Supplementary information

Generalized Machine Learning Potential Models for Elemental Nanoclusters

Suvo Banik[1], Abhishek Aggarwal[1,2], Sukriti Manna[1,2], Partha Sarathi Dutta[1,2], and Subramanian KRS Sankaranarayanan[1,2]

[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, Illinois 60439, United States
[2]Department of Mechanical and Industrial Engineering, University of Illinois, Chicago, Illinois 60607, United States

July 12, 2025

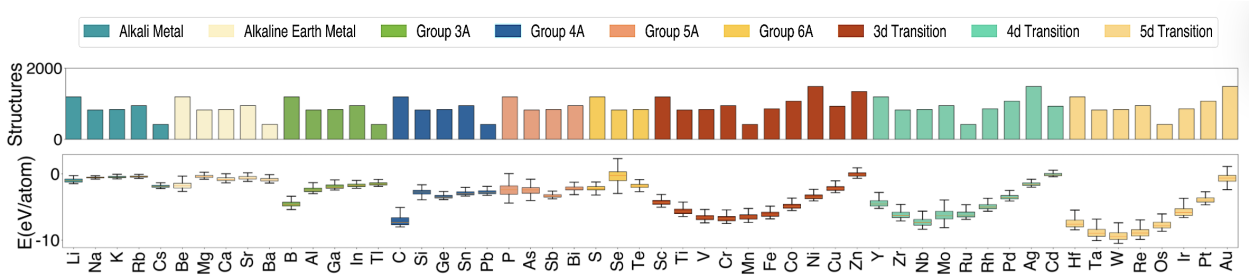

Figure S1: *Elements in the test dataset belonging to the Alkaline Earth Metals, Groups 3A to 6A, and the 3d, 4d, and 5d Transition Metals. The plot shows both the number of clusters and the corresponding potential energy distributions within each category.*

