Supplementary Information for "DART: Deep Learning Enabled Topological Interaction Model for Energy Prediction of Metal Clusters and its Application in Identifying Unique Low Energy Isomers"

Rohit Modee[a], Sheena Agarwal[b,c], Ashwini Verma[b], Kavita Joshi[*b,c], U. Deva Priyakumar[*a]

[a] *Center for Computational Natural Sciences and Bioinformatics, International Institute of Information Technology, Hyderabad 500032, India*
[b] *Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune-411008, India.*
[c] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, Uttar Pradesh- 201002, India.*

Model	DART (values in kcal/mol)		
	MAE	RMSE	# structures
Test case 1 (overall)	4.77	6.16	427
Test set Ga-46	10.13	10.81	48
Test set Ga-57	3.59	4.82	197
Test set Ga-60	4.63	5.77	182

Table 1: Performance of DART model on first test case which has total of 427 structures in the test set consisting of Ga - 46, 57, and 60 size clusters.

Model	DART (values in kcal/mol)		
	MAE	RMSE	# structures
Test case 2 (overall)	4.76	6.02	436
Test set Ga-46	7.45	8.07	48
Test set Ga-57	4.15	5.59	197
Test set Ga-66	4.72	5.84	191

Table 2: Performance of DART model on second test case which has total of 436 structures in the test set consisting of Ga - 46, 57, and 66 size clusters.

Model	DART (values in kcal/mol)		
	MAE	RMSE	# structures
Test case 3 (overall)	4.34	5.58	570
Test set Ga-57	3.69	4.78	197
Test set Ga-60	4.93	6.15	182
Test set Ga-66	4.45	5.77	191

Table 3: Performance of DART model on third test case which has total of 570 structures in the test set consisting of Ga - 57, 60, and 66 size clusters.