Supplementary Information for "A Data-Driven Method for Optimization of Classical Interatomic Potentials"

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Given parameters	Description	Ni Ref	Ni OptNN
elt	text string, element name	Ni	Ni
lat	text string, lattice structure (reference configuration)	FCC	FCC
z	number of nearest neighbors in reference structure	12	12
ielement	atomic number	0	4.46E-07
atwt	atomic weight	58.69	58.69
alat	lattice constant of reference structure	3.52	3.52
ibar	selects the form of the function ‘G(Gamma)‘ used to compute the electron density; will be selected/provided prior to fitting optNN.	3	3
rho	relative density of element	1	1
re	equilibrium distance between atoms in reference structure	2.49	2.49
zbl	blend the MEAM I-J pair potential with the ZBL potential for small atom separations (ZBL) (default = 1)	0.00	0.00

Table 1: Given parameters for OptNN

1 MEAM Parameters

Parameter descriptions given are from the readme file for [1].

1.1 Given parameters

Table 1 shows the given parameters for the optimization problem demonstration.

1.2 Fitted parameters

Table 2 shows the fitted parameters determined as a result of the optimization problem demonstration.

2 Models used

The models used in this work to train PredNN were originally published and also archived in OpenKIM through the following references: [1]–[117]

Fitted parameters	Description	Ni Ref	Ni OptNN	notes
alpha	alpha parameter for pair potential between I and J (can be computed from bulk modulus of reference structure	5.08	5.03	
b0	standard beta parameters	2.56	3.52	
b1		1.5	0.29	
b2		6	4.57	
b3		1.5	1.48	
esub	(energy per atom in ref structure at equilibrium)	4.45	3.89	
asub	(A parameter for meam, see pg 6090 of baskes)	0.94	0.94	
t1	standard meam parameters	3.1	2.54	
t2		1.8	0.64	
t3		4.36	4.20	
rozero	element-dependent density scaling that weights the reference background density (see, e.g., equation 4.5 in [[9](#references)]) and Is typically 1.0 for single-element systems	1	0.90	
rc	cutoff radius for cutoff function. (default = 4.0)	4.8	4.50	
delr	length of smoothing distance for cutoff function. (default = 0.1)	0.1	0.14	
attrac	additional cubic attraction term in Rose energy I-J pair potential (default = 0)	0.05	-0.02	
repuls	additional cubic repulsive term in Rose energy I-J pair potential (default = 0)	0.05	0.07	
Cmin	Cmin screening parameter when I-J pair is screened by K (I<=J); Default = 2.0	0.81	0.71	
Cmax	Cmax screening parameter when I-J pair is screened by K (I<=J); Default = 2.8	2.8	2.76	
Ec	cohesive energy of reference structure for I-J mixture	4.45	4.49	
emb_lin_neg	integer to set embedding function (default = 0)	0	0.08	OptNN value Rounded to nearest int
bkgd_dyn	integer value to select background density formula (default = 0)	0	0.23	OptNN value rounded to nearest int

Table 2: Fitted parameters values from OptNN

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