Supporting information

Material Discovery by Combining Stochastic Surface Walking Global Optimization with Neural Network

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1. Derivation for the gradient of J_σ with respect to NN parameters

In the following, we derive the gradient of stress part of performance funciton J_σ with respect to NN parameters (see Figure 1 in main text for the NN architecture). In each subnet m (also network for element m), the value of node x in layer *l*, $a^{l,m}_x$, is constructed according to:

$$a^{l,m}_x = f^{l,m}\left(\sum_y w^{l,m}_{xy} a^{l-1,m}_y + b^{l,m}_x\right) \quad \text{(S1)}$$

$$z^{l,m}_x = \sum_y w^{l,m}_{xy} a^{l-1,m}_y + b^{l,m}_x \quad \text{(S2)}$$

where $w^{l,m}_{xy}$ is the weight of the subnet m that connects the node x in layer *l* and the node y in layer *l*-1; $b^{l,m}_i$ is the bias, and $f^{l,m}$ is the activation function. The stress part of performance function is written as:

$$J_\sigma = \frac{1}{18}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\left(\sigma^{NN}_{\alpha\beta} - \sigma^{real}_{\alpha\beta}\right)^2 \quad \text{(S3)}$$

$$\sigma^{NN}_{\alpha\beta} = -\frac{1}{V}\sum_{m=1}^{N_{ele}}\sum_{i=1}^{N_{atm,m}}\sum_{j=1}^{M_{i,m}}\sum_{d=1}^{D_{j,i,m}}\frac{(r_d)_\alpha (r_d)_\beta}{r_d}\frac{\partial E^m_i}{\partial G_{j,i,m}}\frac{\partial G_{j,i,m}}{\partial r_d} \quad \text{(S4)}$$

where $\sigma^{NN}_{\alpha\beta}$, $\sigma^{real}_{\alpha\beta}$ are the stress tensor matrix element in NN PES and DFT, respectively; $G_{j,i,m}$ is the j-th symmetry function describing atom i of element m; r_d is the distance vector with the module r_d constituing the symmtry function; V is the volume of structure.

Combinging Eqs. (S3-4) with Eqs. (S1-2), the gradient for the stress part of performance function with respect to a network weight and bias follows the expression:

$$\frac{\partial J_\sigma}{\partial w^{l,m}_{xy}} = -\frac{1}{9V}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\left[\left(\sigma^{NN}_{\alpha\beta} - \sigma^{real}_{\alpha\beta}\right)\sum_{m=1}^{N_{ele}}\sum_{i=1}^{N_{atm,m}}\sum_{j=1}^{M_{i,m}}\sum_{d=1}^{D_{j,i,m}}\frac{(r_d)_\alpha (r_d)_\beta}{r_d}\frac{\partial G_{j,i,m}}{\partial r_d}\frac{\partial}{\partial w^{l,m}_{xy}}\frac{\partial E^m_i}{\partial G_{j,i,m}}\right] \quad \text{(S5)}$$

$$\frac{\partial J_\sigma}{\partial b^{l,m}_x} = -\frac{1}{9V}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\left[\left(\sigma^{NN}_{\alpha\beta} - \sigma^{real}_{\alpha\beta}\right)\sum_{m=1}^{N_{ele}}\sum_{i=1}^{N_{atm,m}}\sum_{j=1}^{M_{i,m}}\sum_{d=1}^{D_{j,i,m}}\frac{(r_d)_\alpha (r_d)_\beta}{r_d}\frac{\partial G_{j,i,m}}{\partial r_d}\frac{\partial}{\partial b^{l,m}_x}\frac{\partial E^m_i}{\partial G_{j,i,m}}\right] \quad \text{(S6)}$$

For simplicity, we define the following terms:

$$fac_{j,i,m} = -\frac{1}{9V}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\sum_{d=1}^{D_{j,i,m}}\left(\sigma^{NN}_{\alpha\beta} - \sigma^{real}_{\alpha\beta}\right)\frac{(r_d)_\alpha (r_d)_\beta}{r_d}\frac{\partial G_{j,i,m}}{\partial r_d} \quad \text{(S7)}$$

$$u_{i,j,x}^{l,m} = fac_{j,i,m} \frac{\partial E_i^m}{\partial z_{i,x}^{l,m}} \text{ (S8)}$$

$$v_{i,x}^{l,m} = \sum_{j=1}^{M_{i,m}} fac_{j,i,m} \frac{\partial \quad \partial E_i^m}{\partial G_{j,i,m} \partial z_{i,x}^{l,m}} \text{ (S9)}$$

to reduce Eqs. S5-6 as:

$$\frac{\partial J_\sigma}{\partial w_{xy}^{l,m}} = \sum_{i=1}^{N_{atm,m}} \sum_{j=1}^{M_{i,m}} \frac{\partial a_{i,y}^{l-1,m}}{\partial G_{j,i,m}} u_{i,j,x}^{l,m} + \sum_{i=1}^{N_{atm,m}} a_{i,y}^{l-1,m} v_{i,x}^{l,m} \text{ (S10)}$$

$$\frac{\partial J_\sigma}{\partial b_x^{l,m}} = \sum_{i=1}^{N_{atm,m}} v_{i,x}^{l,m} \text{ (S11)}$$

To get the derivatives in Eqs. S10-11, we need to compute the following three terms $\frac{\partial a_{i,x}^{l,m}}{\partial G_{j,i,m}}$, $u_{i,j,x}^{l,m}$ and $v_{i,x}^{l,m}$,. The first term is updated forwardly from layer to layer using:

$$\frac{\partial a_{i,x}^{l,m}}{\partial G_{j,i,m}} = f'\left(z_{i,x}^{l,m}\right) \sum_{k=1}^{S_{l-1}} w_{xk}^{l,m} \frac{\partial a_{i,k}^{l-1,m}}{\partial G_{j,i,m}} \text{ (S12)}$$

which is initialized at the first layer with

$$\frac{\partial a_{i,x}^{l,m}}{\partial G_{j,i,m}} = \begin{cases} 1, & x = j \\ 0, & x \neq j \end{cases} \text{ (S13)}$$

The other two terms $u_{i,j,x}^{l,m}$ and $v_{i,x}^{l,m}$ are updated back-propagatedly from layer to layer using:

$$u_{i,j,x}^{l,m} = f'\left(z_{i,x}^{l,m}\right) \sum_{k=1}^{S_{l+1}} w_{kx}^{l+1,m} u_{i,j,k}^{l+1,m} \text{ (S14)}$$

$$v_{i,x}^{l,m} = f'\left(z_{i,x}^{l,m}\right) \sum_{k=1}^{S_{l+1}} w_{kx}^{l+1,m} v_{i,j,k}^{l+1,m} + \sum_{j=1}^{M_{i,m}} \frac{\partial f'\left(z_{i,x}^{l,m}\right)}{\partial G_{j,i,m}} \sum_{k=1}^{S_{l+1}} w_{kx}^{l+1,m} u_{i,j,k}^{l+1,m} \text{ (S15)}$$

which is initialized at the last layer (layer L) using:

$$u_{i,j,x}^{L,m} = fac_{j,i,m} \cdot f'\left(z_{i,x}^{L,m}\right) \text{ (S16)}$$

$$v_{i,x}^{L,m} = \sum_{j=1}^{M_{i,m}} fac_{j,i,m} \cdot \frac{\partial f'\left(z_{i,x}^{L,m}\right)}{\partial G_{j,i,m}} \text{ (S17)}$$

2. DFT calculation setups

All DFT calculations are performed using the periodic plane wave method as implemented in the VASP package[1-2]. The ionic core electrons are described using the projector augmented wave (PAW) pseudopotential[3], where the semicore electrons are included in the Ti potential ($3p^6 3d^2 4s^2$) .The electron exchange and correlation effects are described by the GGA-PBE functional[4]. For the low accuracy calculations used in SSW sampling to collect raw data set (Scheme 1 in text), the kinetic energy cutoff utilized is 400 eV; the first Brillouin zone is sampled using the Monkhorst−Pack scheme[5] with a (4 × 4 × 4). For the high accuracy calculations used in single-point energy refinement calculations to build the global data set, these two quantities increase to 600 eV and (6 × 6 × 6), respectively.

(1) Kresse, G.; Hafner, J., *Physical Review B* **1993,** *47*, 558.

(2) Kresse, G.; Furthmüller, J., *Computational Materials Science* **1996,** *6*, 15-50.

(3) Kresse, G.; Joubert, D., *Physical Review B* **1999,** *59*, 1758.

(4) Perdew, J. P.; Burke, K.; Ernzerhof, M., *Physical review letters* **1996,** *77*, 3865.

(5) Monkhorst, H. J.; Pack, J. D., *Physical review B* **1976,** *13*, 5188.

