	90	H	H	0.0000	90
H	3.461580230	9.722070246	10.814486902 CORE	91	H	H	0.0000	91
H	9.677594459	9.443059657	10.819118746 CORE	92	H	H	0.0000	92
H	3.807210224	3.597645019	10.830435375 CORE	93	H	H	0.0000	93
H	3.272114350	6.480050465	10.868319352 CORE	94	H	H	0.0000	94
H	6.456409720	3.983886581	10.797759866 CORE	95	H	H	0.0000	95
H	6.729255273	0.696104045	11.321109740 CORE	96	H	H	0.0000	96
H	0.630831792	3.283736196	11.337998832 CORE	97	H	H	0.0000	97
H	6.431605878	9.043209833	11.320909311 CORE	98	H	H	0.0000	98
H	10.808651244	5.299810763	13.253354650 CORE	99	H	H	0.0000	99
H	10.972031490	7.964724291	13.253169459 CORE	100	H	H	0.0000	100
H	8.127762717	10.793317660	13.275813342 CORE	101	H	H	0.0000	101
H	10.749522864	11.054872041	13.239407454 CORE	102	H	H	0.0000	102
H	2.011953976	8.126605762	13.245490670 CORE	103	H	H	0.0000	103
H	4.938713961	10.745869024	13.231031615 CORE	104	H	H	0.0000	104
H	7.863097677	2.390430360	13.280070899 CORE	105	H	H	0.0000	105
H	4.652809534	7.936923033	13.296975858 CORE	106	H	H	0.0000	106
H	5.046246312	2.335005182	13.301747869 CORE	107	H	H	0.0000	107
H	2.010181620	11.035753524	13.245972708 CORE	108	H	H	0.0000	108
H	10.596777497	2.113664187	13.259298526 CORE	109	H	H	0.0000	109
H	8.048593392	8.151004030	13.276667722 CORE	110	H	H	0.0000	110
H	2.232721431	1.944050501	13.287552986 CORE	111	H	H	0.0000	111
H	1.917981009	5.046044773	13.213550983 CORE	112	H	H	0.0000	112
H	8.308434905	5.843644726	15.865642167 CORE	113	H	H	0.0000	113
H	4.722826048	4.918915761	13.254971865 CORE	114	H	H	0.0000	114
H	8.119014969	5.043003906	13.177001094 CORE	115	H	H	0.0000	115

C	7.250615871	5.646820086	16.091901028	CORE	116 C	C	0.0000	116
C	6.319503992	6.590549372	15.378009495	CORE	117 C	C	0.0000	117
H	7.118051812	5.778165732	17.183932080	CORE	118 H	H	0.0000	118
H	6.539991138	7.650471757	15.567458676	CORE	119 H	H	0.0000	119
H	5.257840432	6.382785072	15.567669954	CORE	120 H	H	0.0000	120
H	7.038423136	4.591941174	15.863793922	CORE	121 H	H	0.0000	121

end

end

TS from ethyl to ethane on Pd_4H_3(100). The energy from VASP is -528.982653 eV.

PBC	11.60000000	11.60000000	20.00000000	90.00000000	90.00000000	90.00000000		
Pd	10.782813856	5.016247660	7.193226476	CORE	1 Pd	Pd	0.0000	1
Pd	4.983148483	10.816790048	7.193170144	CORE	2 Pd	Pd	0.0000	2
Pd	2.085019604	5.016620832	7.193299683	CORE	3 Pd	Pd	0.0000	3
Pd	7.884901240	10.816521313	7.193479525	CORE	4 Pd	Pd	0.0000	4
Pd	4.983416221	2.117754835	7.193565625	CORE	5 Pd	Pd	0.0000	5
Pd	2.083689210	2.116303795	7.193523055	CORE	6 Pd	Pd	0.0000	6
Pd	2.083337101	10.816628396	7.193560017	CORE	7 Pd	Pd	0.0000	7
Pd	10.783357174	2.116005107	7.193717507	CORE	8 Pd	Pd	0.0000	8
Pd	7.884314250	7.916229331	7.194179624	CORE	9 Pd	Pd	0.0000	9
Pd	2.084485458	7.917186866	7.193893349	CORE	10 Pd	Pd	0.0000	10
Pd	10.783518995	7.917095999	7.193878528	CORE	11 Pd	Pd	0.0000	11
Pd	10.784183220	10.816439879	7.193774103	CORE	12 Pd	Pd	0.0000	12
Pd	7.883464201	5.016721878	7.194093710	CORE	13 Pd	Pd	0.0000	13
Pd	4.984519188	5.017098245	7.194084067	CORE	14 Pd	Pd	0.0000	14
Pd	7.884069627	2.117381531	7.193905540	CORE	15 Pd	Pd	0.0000	15
Pd	4.984015372	7.916443018	7.194219365	CORE	16 Pd	Pd	0.0000	16
Pd	0.634013228	6.466332063	9.009721539	CORE	17 Pd	Pd	0.0000	17
Pd	6.433640859	0.666804909	9.009776069	CORE	18 Pd	Pd	0.0000	18
Pd	0.633707465	3.566812798	9.009902151	CORE	19 Pd	Pd	0.0000	19
Pd	6.434087100	9.367309174	9.010160968	CORE	20 Pd	Pd	0.0000	20
Pd	3.533869947	0.666899228	9.010240576	CORE	21 Pd	Pd	0.0000	21
Pd	0.633969081	9.366447775	9.010826567	CORE	22 Pd	Pd	0.0000	22
Pd	0.633676922	0.666672598	9.010533542	CORE	23 Pd	Pd	0.0000	23
Pd	6.433782001	3.566623726	9.011031260	CORE	24 Pd	Pd	0.0000	24
Pd	9.333604600	0.666638656	9.010546436	CORE	25 Pd	Pd	0.0000	25
Pd	9.334234437	6.466445910	9.010863765	CORE	26 Pd	Pd	0.0000	26
Pd	6.434155127	6.466929211	9.011104041	CORE	27 Pd	Pd	0.0000	27
Pd	3.534124022	9.367105408	9.010616024	CORE	28 Pd	Pd	0.0000	28
Pd	3.533628327	3.566955412	9.010687856	CORE	29 Pd	Pd	0.0000	29
Pd	3.533991674	6.466788159	9.010808806	CORE	30 Pd	Pd	0.0000	30
Pd	9.333852689	3.566664034	9.010894518	CORE	31 Pd	Pd	0.0000	31
Pd	9.333931906	9.366801997	9.011053461	CORE	32 Pd	Pd	0.0000	32
H	9.580275272	3.552800903	6.954668839	CORE	33 H	H	0.0000	33

