Supplementary Information Iterative training set refinement enables reactive molecular dynamics via machine learned forces

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Radial, angular narrow and angular wide symmetry functions are defined as (1-3) respectively that are originally from Ref.¹⁻³.

$$G_{i}^{rad} = \sum_{i \neq i} e^{-\eta (R_{ij} - R_s)^2} f_c(R_{ij})$$
(1)

$$G_{i}^{ang.n.} = 2^{1-\zeta} \sum_{\substack{j,k \neq i \\ j < k}}^{all} (1 + \lambda \cos \theta_{ijk})^{\zeta} e^{-\eta \left(R_{ij}^{2} + R_{ik}^{2} + R_{jk}^{2}\right)} f_{c}(R_{ij}) f_{c}(R_{ik}) f_{c}(R_{jk})$$
(2)

$$G_{i}^{ang.w.} = 2^{1-\zeta} \sum_{\substack{j,k \neq i \\ j < k}}^{all} (1 + \lambda \cos \theta_{ijk})^{\zeta} e^{-\eta \left(R_{ij}^{2} + R_{ik}^{2}\right)} f_{c}(R_{ij}) f_{c}(R_{ik})$$
(3)

Table S1 Parameters of symmetry functions employed to describe the local atomic environments in the input layer of neural network. R_c is the cutoff radius and the meaning of the rest parameters refer to the definitions in articles.¹⁻³

	Syn	nmetry functi	ons of type (rad i
No.		η (Bohr ⁻²)	^R s (Bohr)	^R _c (Bohr)
1		1.3	2.0	13.0
2		1.0	3.0	13.0
3		0.7	3.8	13.0
4		0.7	4.6	13.0
5		0.7	5.4	13.0
6		0.7	6.2	13.0
7		0.7	7.0	13.0
8		0.7	8.5	13.0
9		0.7	10.0	13.0
	Sym	netry functions of type $G^{ang.n}_{i}$		
No.	η (Bohr ⁻²)	λ	ζ	^R _c (Bohr)
1	0.2283	-1	1.0	13.0

2	0.2283	1	1.0	13.0
3	0.2283	-1	4.0	13.0
4	0.2283	1	4.0	13.0
5	0.2283	-1	9.0	13.0
6	0.2283	1	9.0	13.0
7	0.2283	-1	1.0	13.0
8	0.2283	1	1.0	13.0
9	0.2283	-1	4.0	13.0
10	0.2283	1	4.0	13.0
11	0.2283	-1	9.0	13.0
12	0.2283	1	9.0	13.0
13	0.2283	-1	1.0	13.0
14	0.2283	1	1.0	13.0
15	0.2283	-1	4.0	13.0
16	0.2283	1	4.0	13.0
17	0.2283	-1	9.0	13.0
18	0.2283	1	9.0	13.0
19	0.2283	-1	1.0	13.0
20	0.2283	1	1.0	13.0
21	0.2283	-1	4.0	13.0
22	0.2283	1	4.0	13.0
23	0.2283	-1	9.0	13.0
24	0.2283	1	9.0	13.0
	Symm	etry functi	ons of type G	ang.w i
No.	Symm η (Bohr-²)	etry functi λ	ons of type $\frac{G}{\zeta}$	ang.w i ^R c(Bohr)
No. 1	Symm η (Bohr ⁻²) 0.7	etry functi λ -1	ons of type G ζ 1.0	ang.w i R _c (Bohr) 13.0
No. 1 2	Symm η (Bohr ⁻²) 0.7 0.7	etry functi λ -1 1	ons of type G ζ 1.0 1.0	ang.w i R _c (Bohr) 13.0 13.0
No. 1 2 3	Symm η (Bohr ⁻²) 0.7 0.7 0.7	etry functi λ -1 1 -1	ons of type G	ang.w i R _c (Bohr) 13.0 13.0 13.0
No. 1 2 3 4	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1	ons of type G ζ 1.0 1.0 6.0 6.0	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1	ons of type G ζ 1.0 1.0 6.0 6.0 1.0	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1	ons of type G	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 1.0 6.0	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7 8	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 6.0 6.0	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7 8 9	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1 -1	ons of type G ζ 1.0 1.0 6.0 1.0 1.0 1.0 6.0 6.0 1.0 1.0 1.0 1.0	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7 8 9 10	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1 -1 1	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 1.0 1.0 1.0 1.0	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7 8 9 10 11	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -1	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 6.0 1.0 1.0 1.0 6.0 1.0 6.0 1.0 6.0	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7 8 9 10 11 12	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 1	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 6.0 1.0 6.0 6.0 6.0 6.0 6.0 6.0 6.0 6	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7 8 9 10 11 12 13	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
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No. 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 6.0 1.0 1.0 6.0 1.0 1.0 6.0 1.0 1.0 6.0 6.0 1.0 6.0 6.0 1.0 6.0 6.0 6.0 6.0 6.0 6.0 6.0 6	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 6.0 6.0 6.0 6.0 6.0 6	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
No. 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	Symm η (Bohr ⁻²) 0.7 0.7 0.7 0.7 0.7 0.7 0.7 0.7	etry functi λ -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -	ons of type G ζ 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 1.0 1.0 6.0 6.0 1.0 1.0 6.0 6.0 1.0 6.0 6.0 6.0 6.0 6.0 6.0 6.0 6	ang.w i R _c (Bohr) 13.0 13.0 13.0 13.0 13.0 13.0 13.0 13.0
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