3. Parameters of atom-centered symmetry functions for generating TiO_2 NN potential

Table S1. Parameters of the radial symmetry functions G^1 (see Eq. 3 in the main text) used to describe the local atomic environment ('Cent ele' in table). R_c is the cutoff radius, and 'Neigb ele' is the neighboring element taken into account.

Cent ele	No.	R_c (Å)	Neigb ele	Cent ele	No.	R_c (Å)	Neigb ele
O	1	3.30	O	O	3	6.00	O
O	2	3.30	Ti	O	4	6.00	Ti
Ti	1	3.30	O	Ti	3	6.00	O
Ti	2	3.30	Ti	Ti	4	6.00	Ti

Table S2. Parameters of the radial symmetry functions G^2 (see Eq. 4 in main text) used to describe the local atomic environment. Also see Table S1 caption for explanations.

Cent ele	R_c (Å)	No.	Neigb ele	η ($Å^{-2}$)	R_s (Å)	Cent ele	R_c (Å)	No.	Neigb ele	η ($Å^{-2}$)	R_s (Å)
O	3.30	1	O	0.042	1.8	O	6.00	9	O	0.014	2.0
O	3.30	2	O	0.280	0.2	O	6.00	10	O	0.028	1.0
O	3.30	3	O	0.280	0.5	O	6.00	11	O	0.140	0.5
O	3.30	4	O	0.560	1.0	O	6.00	12	O	0.504	1.8
O	3.30	5	Ti	0.042	2.0	O	6.00	13	Ti	0.014	2.0
O	3.30	6	Ti	0.280	0.2	O	6.00	14	Ti	0.028	1.0
O	3.30	7	Ti	0.280	0.5	O	6.00	15	Ti	0.140	0.5
O	3.30	8	Ti	0.560	1.0	O	6.00	16	Ti	0.504	1.8
Ti	3.30	1	O	0.042	2.0	Ti	6.00	9	O	0.014	2.0
Ti	3.30	2	O	0.280	0.2	Ti	6.00	10	O	0.028	1.0
Ti	3.30	3	O	0.280	0.5	Ti	6.00	11	O	0.140	0.5
Ti	3.30	4	O	0.560	1.0	Ti	6.00	12	O	0.504	1.8
Ti	3.30	5	Ti	0.042	2.2	Ti	6.00	13	Ti	0.014	2.2
Ti	3.30	6	Ti	0.280	0.2	Ti	6.00	14	Ti	0.028	1.0
Ti	3.30	7	Ti	0.280	0.5	Ti	6.00	15	Ti	0.140	0.5
Ti	3.30	8	Ti	0.560	1.0	Ti	6.00	16	Ti	0.504	1.8

Table S3. Parameters of the radial symmetry functions G^3 (see Eq. 5 in main text) used to describe the local atomic environments. Also see Table S1 caption for explanations.

Cent ele	R_c (Å)	No.	Neigb ele	κ (Å^{-1})	Cent ele	R_c (Å)	No.	Neigb ele	κ (Å^{-1})
O	3.30	1	O	0.265	O	3.30	4	Ti	0.794
O	3.30	2	O	0.794	O	6.00	5	O	0.529
O	3.30	3	Ti	0.265	O	6.00	6	Ti	0.529
Ti	3.30	1	O	0.265	Ti	3.30	4	Ti	0.794
Ti	3.30	2	O	0.794	Ti	6.00	5	O	0.529
Ti	3.30	3	Ti	0.265	Ti	6.00	6	Ti	0.529

Table S4. Parameters of the radial symmetry functions G^4 (see Eq. 6 in main text) used to describe the local atomic environment. Also see Table S1 caption for explanations.

Cent ele	R_c (Å)	No.	Neigb ele1	Neigb ele2	η (Å^{-2})	λ	ζ	Cent ele	R_c (Å)	No.	Neigb ele1	Neigb ele2	η (Å^{-2})	λ	ζ
O	3.30	1	O	O	0.000	1.0	-1.0	O	3.30	16	Ti	Ti	0.011	4.0	1.0
O	3.30	2	O	O	0.000	1.0	1.0	O	3.30	17	Ti	Ti	0.022	1.0	-1.0
O	3.30	3	O	O	0.011	1.0	-1.0	O	3.30	18	Ti	Ti	0.022	1.0	1.0
O	3.30	4	O	O	0.011	4.0	1.0	O	6.00	19	O	O	0.003	1.0	-1.0
O	3.30	5	O	O	0.022	1.0	-1.0	O	6.00	20	O	O	0.003	4.0	1.0
O	3.30	6	O	O	0.022	1.0	1.0	O	6.00	21	O	O	0.014	1.0	-1.0
O	3.30	7	O	Ti	0.000	1.0	-1.0	O	6.00	22	O	O	0.014	2.0	1.0
O	3.30	8	O	Ti	0.000	1.0	1.0	O	6.00	23	O	Ti	0.003	1.0	-1.0
O	3.30	9	O	Ti	0.011	1.0	-1.0	O	6.00	24	O	Ti	0.003	4.0	1.0
O	3.30	10	O	Ti	0.011	4.0	1.0	O	6.00	25	O	Ti	0.014	1.0	-1.0
O	3.30	11	O	Ti	0.022	1.0	-1.0	O	6.00	26	O	Ti	0.014	2.0	1.0
O	3.30	12	O	Ti	0.022	4.0	1.0	O	6.00	27	Ti	Ti	0.003	1.0	-1.0
O	3.30	13	Ti	Ti	0.000	1.0	-1.0	O	6.00	28	Ti	Ti	0.003	4.0	1.0
O	3.30	14	Ti	Ti	0.000	1.0	1.0	O	6.00	29	Ti	Ti	0.014	1.0	-1.0
O	3.30	15	Ti	Ti	0.011	1.0	-1.0	O	6.00	30	Ti	Ti	0.014	2.0	1.0
Ti	3.30	1	O	O	0.000	1.0	-1.0	Ti	6.00	13	O	O	0.003	1.0	-1.0
Ti	3.30	2	O	O	0.000	1.0	1.0	Ti	6.00	14	O	O	0.003	4.0	1.0
Ti	3.30	3	O	O	0.011	1.0	-1.0	Ti	6.00	15	O	O	0.014	1.0	-1.0
Ti	3.30	4	O	O	0.011	4.0	1.0	Ti	6.00	16	O	O	0.014	2.0	1.0
Ti	3.30	5	O	O	0.022	1.0	-1.0	Ti	6.00	17	O	Ti	0.003	1.0	-1.0
Ti	3.30	6	O	O	0.022	1.0	1.0	Ti	6.00	18	O	Ti	0.003	4.0	1.0
Ti	3.30	7	O	Ti	0.000	1.0	-1.0	Ti	6.00	19	O	Ti	0.014	1.0	-1.0
Ti	3.30	8	O	Ti	0.000	1.0	1.0	Ti	6.00	20	O	Ti	0.014	2.0	1.0
Ti	3.30	9	O	Ti	0.011	1.0	-1.0	Ti	6.00	21	Ti	Ti	0.003	1.0	-1.0
Ti	3.30	10	O	Ti	0.011	4.0	1.0	Ti	6.00	22	Ti	Ti	0.003	4.0	1.0
Ti	3.30	11	O	Ti	0.022	1.0	-1.0	Ti	6.00	23	Ti	Ti	0.014	1.0	-1.0
Ti	3.30	12	O	Ti	0.022	1.0	1.0	Ti	6.00	24	Ti	Ti	0.014	2.0	1.0

Table S5. Parameters of the radial symmetry functions G^5 (see Eq. 7 in main text) used to describe the local atomic environment. Also see Table 1 caption for explanations.