H	3.295746757	3.547762072	6.962678283	CORE	34	H	H	0.0000	34
H	9.086881997	9.341519786	6.949637981	CORE	35	H	H	0.0000	35
H	0.584442804	9.413295161	7.028496754	CORE	36	H	H	0.0000	36
H	3.745807373	9.375081903	6.966885887	CORE	37	H	H	0.0000	37
H	6.434765974	3.610391075	7.040123954	CORE	38	H	H	0.0000	38
H	9.579247705	6.450013154	6.934030077	CORE	39	H	H	0.0000	39
H	3.288603653	6.446999111	6.952815561	CORE	40	H	H	0.0000	40
H	3.843604606	0.664546205	6.896175203	CORE	41	H	H	0.0000	41
H	0.655067259	0.565014710	7.024166018	CORE	42	H	H	0.0000	42
H	6.409107817	6.337967854	7.025746693	CORE	43	H	H	0.0000	43
H	9.051661337	0.667038575	6.904917138	CORE	44	H	H	0.0000	44
H	5.148172690	10.776144117	9.318939480	CORE	45	H	H	0.0000	45
H	10.943859652	4.955687958	9.346146877	CORE	46	H	H	0.0000	46
H	1.947844561	4.898465719	9.314227342	CORE	47	H	H	0.0000	47
H	7.863646690	10.714276031	9.298683968	CORE	48	H	H	0.0000	48
H	4.942919882	1.916526292	9.333046890	CORE	49	H	H	0.0000	49
H	1.929986792	7.933294934	9.306319839	CORE	50	H	H	0.0000	50
H	8.010473952	2.015176908	9.313595515	CORE	51	H	H	0.0000	51
H	10.730630473	7.711554998	9.370502570	CORE	52	H	H	0.0000	52
H	5.124066584	7.787239334	9.316356954	CORE	53	H	H	0.0000	53
H	2.058528079	1.758962307	9.431083334	CORE	54	H	H	0.0000	54
H	10.808973037	1.757212179	9.437471070	CORE	55	H	H	0.0000	55
H	7.869842005	7.529248067	9.452210517	CORE	56	H	H	0.0000	56
Pd	2.092577296	10.828554322	11.068265928	CORE	57	Pd	Pd	0.0000	57
Pd	2.106095030	7.899918620	11.104572232	CORE	58	Pd	Pd	0.0000	58
Pd	2.071695307	2.098171404	11.149528648	CORE	59	Pd	Pd	0.0000	59
Pd	10.773645717	7.945020233	11.119109479	CORE	60	Pd	Pd	0.0000	60
Pd	5.003159529	7.870626273	11.116209991	CORE	61	Pd	Pd	0.0000	61
Pd	7.845412506	5.084472345	11.152578040	CORE	62	Pd	Pd	0.0000	62
Pd	4.950712766	2.113854389	11.105226755	CORE	63	Pd	Pd	0.0000	63
Pd	7.888121450	2.151561812	11.098453336	CORE	64	Pd	Pd	0.0000	64
Pd	7.878562910	7.914744905	11.179724869	CORE	65	Pd	Pd	0.0000	65
Pd	10.787557762	2.116963267	11.160568007	CORE	66	Pd	Pd	0.0000	66
Pd	4.979507269	5.017607277	11.116700682	CORE	67	Pd	Pd	0.0000	67
Pd	10.799559897	10.856474429	11.096115858	CORE	68	Pd	Pd	0.0000	68
Pd	7.919196727	10.847014537	11.097635506	CORE	69	Pd	Pd	0.0000	69
Pd	4.966597035	10.811556142	11.114678579	CORE	70	Pd	Pd	0.0000	70
Pd	10.741404459	5.035671184	11.112953409	CORE	71	Pd	Pd	0.0000	71
Pd	2.085760514	5.007402139	11.110694600	CORE	72	Pd	Pd	0.0000	72
Pd	3.537305617	9.326296037	13.097122131	CORE	73	Pd	Pd	0.0000	73
Pd	0.659464358	9.382965686	13.119064769	CORE	74	Pd	Pd	0.0000	74
Pd	9.366871955	9.394797837	13.152232834	CORE	75	Pd	Pd	0.0000	75
Pd	6.417675027	3.583156262	13.133407945	CORE	76	Pd	Pd	0.0000	76
Pd	3.518464382	6.376947291	13.148884222	CORE	77	Pd	Pd	0.0000	77