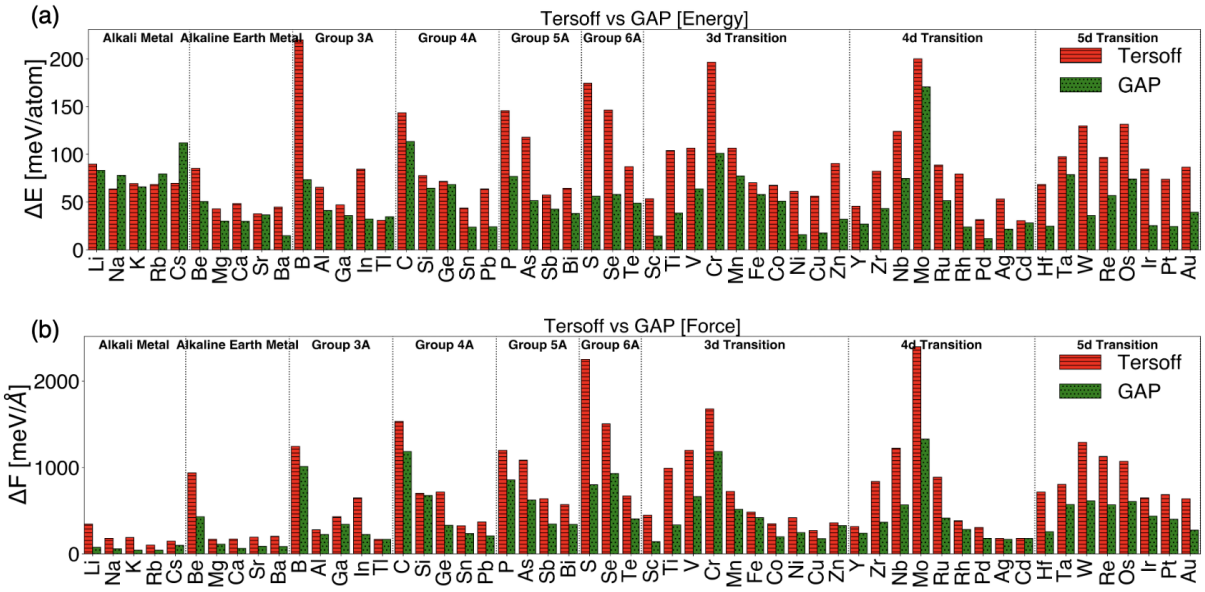

Figure S2: *Comparison of the performance of the GAP models on the test dataset for elements in the Alkaline Earth Metals, Groups 3A to 6A, and 3d, 4d, and 5d Transition Metals categories. (a) The energy error predicted by the GAP models and the corresponding energy errors by the Tersoff models by Manna et al. (b) Comparison of force errors between the GAP model and the Tersoff models.*

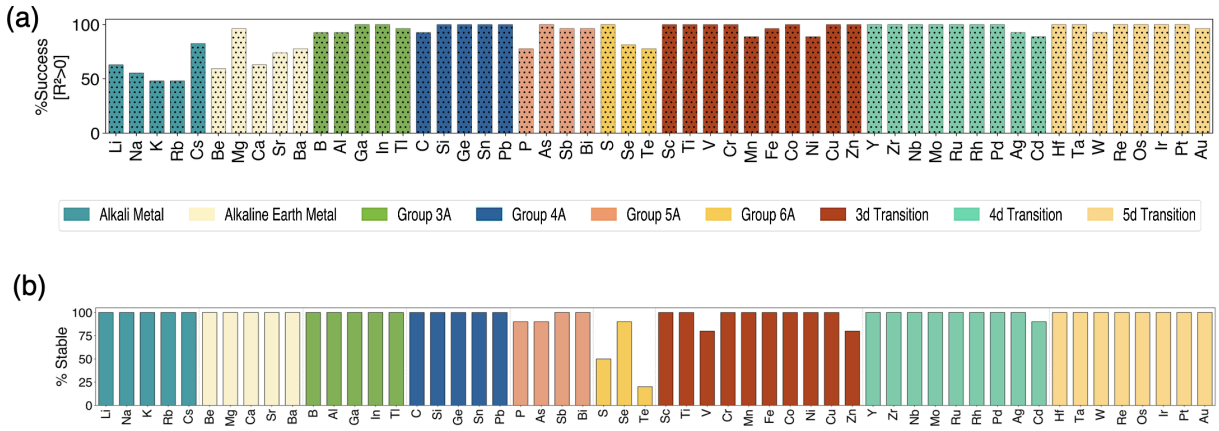

Figure S3: *The success rate in predicting normal modes using our trained GAP models. The success rate is defined as predicting all the modes to be positive for stable nanoclusters.*

Table 1: Temperatures used for performing dynamics simulation.

Element	Temperature (K)	Element	Temperature(K)
Ag	300	Cs	150
Al	300	Cu	300
As	300	Fe	300
Au	300	Ga	150
B	300	Ge	300
Ba	300	Hf	300
Be	300	In	200
Bi	200	Ir	300
C	300	K	150
Ca	300	Li	200
Cd	200	Mg	300
Co	300	Mn	300
Cr	300	Mo	300
Cs	150	Na	200
Cu	300	Nb	300
Fe	300	Ni	300
Ga	150	Os	300
Ge	300	Pd	300
Hf	300	Pt	300
In	200	Re	300
Ir	300	Rh	300
K	150	Ru	300
Li	200	S	200
Mg	300	Sb	300
Mn	300	Sc	300
Mo	300	Se	300
Na	200	Si	300
Nb	300	Sn	200
Ni	300	Sr	300
Os	300	Ta	300
P	150	Te	300
Pb	300	Ti	300
Pd	300	Tl	200
Pt	300	V	300
Rb	150	W	300
Re	300	Y	300
Rh	300	Zn	300
Ru	300	Zr	300