Cent ele	R_c (Å)	No.	Neigb ele1	Neigb ele2	η (Å^{-2})	λ	ζ	Cent ele	R_c (Å)	No.	Neigb ele1	Neigb ele2	η (Å^{-2})	λ	ζ
O	3.30	1	O	O	0.112	1.0	-1.0	O	6.00	16	O	O	0.140	4.0	1.0
O	3.30	2	O	O	0.112	4.0	1.0	O	6.00	17	O	O	0.196	1.0	1.0
O	3.30	3	O	O	0.168	1.0	-1.0	O	6.00	18	O	O	0.196	4.0	-1.0
O	3.30	4	O	O	0.224	1.0	1.0	O	6.00	19	O	Ti	0.007	1.0	-1.0
O	3.30	5	O	Ti	0.112	1.0	-1.0	O	6.00	20	O	Ti	0.007	2.0	1.0
O	3.30	6	O	Ti	0.112	4.0	1.0	O	6.00	21	O	Ti	0.140	1.0	-1.0
O	3.30	7	O	Ti	0.168	1.0	-1.0	O	6.00	22	O	Ti	0.140	4.0	1.0
O	3.30	8	O	Ti	0.224	1.0	1.0	O	6.00	23	O	Ti	0.196	1.0	1.0
O	3.30	9	Ti	Ti	0.112	1.0	-1.0	O	6.00	24	O	Ti	0.196	4.0	-1.0
O	3.30	10	Ti	Ti	0.112	4.0	1.0	O	6.00	25	Ti	Ti	0.007	1.0	-1.0
O	3.30	11	Ti	Ti	0.168	1.0	-1.0	O	6.00	26	Ti	Ti	0.007	2.0	1.0
O	3.30	12	Ti	Ti	0.224	1.0	1.0	O	6.00	27	Ti	Ti	0.140	1.0	-1.0
O	6.00	13	O	O	0.007	1.0	-1.0	O	6.00	28	Ti	Ti	0.140	4.0	1.0
O	6.00	14	O	O	0.007	2.0	1.0	O	6.00	29	Ti	Ti	0.196	1.0	1.0
O	6.00	15	O	O	0.140	1.0	-1.0	O	6.00	30	Ti	Ti	0.196	4.0	-1.0
Ti	3.30	1	O	O	0.112	1.0	-1.0	Ti	6.00	16	O	O	0.140	4.0	1.0
Ti	3.30	2	O	O	0.112	4.0	1.0	Ti	6.00	17	O	O	0.196	1.0	1.0
Ti	3.30	3	O	O	0.168	1.0	-1.0	Ti	6.00	18	O	O	0.196	4.0	-1.0
Ti	3.30	4	O	O	0.224	1.0	1.0	Ti	6.00	19	O	Ti	0.007	1.0	-1.0
Ti	3.30	5	O	Ti	0.112	1.0	-1.0	Ti	6.00	20	O	Ti	0.007	2.0	1.0
Ti	3.30	6	O	Ti	0.112	4.0	1.0	Ti	6.00	21	O	Ti	0.140	1.0	-1.0
Ti	3.30	7	O	Ti	0.168	1.0	-1.0	Ti	6.00	22	O	Ti	0.140	4.0	1.0
Ti	3.30	8	O	Ti	0.224	1.0	1.0	Ti	6.00	23	O	Ti	0.196	1.0	1.0
Ti	3.30	9	Ti	Ti	0.112	1.0	-1.0	Ti	6.00	24	O	Ti	0.196	4.0	-1.0
Ti	3.30	10	Ti	Ti	0.112	4.0	1.0	Ti	6.00	25	Ti	Ti	0.007	1.0	-1.0
Ti	3.30	11	Ti	Ti	0.168	1.0	-1.0	Ti	6.00	26	Ti	Ti	0.007	2.0	1.0
Ti	3.30	12	Ti	Ti	0.224	1.0	1.0	Ti	6.00	27	Ti	Ti	0.140	1.0	-1.0
Ti	6.00	13	O	O	0.007	1.0	-1.0	Ti	6.00	28	Ti	Ti	0.140	4.0	1.0
Ti	6.00	14	O	O	0.007	2.0	1.0	Ti	6.00	29	Ti	Ti	0.196	1.0	1.0
Ti	6.00	15	O	O	0.140	1.0	-1.0	Ti	6.00	30	Ti	Ti	0.196	4.0	-1.0

4. Comparison of the performance for symmetry functions with different numbers of cutoff radii.

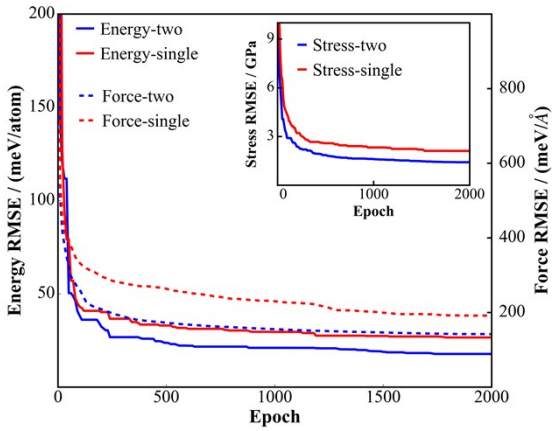

Figure S1. Comparison of the performance for symmetry functions with 2-cutoffs (blue) and single-cutoff (red) radius (R_c in Eq. 2 of main text) by showing the evolution of RMSEs of energy (meV / atom) and force (meV / Å) in the training set during the NN training. 2-cutoffs symmetry functions correspond to Table S1-S5 NN parameters; 1-cutoff symmetry functions correspond to Table S1-S5 NN parameters except all R_c=3.3 are replaced by R_c=6.0. Solid lines: RMSEs of energy; Dashed lines: RMSEs of forces. The inset is the comparison for the stress.

5. Comparison of the computational cost for NN and DFT calculations.

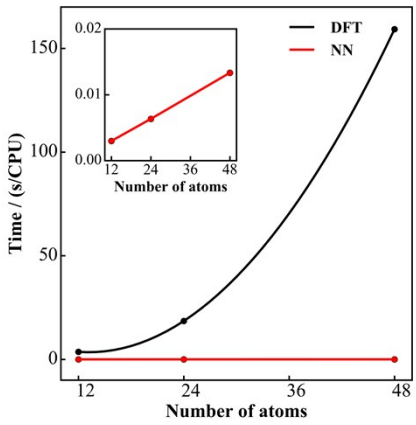

Figure S2. Computational time (s/CPU) of single point calculation for different size TiO_2 systems (12, 24 and 48 atoms in a unit cell) by DFT (black) and NN (red). The inset rescales y-axis to illustrate the NN performance better. Also see Table S7 for the data.

Table S7. Computation time (seconds per CPU, each CPU contains 24 cores) in a single point energy calculation for different TiO_2 systems (12, 24 and 48 atoms in one unit cell) by DFT and by NN.

TiO_2	T_{low}*	T_{high}*	T_{NN}*	S_{low}‡	S_{high}‡
12-atom	7.2	96.0	0.13	55	738
24-atom	62.4	672.0	0.26	240	2584
48-atom	631.2	8205.6	0.39	1618	21040

* T_{low}: time using low precision DFT ((Ti PAW potential with 4 electrons (Ti: $3d^24s^2$); (4×4×4) k-points and 400 eV cutoff); T_{high}: time using high precision DFT (Ti PAW potential with 10 electrons (Ti: $3p^63d^24s^2$); (6×6×6) k-points and 600 eV cutoff); $T_{NN:}$ time using NN calculations that utilizes only one CPU core per run.

‡ S_{low}/S_{high}: The scaling of NN with respect to low/high precision DFT.

Table S8 shows that tthe overall cost of SSW-NN for the global PES search of TiO_2 in 48-atom cell is still roughly four orders of magnitude lower than that of SSW-DFT.

Table S8. Computation time (10^6 seconds per CPU, each CPU contains 24 cores) of SSW global search for TiO_2 in 48-atom cell.

	SSW-NN	SSW-DFT_{low}	SSW-DFT_{high}
Comput. time	12.76 (0.94/4.80/7.02)	$1.14*10^4$	$1.48*10^5$

* The overall computational cost in SSW-NN is contributed from three sources, (i) SSW global search using low-precision DFT in 12-atom cell, which collects 130,000 structures from SSW trajectories; (ii) the high-precision DFT single-point calculations to construct training data set (50,000 structures); and (iii) SSW global search in 48-atom cell ($1.8*10^7$ energy/force evaluations to glean 60,000 minima). The data in parenthesis list the computation time for each part.

** The computational cost in SSW-DFT-low/high is estimated from SSW global search in 48-atom cell ($1.8*10^7$ energy/force evaluations) to identify 60,000 minima with the low/high DFT accuracy setups (also see Table S7).

6. Comparison of structural properties of experimentally known TiO_2 phase using NN and DFT PES.

Table S9. Comparison of the energy and lattice parameters of experimentally known structures of TiO_2 using NN PES and DFT calculations. All energies are with reference to that of GM (TiO_2-B).

No	Species	SG*	OP_2*	E_{DFT}/eV/f.u.	E_{NN}/eV/f.u.	dE**/eV/f.u.	V_{DFT}/Å^3/f.u.	V_{NN}/Å^3/f.u.	dV**/Å^3/f.u.
1	rutile	136	0.28	0.11	0.11	0.00	32.15	32.20	0.05
2	anatase	141	0.37	0.02	0.01	-0.01	35.19	35.17	-0.02
3	brookite	61	0.30	0.05	0.05	0.00	33.06	33.07	0.01
4	TiO_2(B)	12	0.52	0.00	-0.01	-0.01	36.66	36.82	0.16
5	TiO_2(H)	87	0.65	0.18	0.22	0.04	39.56	39.89	0.33
6	TiO_2(R)	62	0.34	0.18	0.19	0.01	35.31	35.69	0.38
7	TiO_2(II)	60	0.23	0.09	0.10	0.01	31.54	31.72	0.18
8	baddeleyite	14	0.18	0.20	0.21	0.01	29.89	29.91	0.02
9	TiO_2-OI	61	0.14	0.35	0.36	0.01	28.50	28.65	0.15
10	TiO_2-OII	62	0.02	0.87	0.85	-0.02	26.25	26.35	0.10

*SG: symmetry group; OP_2: Steinhardt-type order parameter (see Eq. 11);

** dE and dV: deviation of energy and volume from NN PES with respect to those (E_{DFT} and V_{DFT}) from DFT PES, respectively.