Pd	3.538945985	3.444058150	13.168695391	CORE	78	Pd	Pd	0.0000	78
Pd	9.292245769	3.549880293	13.152054635	CORE	79	Pd	Pd	0.0000	79
Pd	0.617112965	6.503988185	13.101841673	CORE	80	Pd	Pd	0.0000	80
Pd	0.613686989	3.633789483	13.140108429	CORE	81	Pd	Pd	0.0000	81
Pd	6.426858315	0.725646969	13.110970340	CORE	82	Pd	Pd	0.0000	82
Pd	9.344849958	6.470195826	13.137857904	CORE	83	Pd	Pd	0.0000	83
Pd	6.460269687	9.451054432	13.128572541	CORE	84	Pd	Pd	0.0000	84
Pd	0.643144593	0.663324201	13.145563779	CORE	85	Pd	Pd	0.0000	85
Pd	9.375184857	0.652448889	13.142166170	CORE	86	Pd	Pd	0.0000	86
Pd	6.399294010	6.548609489	13.314653663	CORE	87	Pd	Pd	0.0000	87
Pd	3.487482537	0.583468656	13.143352679	CORE	88	Pd	Pd	0.0000	88
H	0.645946289	9.756692879	10.820190783	CORE	89	H	H	0.0000	89
H	9.269279101	3.907200090	10.806903984	CORE	90	H	H	0.0000	90
H	3.463712782	9.576582575	11.241792868	CORE	91	H	H	0.0000	91
H	9.607702509	9.506766440	10.812843660	CORE	92	H	H	0.0000	92
H	3.724492693	3.563275709	10.826935705	CORE	93	H	H	0.0000	93
H	3.429202289	6.458965684	10.849892459	CORE	94	H	H	0.0000	94
H	6.460654415	3.950185162	10.804803409	CORE	95	H	H	0.0000	95
H	6.663964022	0.708370640	11.326377225	CORE	96	H	H	0.0000	96
H	0.649920745	3.334122401	11.339179777	CORE	97	H	H	0.0000	97
H	6.404455303	9.081134902	11.374795901	CORE	98	H	H	0.0000	98
H	10.802788427	5.248348193	13.308358289	CORE	99	H	H	0.0000	99
H	10.943464552	7.986924308	13.252841370	CORE	100	H	H	0.0000	100
H	8.194065091	10.829903725	13.346145150	CORE	101	H	H	0.0000	101
H	10.768430350	10.947728125	13.304537807	CORE	102	H	H	0.0000	102
H	1.999827900	7.995431287	13.227402787	CORE	103	H	H	0.0000	103
H	4.918651921	10.669102359	13.242824014	CORE	104	H	H	0.0000	104
H	7.823633576	2.364497054	13.333626351	CORE	105	H	H	0.0000	105
H	5.000383276	6.792448494	14.192518000	CORE	106	H	H	0.0000	106
H	5.054122173	2.317559144	13.328035428	CORE	107	H	H	0.0000	107
H	1.973475530	11.026519872	13.359291128	CORE	108	H	H	0.0000	108
H	10.702719484	2.096174363	13.222314919	CORE	109	H	H	0.0000	109
H	8.144982903	8.020786369	13.223616345	CORE	110	H	H	0.0000	110
H	2.195091451	1.842728964	13.349168308	CORE	111	H	H	0.0000	111
H	1.883448401	5.090101283	13.254552708	CORE	112	H	H	0.0000	112
H	8.014441271	6.165685461	15.831223355	CORE	113	H	H	0.0000	113
H	4.669534220	4.831083353	13.125502234	CORE	114	H	H	0.0000	114
H	8.163987261	4.987078618	13.226285369	CORE	115	H	H	0.0000	115
C	6.977895387	5.967797459	16.134570267	CORE	116	C	C	0.0000	116
C	5.989261022	6.910278827	15.474072254	CORE	117	C	C	0.0000	117
H	6.911956798	6.108596217	17.230928796	CORE	118	H	H	0.0000	118
H	6.263018954	7.970437834	15.540407746	CORE	119	H	H	0.0000	119
H	4.992430716	6.794475929	15.919974092	CORE	120	H	H	0.0000	120
H	6.756674131	4.910445368	15.932110878	CORE	121	H	H	0.0000	121

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end
end
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