7. XYZ coordination of structures.

TiO2-B Energy from VASP is -107.69

```
!DATE
PBC      6.4304      3.7628      6.6265     89.9908    106.2060     72.9920
O      0.583206356     1.842667707     0.611031485     CORE     1     O     O     0.0000     1
O      4.852912827     0.536925427     5.001861099     CORE     2     O     O     0.0000     2
O      3.267794823     2.989255309     5.149575118     CORE     3     O     O     0.0000     3
O      3.268834054     2.988334428     0.463463701     CORE     4     O     O     0.0000     4
O      4.822747234     2.512947509     2.829482641     CORE     5     O     O     0.0000     5
O      0.545506551     1.854904490     4.666370234     CORE     6     O     O     0.0000     6
O      1.713743047     3.464882796     2.783458911     CORE     7     O     O     0.0000     7
O      4.890581050     0.524616285     0.946684241     CORE     8     O     O     0.0000     8
Ti     5.030237067     2.450060374     4.595621732     CORE     9     Ti    Ti    0.0000     9
Ti     1.549049436     3.515142833     4.644133649     CORE     10    Ti    Ti    0.0000     10
Ti     1.506476318     3.527856727     1.017392971     CORE     11    Ti    Ti    0.0000     11
Ti     4.987475916     2.462268399     0.968835576     CORE     12    Ti    Ti    0.0000     12
end
end
```

anatase Energy from VASP is -107.62

```
!DATE
PBC      5.3814      5.3813      5.5546    118.9567     89.9897     89.9978
O      4.194198606     0.856082428     2.579820839     CORE     1     O     O     0.0000     1
O      0.158673073     4.892198289     0.149748701     CORE     2     O     O     0.0000     2
O      1.503583919     3.546716138     2.579809188     CORE     3     O     O     0.0000     3
O      4.194514209     3.546897938     1.733259159     CORE     4     O     O     0.0000     4
O      2.849294535     2.201561852     0.149734903     CORE     5     O     O     0.0000     5
O      2.850637267     2.203090838     4.163341984     CORE     6     O     O     0.0000     6
O      1.503713032     0.856256749     1.733261386     CORE     7     O     O     0.0000     7
O      0.159823349     -0.487541830    4.163349920     CORE     8     O     O     0.0000     8
Ti     2.848871027     2.201289809     2.156503676     CORE     9     Ti    Ti    0.0000     9
Ti     4.196250059     0.857770012     4.586677458     CORE     10    Ti    Ti    0.0000     10
Ti     0.158051496     -0.489353156    2.156505204     CORE     11    Ti    Ti    0.0000     11
Ti     1.505462630     -1.832849123    4.586689365     CORE     12    Ti    Ti    0.0000     12
end
end
```

TiO2-II Energy from VASP is -107.32

```
!DATE
PBC      5.5782      4.5845      4.9336     89.9986     90.0000     89.9982
O      2.655829461     4.573045084     3.201128877     CORE     1     O     O     0.0000     1
O      3.987086485     4.573020961     0.734325392     CORE     2     O     O     0.0000     2
O      1.197925484     2.280816988     4.003218636     CORE     3     O     O     0.0000     3
O      5.444742859     2.280728980     1.536376872     CORE     4     O     O     0.0000     4
O      3.987017536     2.085187894     4.003065820     CORE     5     O     O     0.0000     5
O      2.655611840     2.085119376     1.536287472     CORE     6     O     O     0.0000     6
O      5.444867602     4.377405597     3.201102411     CORE     7     O     O     0.0000     7
O      1.197990440     4.377370075     0.734361893     CORE     8     O     O     0.0000     8
Ti     2.336869024     1.036666902     4.835611361     CORE     9     Ti    Ti    0.0000     9
Ti     5.125943791     3.328912914     4.835518682     CORE     10    Ti    Ti    0.0000     10
Ti     4.305828900     1.036696731     2.368706908     CORE     11    Ti    Ti    0.0000     11
Ti     1.516894587     3.328971422     2.368821752     CORE     12    Ti    Ti    0.0000     12
end
end
```

rutile Energy from VASP is -107.25

```
!DATE
PBC       5.5231       5.5229       4.6491      90.0127      89.9874     114.9372
O      3.206710125     4.875312726     4.082738586     CORE       1       O       O     0.0000       1
O      3.135355807     1.398276571     2.264141858     CORE       2       O       O     0.0000       2
O      1.971011238     3.902335742     1.763171760     CORE       3       O       O     0.0000       3
O      1.609429377     2.371291940     4.082724135     CORE       4       O       O     0.0000       4
O      4.371392056     2.371015026     4.593864082     CORE       5       O       O     0.0000       5
O      0.445521159     4.875053112     4.593852397     CORE       6       O       O     0.0000       6
O      0.373751649     1.398335351     1.763174150     CORE       7       O       O     0.0000       7
O     -0.790550723     3.902325833     2.264134949     CORE       8       O       O     0.0000       8
Ti     3.120578828     3.166075662     3.162235067     CORE       9      Ti      Ti     0.0000       9
Ti     0.359450991     3.165707320     0.860251469     CORE      10      Ti      Ti     0.0000      10
Ti     4.285121573     0.661759475     0.859772344     CORE      11      Ti      Ti     0.0000      11
Ti     1.523354732     0.662112520     3.162098123     CORE      12      Ti      Ti     0.0000      12
end
end
```

Str-1 Energy from VASP is -107.20

```
!DATE
PBC       8.0611       8.0631       5.9485      68.4633     111.6457      92.8532
O     -1.302320157     5.040501508     4.137228810     CORE       1       O       O     0.0000       1
O     -0.195070727     3.994643706     1.582453061     CORE       2       O       O     0.0000       2
O      1.268578344     3.506011922     4.149575341     CORE       3       O       O     0.0000       3
O     -1.330465840     2.143301850     3.585507681     CORE       4       O       O     0.0000       4
O      4.933092024     0.930782837     1.587825913     CORE       5       O       O     0.0000       5
O      3.838716495     1.968275715     4.151339823     CORE       6       O       O     0.0000       6
O      5.098199777     7.531279249     4.149822886     CORE       7       O       O     0.0000       7
O      3.869874762     4.863501881     4.711176136     CORE       8       O       O     0.0000       8
Ti     4.843603654     9.159627174     3.375242474     CORE       9      Ti      Ti     0.0000       9
Ti     2.906385832     3.329820636     4.925161378     CORE      10      Ti      Ti     0.0000      10
Ti    -0.367576692     3.677321107     3.369516885     CORE      11      Ti      Ti     0.0000      11
Ti     5.355308420     5.900904752     4.919529377     CORE      12      Ti      Ti     0.0000      12
end
end
```

Str-2 Energy from VASP is -107.14

```
!DATE
PBC       5.8993       6.8748       6.1557     102.3379     117.9044      93.7558
O      1.801955829     3.569277669     0.060420798     CORE       1       O       O     0.0000       1
O     -0.191671612     5.225018718     1.282291004     CORE       2       O       O     0.0000       2
O     -2.070751520     4.748257556     3.850519296     CORE       3       O       O     0.0000       3
O     -0.077009894     3.092450350     2.629024480     CORE       4       O       O     0.0000       4
O      0.906188426     4.887035630     4.437929689     CORE       5       O       O     0.0000       5
O      0.232094015     1.299884064     0.574971091     CORE       6       O       O     0.0000       6
O     -0.050869794     0.157576473     3.335994357     CORE       7       O       O     0.0000       7
O      1.843594573     1.923928726     4.699894788     CORE       8       O       O     0.0000       8
Ti    -0.423023291     5.167385441     3.200288158     CORE       9      Ti      Ti     0.0000       9
Ti     2.576905751     4.991864681     5.156494505     CORE      10      Ti      Ti     0.0000      10
Ti     0.154172001     3.150187049     0.710730356     CORE      11      Ti      Ti     0.0000      11
Ti     0.172825678     1.818389519     3.981545837     CORE      12      Ti      Ti     0.0000      12
end
end
```

lepidocrocite Energy from VASP is -106.99

```
!DATE
PBC       4.8158       4.8158       9.2595      58.5131      96.2773     102.1620
O      1.322927203     5.796281737     3.577153131     CORE       1       O       O     0.0000       1
O      1.322872063     5.796766856     6.240600409     CORE       2       O       O     0.0000       2
```

```
O     -1.085077270    5.796434527    1.931730499    CORE    3    O    O    0.0000    3
O     1.830312750     3.442532548    4.595204295    CORE    4    O    O    0.0000    4
O     -1.084860546    5.796410092    4.595204295    CORE    5    O    O    0.0000    5
O     -1.592301233    8.150644399    6.240600409    CORE    6    O    O    0.0000    6
O     1.830096026     3.442556984    1.931730500    CORE    7    O    O    0.0000    7
O     -0.577657656    3.442404193    3.577153130    CORE    8    O    O    0.0000    8
Ti    0.372833114     4.619615543    5.205280234    CORE    9    Ti   Ti   0.0000    9
Ti    2.780490140     4.619381317    2.967076083    CORE    10   Ti   Ti   0.0000    10
Ti    2.273417972     6.973493087    5.205280234    CORE    11   Ti   Ti   0.0000    11
Ti    0.879905282     2.265503774    2.967076082    CORE    12   Ti   Ti   0.0000    12
end
end

    TiO2-R          Energy from VASP is -106.98
!DATE
PBC     9.5346      2.9807      4.9697      90.0000     89.9874     90.0000
O     9.250472601     0.745186196     3.955928451     CORE    1    O    O    0.0000    1
O     2.543027823     0.745185938     1.820819256     CORE    2    O    O    0.0000    2
O     5.053269320     2.235515369     1.471344893     CORE    3    O    O    0.0000    3
O     2.225413683     2.235514994     4.305858904     CORE    4    O    O    0.0000    4
O     0.285213295     2.235515242     1.013718398     CORE    5    O    O    0.0000    5
O     6.992711083     2.235515024     3.148735299     CORE    6    O    O    0.0000    6
O     4.482492335     0.745185796     3.498364500     CORE    7    O    O    0.0000    7
O     7.310159186     0.745185664     0.663745731     CORE    8    O    O    0.0000    8
Ti    1.312515779     0.745186028     0.398085138     CORE    9    Ti   Ti   0.0000    9
Ti    3.455318003     2.235515784     2.882509640     CORE    10   Ti   Ti   0.0000    10
Ti    8.223160766     2.235515853     4.571564302     CORE    11   Ti   Ti   0.0000    11
Ti    6.080341397     0.745186182     2.087224789     CORE    12   Ti   Ti   0.0000    12
end
end

    TiO2-H          Energy from VASP is -106.97
!DATE
PBC     7.4357      7.4367      2.9812      78.4418     101.5642    92.3150
O     2.301270862     7.153607639     0.598271524     CORE    1    O    O    0.0000    1
O     5.033741933     2.908725785     0.467579271     CORE    2    O    O    0.0000    2
O     4.236413917     0.850632071     2.265509473     CORE    3    O    O    0.0000    3
O     1.503947385     5.095569340     2.396193876     CORE    4    O    O    0.0000    4
O     6.755523488     4.811372539     0.445757690     CORE    5    O    O    0.0000    5
O     2.403391580     2.499104005     1.552667186     CORE    6    O    O    0.0000    6
O     -0.217821413    3.192921995     2.418009631     CORE    7    O    O    0.0000    7
O     4.134231022     5.505209580     1.311084134     CORE    8    O    O    0.0000    8
Ti    3.830110043     1.470289167     0.505210106     CORE    9    Ti   Ti   0.0000    9
Ti    2.707567933     6.533979771     2.358563092     CORE    10   Ti   Ti   0.0000    10
Ti    1.015337433     3.648749000     1.032638809     CORE    11   Ti   Ti   0.0000    11
Ti    5.522360072     4.355517238     1.831132974     CORE    12   Ti   Ti   0.0000    12
end
end

    baddeleyite         Energy from VASP is -106.91
!DATE
PBC     4.8534      5.0956      4.9099      89.9962     90.0001     100.0987
O     0.092611133     0.124278447     4.231390402     CORE    1    O    O    0.0000    1
O     2.724459787     2.093200823     2.166300671     CORE    2    O    O    0.0000    2
O     2.277789540     4.601478183     2.085133135     CORE    3    O    O    0.0000    3
O     2.286959669     1.703460486     4.540088916     CORE    4    O    O    0.0000    4
O     -0.354166690    2.632313847     0.019959797     CORE    5    O    O    0.0000    5
O     1.840153772     4.211787267     4.621178328     CORE    6    O    O    0.0000    6
```

```
O     0.512243252    1.163912441    1.776383844    CORE    7    O    O    0.0000    7
O     0.065435937    3.672271260    2.474995621    CORE    8    O    O    0.0000    8
Ti    3.335423032    3.323631682    3.629101341    CORE    9    Ti   Ti   0.0000    9
Ti    1.229069439    2.981079673    1.174206246    CORE    10   Ti   Ti   0.0000    10
Ti    3.782401731    0.815101600    0.622169350    CORE    11   Ti   Ti   0.0000    11
Ti    1.676014186    0.472891497    3.077286429    CORE    12   Ti   Ti   0.0000    12
end
end
```

Str-3 Energy from VASP is -106.79

```
!DATE
PBC     8.1377     5.5827     8.1097    77.2279   115.0775    77.5175
O     5.868971635    2.012104575    2.484667731    CORE    1    O    O    0.0000    1
O     7.945226094    5.276560441    0.686121521    CORE    2    O    O    0.0000    2
O     2.408985841    4.182532096    5.298365462    CORE    3    O    O    0.0000    3
O     6.969795475    4.623058661    3.426951470    CORE    4    O    O    0.0000    4
O     1.450988860    5.966791209    3.087043011    CORE    5    O    O    0.0000    5
O     3.804742005    6.732636391    4.837565122    CORE    6    O    O    0.0000    6
O     4.073939819    4.471017281    2.912760957    CORE    7    O    O    0.0000    7
O     5.055918829    2.948190089    5.156470215    CORE    8    O    O    0.0000    8
Ti    7.896030614    5.833088035    2.421635761    CORE    9    Ti   Ti   0.0000    9
Ti    2.908326187    5.376341016    4.007982538    CORE    10   Ti   Ti   0.0000    10
Ti    5.528888989    3.505460168    3.474252040    CORE    11   Ti   Ti   0.0000    11
Ti    3.339085169    2.676406857    5.752840050    CORE    12   Ti   Ti   0.0000    12
end
end
```

Str-4 Energy from VASP is -106.30

```
!DATE
PBC     3.4169     5.1875     8.6754    86.5497   101.3448    90.0459
O     1.076042399    1.141835544    6.709397986    CORE    1    O    O    0.0000    1
O     1.072230667    0.973182634    0.168346101    CORE    2    O    O    0.0000    2
O    -0.635863520    4.229521003    8.440496119    CORE    3    O    O    0.0000    3
O     1.074018404    2.126248253    2.831485910    CORE    4    O    O    0.0000    4
O     1.069697213    5.176622951    4.046253139    CORE    5    O    O    0.0000    5
O    -0.634037322    2.366902594    5.158369917    CORE    6    O    O    0.0000    6
O     1.072697533    3.593860196    6.927404914    CORE    7    O    O    0.0000    7
O     2.777727059    4.935909383    1.719574827    CORE    8    O    O    0.0000    8
Ti   -0.636038875    2.653687518    7.226786687    CORE    9    Ti   Ti   0.0000    9
Ti    1.073479671    0.424982420    2.216746229    CORE    10   Ti   Ti   0.0000    10
Ti    1.072823954    5.169858995    8.141136709    CORE    11   Ti   Ti   0.0000    11
Ti    1.074374377    1.690370849    4.660907849    CORE    12   Ti   Ti   0.0000    12
end
end
```

Str-5 Energy from VASP is -106.29

```
!DATE
PBC     8.0307     8.0256     5.8150   110.8864    69.0818    82.9311
O     3.591884064    1.911379118    2.172448537    CORE    1    O    O    0.0000    1
O     6.068317433    1.174807338    0.410385099    CORE    2    O    O    0.0000    2
O     8.924878934    3.132443563    2.367895761    CORE    3    O    O    0.0000    3
O     9.220231305    0.205872842    2.840501788    CORE    4    O    O    0.0000    4
O     8.040887783    5.960827269    2.547620878    CORE    5    O    O    0.0000    5
O     6.635925578    0.545533258    4.311507528    CORE    6    O    O    0.0000    6
O     6.058637220    3.780450726    1.884495975    CORE    7    O    O    0.0000    7
O    10.221167175    2.179108589    4.813112225    CORE    8    O    O    0.0000    8
Ti    1.988922690    1.844426812    3.034503581    CORE    9    Ti   Ti   0.0000    9
Ti    5.001858090    2.478630288    1.157684187    CORE    10   Ti   Ti   0.0000    10
```

```
Ti     7.782585370     4.373609951     1.692428650     CORE     11     Ti     Ti     0.0000     11
Ti     7.793761871     -0.677949975    3.564450202     CORE     12     Ti     Ti     0.0000     12
end
end
```

Str-6 Energy from VASP is -105.96

```
!DATE
PBC     3.1722     7.5314     6.0514    104.7018    105.1494     77.9269
O     1.983414512     0.354015447     0.678750650     CORE     1     O     O     0.0000     1
O     0.390478552     4.325732397     5.242460023     CORE     2     O     O     0.0000     2
O     1.979767882     1.581323454     4.160842142     CORE     3     O     O     0.0000     3
O     1.975711568     2.929227058     0.249614211     CORE     4     O     O     0.0000     4
O     0.390723125     1.725342645     2.238470063     CORE     5     O     O     0.0000     5
O     1.974254360     6.514999894     2.667678506     CORE     6     O     O     0.0000     6
O     -1.186828335    -0.734684252    4.466161101     CORE     7     O     O     0.0000     7
O     1.977183456     3.886057570     3.385642779     CORE     8     O     O     0.0000     8
Ti     1.974708686     5.408297113     4.470116849     CORE     9     Ti     Ti     0.0000     9
Ti     0.393336880     2.803540473     4.157750333     CORE     10     Ti     Ti     0.0000     10
Ti     0.384928593     1.799976290     0.307226417     CORE     11     Ti     Ti     0.0000     11
Ti     1.990539418     0.279140984     2.610300749     CORE     12     Ti     Ti     0.0000     12
end
end
```

Str-7 Energy from VASP is -105.82

```
!DATE
PBC     2.9553     5.9700     9.3990     74.2814     89.9993     90.0006
O     0.791684930     7.615440174     8.610241779     CORE     1     O     O     0.0000     1
O     0.791609498     3.553443003     3.929106915     CORE     2     O     O     0.0000     2
O     2.269279723     5.755215887     2.760823043     CORE     3     O     O     0.0000     3
O     0.791452990     7.283976966     5.001353159     CORE     4     O     O     0.0000     4
O     2.269339579     3.678447097     1.377576459     CORE     5     O     O     0.0000     5
O     2.269342529     4.007270431     9.008612214     CORE     6     O     O     0.0000     6
O     2.269293666     3.123995044     6.574284777     CORE     7     O     O     0.0000     7
O     0.791670891     5.445471125     7.581615779     CORE     8     O     O     0.0000     8
Ti     2.269160985     2.402132863     4.869459463     CORE     9     Ti     Ti     0.0000     9
Ti     0.791742354     3.422232939     7.972954274     CORE     10     Ti     Ti     0.0000     10
Ti     0.791610701     4.682557242     2.482100854     CORE     11     Ti     Ti     0.0000     11
Ti     2.269347594     6.139620602     8.599850851     CORE     12     Ti     Ti     0.0000     12
end
end
```

Str-8 Energy from VASP is -105.65

```
!DATE
PBC     7.8704     7.5524     2.9162     89.4477     83.9347    107.5610
O     4.852963740     3.741068877     1.008911947     CORE     1     O     O     0.0000     1
O     4.234893082     0.251018308     1.275088135     CORE     2     O     O     0.0000     2
O     6.432399842     1.747424407     2.362241556     CORE     3     O     O     0.0000     3
O     2.830709831     5.037127687     2.642726719     CORE     4     O     O     0.0000     4
O     -0.504853174    3.930222178     0.729971767     CORE     5     O     O     0.0000     5
O     1.728457693     0.180006311     1.544180721     CORE     6     O     O     0.0000     6
O     4.448837054     6.540980642     0.924996734     CORE     7     O     O     0.0000     7
O     2.855866076     2.517891426     2.759485564     CORE     8     O     O     0.0000     8
Ti     3.075327481     3.840485504     1.199371540     CORE     9     Ti     Ti     0.0000     9
Ti     6.494366268     3.518367029     2.302938373     CORE     10     Ti     Ti     0.0000     10
Ti     3.653969657     7.165554947     2.410480133     CORE     11     Ti     Ti     0.0000     11
Ti     2.910818236     0.654561615     2.856968722     CORE     12     Ti     Ti     0.0000     12
end
end
```

TiO2-OII Energy from VASP is -104.21

```
!DATE
PBC      3.1747      6.3125      5.2386     90.1138     89.9999     90.0110
O      2.410624712     5.292048280     2.667179022     CORE     1     O     O     0.0000     1
O      0.824035880     2.129203698     5.156664289     CORE     2     O     O     0.0000     2
O      0.824557299     0.897448688     2.539497205     CORE     3     O     O     0.0000     3
O      2.411480559     4.061321129     0.056831716     CORE     4     O     O     0.0000     4
O      0.823564506     5.721239749     4.509014515     CORE     5     O     O     0.0000     5
O      2.411560690     2.570818515     3.319468222     CORE     6     O     O     0.0000     6
O      2.411729665     0.466341321     0.697486462     CORE     7     O     O     0.0000     7
O      0.823871852     3.616592051     1.893824964     CORE     8     O     O     0.0000     8
Ti     2.412113809     0.591082712     3.896715140     CORE     9     Ti    Ti    0.0000     9
Ti     0.824242527     3.745868410     3.932681043     CORE     10    Ti    Ti    0.0000     10
Ti     0.823111421     5.595303970     1.310487526     CORE     11    Ti    Ti    0.0000     11
Ti     2.411312641     2.440943172     1.279314338     CORE     12    Ti    Ti    0.0000     12
end
end
```

TiO2-OI Energy from VASP is -212.57

```
!DATE
PBC      9.4352      4.9894      4.8433     90.0000     90.0000     90.0000
O      6.713616664     4.367977188     0.670449006     CORE     1     O     O     0.0000     1
O      4.951016256     1.185106423     2.403201071     CORE     2     O     O     0.0000     2
O      7.439169497     0.621467312     3.092106240     CORE     3     O     O     0.0000     3
O      9.201774917     3.804305446     4.824871544     CORE     4     O     O     0.0000     4
O      2.721542933     1.873264596     1.751265005     CORE     5     O     O     0.0000     5
O      4.484143627     3.679819340     0.018514634     CORE     6     O     O     0.0000     6
O      1.995993934     3.116180635     4.172941733     CORE     7     O     O     0.0000     7
O      0.233388044     1.309591557     2.440175599     CORE     8     O     O     0.0000     8
O      2.721544373     0.621435397     4.172932236     CORE     9     O     O     0.0000     9
O      4.484145555     3.804305925     2.440180227     CORE     10    O     O     0.0000     10
O      1.995991801     4.367945329     1.751274732     CORE     11    O     O     0.0000     11
O      0.233386381     1.185107458     0.018509614     CORE     12    O     O     0.0000     12
O      6.713618187     3.116148055     3.092116246     CORE     13    O     O     0.0000     13
O      4.951018241     1.309593457     4.824866763     CORE     14    O     O     0.0000     14
O      7.439167329     1.873232129     0.670439300     CORE     15    O     O     0.0000     15
O      9.201773205     3.679820626     2.403205695     CORE     16    O     O     0.0000     16
Ti     1.085403067     2.703701099     1.212470027     CORE     17    Ti    Ti    0.0000     17
Ti     3.632126790     2.285714790     3.634129317     CORE     18    Ti    Ti    0.0000     18
Ti     8.349757185     0.208987620     1.209245214     CORE     19    Ti    Ti    0.0000     19
Ti     5.803036438     4.780427178     3.630918364     CORE     20    Ti    Ti    0.0000     20
Ti     8.349758899     2.285711609     3.630911219     CORE     21    Ti    Ti    0.0000     21
Ti     5.803034034     2.703698102     1.209251901     CORE     22    Ti    Ti    0.0000     22
Ti     1.085404823     4.780424766     3.634136035     CORE     23    Ti    Ti    0.0000     23
Ti     3.632124309     0.208985105     1.212462930     CORE     24    Ti    Ti    0.0000     24
end
end
```

brookite Energy from VASP is -429.98

```
!DATE
PBC     10.7943      5.1725     10.7892     89.9999    118.5747     90.0002
O     -2.875841735     3.602509630     5.348084071     CORE     1     O     O     0.0000     1
O      3.158796423     3.182974405     6.419112255     CORE     2     O     O     0.0000     2
O     -4.215074226     4.353236874     7.815537779     CORE     3     O     O     0.0000     3
O     -0.829921589     1.016098200     8.788134382     CORE     4     O     O     0.0000     4
O      7.750752288     5.018308903     0.708477931     CORE     5     O     O     0.0000     5
O      7.147244304     1.016121625     4.050375749     CORE     6     O     O     0.0000     6
```

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O     0.349244915    2.432212477    6.415862105    CORE    7    O    O    0.0000    7
O    -2.542358525    1.016205180    6.599940841    CORE    8    O    O    0.0000    8
O     3.761790011    4.353217513    3.078210836    CORE    9    O    O    0.0000    9
O     4.263562617    3.182736349    8.968504928    CORE   10    O    O    0.0000   10
O     1.446158320    3.182681086    4.231365665    CORE   11    O    O    0.0000   11
O     5.027170269    5.018640549    5.532239736    CORE   12    O    O    0.0000   12
O     2.209979308    5.018565393    0.795043011    CORE   13    O    O    0.0000   13
O     4.338197434    1.766731192    4.047236609    CORE   14    O    O    0.0000   14
O     2.217472475    0.596637278    5.528751628    CORE   15    O    O    0.0000   15
O     5.434868938    1.016375836    1.862319200    CORE   16    O    O    0.0000   16
O    -1.771143608    3.602268900    7.897626298    CORE   17    O    O    0.0000   17
O     8.326756463    2.432235317    1.678026805    CORE   18    O    O    0.0000   18
O     5.603152946    2.432164998    6.501623918    CORE   19    O    O    0.0000   19
O     5.101572079    3.602663355    0.610672981    CORE   20    O    O    0.0000   20
O    -3.638866570    1.766743497    8.784948191    CORE   21    O    O    0.0000   21
O    10.194928179    0.596727937    0.790887413    CORE   22    O    O    0.0000   22
O     9.014832315    4.353127597    3.162992236    CORE   23    O    O    0.0000   23
O     3.929989888    0.596545484    7.716608522    CORE   24    O    O    0.0000   24
O     1.037852835    4.353014562    7.900730949    CORE   25    O    O    0.0000   25
O     1.614223300    1.767063394    8.869990338    CORE   26    O    O    0.0000   26
O    -1.203075104    1.767126545    4.132688683    CORE   27    O    O    0.0000   27
O    -0.226973028    5.018237874    5.446254238    CORE   28    O    O    0.0000   28
O     0.341619083    3.183011510    1.681903723    CORE   29    O    O    0.0000   29
O     2.785730985    2.432124510    1.764478852    CORE   30    O    O    0.0000   30
O     1.112321211    0.596472371    2.979408037    CORE   31    O    O    0.0000   31
O     6.205984518    3.602322603    3.159895673    CORE   32    O    O    0.0000   32
Ti    9.430142606    4.114803320    1.364630443    CORE   33    Ti   Ti   0.0000   33
Ti    4.563878546    2.670840119    2.259669122    CORE   34    Ti   Ti   0.0000   34
Ti   -2.535737684    0.084365403    8.471877754    CORE   35    Ti   Ti   0.0000   35
Ti    5.441479626    0.084501179    3.733728341    CORE   36    Ti   Ti   0.0000   36
Ti    3.392332004    1.528348276    9.365317407    CORE   37    Ti   Ti   0.0000   37
Ti    1.983732344    4.114583943    2.582663974    CORE   38    Ti   Ti   0.0000   38
Ti   -0.065294441    2.670739032    8.214261317    CORE   39    Ti   Ti   0.0000   39
Ti    1.106274367    1.528594997    1.108290090    CORE   40    Ti   Ti   0.0000   40
Ti    1.452996335    4.114684278    6.102309735    CORE   41    Ti   Ti   0.0000   41
Ti    7.911841666    2.670650138    3.476235527    CORE   42    Ti   Ti   0.0000   42
Ti    0.574655329    1.528216453    4.628511943    CORE   43    Ti   Ti   0.0000   43
Ti    4.801567099    4.114521240    7.319468161    CORE   44    Ti   Ti   0.0000   44
Ti   -2.005179451    0.084388176    4.950897703    CORE   45    Ti   Ti   0.0000   45
Ti   -3.412901056    2.670580066    6.997118548    CORE   46    Ti   Ti   0.0000   46
Ti    3.923261657    1.528501955    5.845690514    CORE   47    Ti   Ti   0.0000   47
Ti    5.972585246    0.084604998    0.213351313    CORE   48    Ti   Ti   0.0000   48
end
end

      phase-87                Energy from VASP is -429.95
!DATE
PBC      3.7505     15.5832     15.5604     94.0894    103.9334     76.0736
O     3.301163236    1.259446670    2.899229677    CORE    1    O    O    0.0000    1
O     3.301276295    7.338823944    2.369563555    CORE    2    O    O    0.0000    2
O     3.301795401    4.557046194    5.685874557    CORE    3    O    O    0.0000    3
O     1.426716811    3.933814346    7.133418440    CORE    4    O    O    0.0000    4
O     1.425523608    5.668962020    1.138626605    CORE    5    O    O    0.0000    5
O     1.425731085    2.713930390    1.179993746    CORE    6    O    O    0.0000    6
O     1.425732264    2.928891975    4.130380043    CORE    7    O    O    0.0000    7
O     1.426294362    5.884212761    4.088889575    CORE    8    O    O    0.0000    8
O     5.176408833    8.822017960    2.899229677    CORE    9    O    O    0.0000    9
O     5.176521892   14.901395234    2.369563555    CORE   10    O    O    0.0000   10
```

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O     5.177040998   12.119617484   5.685874557   CORE   11   O   O   0.0000   11
O     3.301962408   11.496385636   7.133418440   CORE   12   O   O   0.0000   12
O     3.300769205   13.231533310   1.138626605   CORE   13   O   O   0.0000   13
O     3.300976682   10.276501680   1.179993746   CORE   14   O   O   0.0000   14
O     3.300977861   10.491463265   4.130380043   CORE   15   O   O   0.0000   15
O     3.301539959   13.446784051   4.088889575   CORE   16   O   O   0.0000   16
O     1.427738760   1.152357112    10.449747845  CORE   17   O   O   0.0000   17
O     1.427851819   7.231734386    9.920081723   CORE   18   O   O   0.0000   18
O     1.428370925   4.449956636    13.236392725  CORE   19   O   O   0.0000   19
O     -0.446707665  3.826724788    14.683936608  CORE   20   O   O   0.0000   20
O     -0.447900868  5.561872462    8.689144773   CORE   21   O   O   0.0000   21
O     -0.447693391  2.606840832    8.730511914   CORE   22   O   O   0.0000   22
O     -0.447692212  2.821802417    11.680898211  CORE   23   O   O   0.0000   23
O     -0.447130114  5.777123203    11.639407743  CORE   24   O   O   0.0000   24
O     3.302984358   8.714928401    10.449747845  CORE   25   O   O   0.0000   25
O     3.303097417   14.794305675   9.920081723   CORE   26   O   O   0.0000   26
O     3.303616523   12.012527925   13.236392725  CORE   27   O   O   0.0000   27
O     1.428537933   11.389296077   14.683936608  CORE   28   O   O   0.0000   28
O     1.427344730   13.124443751   8.689144773   CORE   29   O   O   0.0000   29
O     1.427552207   10.169412121   8.730511914   CORE   30   O   O   0.0000   30
O     1.427553386   10.384373706   11.680898211  CORE   31   O   O   0.0000   31
O     1.428115484   13.339694492   11.639407743  CORE   32   O   O   0.0000   32
Ti    1.426420275   4.370020276    5.176563333   CORE   33   Ti  Ti  0.0000   33
Ti    1.426091992   6.842279153    2.586646288   CORE   34   Ti  Ti  0.0000   34
Ti    1.424945584   4.228027082    0.092251333   CORE   35   Ti  Ti  0.0000   35
Ti    1.425856300   1.755850795    2.682191476   CORE   36   Ti  Ti  0.0000   36
Ti    3.301665872   11.932591566   5.176563333   CORE   37   Ti  Ti  0.0000   37
Ti    3.301337589   14.404850443   2.586646288   CORE   38   Ti  Ti  0.0000   38
Ti    3.300191181   11.790598372   0.092251333   CORE   39   Ti  Ti  0.0000   39
Ti    3.301101897   9.318422085    2.682191476   CORE   40   Ti  Ti  0.0000   40
Ti    -0.447004201  4.262930718    12.727081501  CORE   41   Ti  Ti  0.0000   41
Ti    -0.447332484  6.735189595    10.137164456  CORE   42   Ti  Ti  0.0000   42
Ti    -0.448478892  4.120937524    7.642769501   CORE   43   Ti  Ti  0.0000   43
Ti    -0.447568176  1.648761237    10.232709644  CORE   44   Ti  Ti  0.0000   44
Ti    1.428241397   11.825502007   12.727081501  CORE   45   Ti  Ti  0.0000   45
Ti    1.427913114   14.297760884   10.137164456  CORE   46   Ti  Ti  0.0000   46
Ti    1.426766706   11.683508813   7.642769501   CORE   47   Ti  Ti  0.0000   47
Ti    1.427677422   9.211332526    10.232709644  CORE   48   Ti  Ti  0.0000   48
end
end

      phase-139                Energy from VASP is -429.25
!DATE
PBC    11.1993    7.5881    11.1803    99.7705    88.4122    99.7535
O     6.077922890   2.803009270   0.972590490   CORE   1   O   O   0.0000   1
O     -0.464606670  5.528084860   6.942270980   CORE   2   O   O   0.0000   2
O     2.459517920   6.030872400   7.614437460   CORE   3   O   O   0.0000   3
O     6.104394510   6.656954600   3.935821890   CORE   4   O   O   0.0000   4
O     0.178186070   1.788869780   6.942153120   CORE   5   O   O   0.0000   5
O     5.615127420   -1.126237140  10.207240810  CORE   6   O   O   0.0000   6
O     1.293664470   1.980742830   10.244170920  CORE   7   O   O   0.0000   7
O     4.630168500   4.478986900   8.689008530   CORE   8   O   O   0.0000   8
O     0.650905370   5.720025120   10.244162900  CORE   9   O   O   0.0000   9
O     6.747128940   2.917784590   3.935789770   CORE   10  O   O   0.0000   10
O     8.119048280   1.228887370   5.819181630   CORE   11  O   O   0.0000   11
O     3.102309860   2.291685310   7.614416540   CORE   12  O   O   0.0000   12
O     7.476264760   4.968148650   5.819233710   CORE   13  O   O   0.0000   13
O     8.161297580   1.236242410   2.076068740   CORE   14  O   O   0.0000   14
```

O 5.435138610 6.542199870 0.972562990 CORE 15 O O 0.0000 15
O 1.593073970 0.107361620 8.726133370 CORE 16 O O 0.0000 16
O 2.511114960 6.039797480 0.301355960 CORE 17 O O 0.0000 17
O 9.937094120 -0.383388890 5.837913900 CORE 18 O O 0.0000 18
O 10.066293800 5.413435430 3.978887860 CORE 19 O O 0.0000 19
O 4.972390110 2.613011070 10.207207470 CORE 20 O O 0.0000 20
O 7.518595730 4.975418680 2.076043250 CORE 21 O O 0.0000 21
O 8.693845160 7.102329910 2.096215840 CORE 22 O O 0.0000 22
O 6.656954300 -0.947149290 6.885787320 CORE 23 O O 0.0000 23
O 5.272874860 0.739833990 8.688996640 CORE 24 O O 0.0000 24
O 9.294383970 3.355767270 5.837900330 CORE 25 O O 0.0000 25
O -0.401175440 5.539234510 1.028702280 CORE 26 O O 0.0000 26
O 0.241593750 1.800035390 1.028570000 CORE 27 O O 0.0000 27
O 6.014190290 2.792022990 6.885862230 CORE 28 O O 0.0000 28
O 9.336560310 3.363198700 2.096216730 CORE 29 O O 0.0000 29
O 3.153816220 2.300596800 0.301371360 CORE 30 O O 0.0000 30
O 0.950311810 3.846588300 8.726095360 CORE 31 O O 0.0000 31
O 10.709082760 1.674228930 3.978898780 CORE 32 O O 0.0000 32
Ti 9.474342310 5.311717500 2.258238810 CORE 33 Ti Ti 0.0000 33
Ti 10.079268550 1.565835970 5.684974360 CORE 34 Ti Ti 0.0000 34
Ti 1.770151710 0.137898300 10.710602680 CORE 35 Ti Ti 0.0000 35
Ti 0.778852070 5.741931740 8.255652100 CORE 36 Ti Ti 0.0000 36
Ti 1.127455250 3.877101980 10.710597330 CORE 37 Ti Ti 0.0000 37
Ti 6.733717470 6.765300950 2.229499790 CORE 38 Ti Ti 0.0000 38
Ti 1.421599720 2.002736320 8.255627760 CORE 39 Ti Ti 0.0000 39
Ti 9.436496190 5.305033530 5.685038490 CORE 40 Ti Ti 0.0000 40
Ti 10.117068730 1.572505780 2.258258810 CORE 41 Ti Ti 0.0000 41
Ti 5.144046100 0.717690910 10.677666460 CORE 42 Ti Ti 0.0000 42
Ti 7.338554770 3.019556600 5.656680890 CORE 43 Ti Ti 0.0000 43
Ti 4.501268540 4.456903090 10.677672760 CORE 44 Ti Ti 0.0000 44
Ti 5.438660070 -1.156533490 8.222609290 CORE 45 Ti Ti 0.0000 45
Ti 7.981277490 -0.719645150 5.656695610 CORE 46 Ti Ti 0.0000 46
Ti 4.795961520 2.582677790 8.222597580 CORE 47 Ti Ti 0.0000 47
Ti 7.376466830 3.026088080 2.229502730 CORE 48 Ti Ti 0.0000 48
end
end

IS (phase-87) of pathway between phase-87 to anatase Energy from VASP is -107.48
!DATE
PBC 3.7347 7.8225 7.7649 94.5674 103.9351 76.1829
O 3.285903140 1.234500890 2.919231410 CORE 1 O O 0.0000 1
O 3.286738670 7.353537630 2.338462710 CORE 2 O O 0.0000 2
O 3.284469530 4.567030680 5.688790040 CORE 3 O O 0.0000 3
O 1.417329970 3.843997050 7.103139280 CORE 4 O O 0.0000 4
O 1.419599090 5.637960560 1.163501350 CORE 5 O O 0.0000 5
O 1.419419960 2.684431140 1.163426780 CORE 6 O O 0.0000 6
O 1.417756340 2.949995190 4.094109870 CORE 7 O O 0.0000 7
O 1.418368710 5.903270370 4.093976730 CORE 8 O O 0.0000 8
Ti 1.416798560 4.369748510 5.164059450 CORE 9 Ti Ti 0.0000 9
Ti 1.419353600 6.847812580 2.586676040 CORE 10 Ti Ti 0.0000 10
Ti 1.420208730 4.218084290 0.093592320 CORE 11 Ti Ti 0.0000 11
Ti 1.418628190 1.740178950 2.670813760 CORE 12 Ti Ti 0.0000 12
end
end
FS (anatase) of pathway between phase-87 to anatase Energy from VASP is -107.62
!DATE
PBC 3.8035 7.7325 5.5562 112.3479 110.0077 75.7697
O 3.347004150 0.471511740 1.119754860 CORE 1 O O 0.0000 1

O 1.445474330 -0.555893800 2.324828440 CORE 2 O O 0.0000 2
O 3.346986970 3.368631000 3.587193420 CORE 3 O O 0.0000 3
O 1.445429830 2.345394590 4.795858920 CORE 4 O O 0.0000 4
O 1.444934360 4.943147220 1.737292520 CORE 5 O O 0.0000 5
O -0.456077130 0.346832350 4.205188400 CORE 6 O O 0.0000 6
O 1.444964430 2.467686990 1.708032810 CORE 7 O O 0.0000 7
O 1.444822080 5.367130390 4.177144380 CORE 8 O O 0.0000 8
Ti 1.445072490 3.642388430 3.263498930 CORE 9 Ti Ti 0.0000 9
Ti -0.455947940 -0.827873940 2.650748680 CORE 10 Ti Ti 0.0000 10
Ti 1.445413030 3.768665230 0.182333090 CORE 11 Ti Ti 0.0000 11
Ti 1.445364800 0.743729020 0.794478750 CORE 12 Ti Ti 0.0000 12
end
end

TS of pathway between phase-87 to anatase Energy from VASP is -106.74
!DATE
PBC 3.7976 8.0543 6.0104 104.4287 108.4121 76.3682
O 3.341917558 0.910533440 1.569423090 CORE 1 O O 0.0000 1
O 1.443324878 -0.377184201 2.509462438 CORE 2 O O 0.0000 2
O 3.341591052 3.746384816 4.051733856 CORE 3 O O 0.0000 3
O 1.443027640 3.146012868 5.504025290 CORE 4 O O 0.0000 4
O 1.443245052 5.568388539 1.368788185 CORE 5 O O 0.0000 5
O -0.455304603 1.043822888 5.412711344 CORE 6 O O 0.0000 6
O 1.442797161 3.073205238 2.150150228 CORE 7 O O 0.0000 7
O 1.443243772 5.883803145 4.063042030 CORE 8 O O 0.0000 8
Ti 1.442807948 4.110225891 3.823426058 CORE 9 Ti Ti 0.0000 9
Ti 1.443182014 6.922422129 2.483566700 CORE 10 Ti Ti 0.0000 10
Ti 1.442857057 3.962878163 0.247236248 CORE 11 Ti Ti 0.0000 11
Ti 1.443006896 1.354981002 1.459212569 CORE 12 Ti Ti 0.0000 12
end
end