Supplementary information

N$_2$ Adsorption on High-Entropy Alloy Surfaces: Unveiling the Role of Local Environments

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Table S1: Lattice constate values used to weight-average to assess the HEA lattice constants.

	Lattice Constant (Å)
Mo	3.99
Cr	3.61
Mn	3.50
Fe	3.65
Co	3.53
Ni	3.54
Cu	3.66
Zn	3.97

Table S2: Average N$_2$ adsorption energies, average d BCs, average Bader Charges

Elements	Average N$_2$ Adsorption Energy (eV)	Averaged d BC for the surface atoms.	Averaged Bader charge
Mo	-0.58	-0.10	0.20
Cr	-0.49	0.06	0.26
Mn	-0.23	-0.18	0.30
Fe	-0.35	-0.79	0.05
Co	-0.43	-0.95	-0.16
Ni	-0.22	-1.19	-0.25
Cu	0.11	-2.43	-0.16

Table S3: Correlation coefficients and mean Absolut errors (MAEs) between the linear model presented in section "**d BCs of the adsorbing element and the Bader charge of the adsorbing element vs. the composition of the *first solvation shell*:**" and the DFT data. Correlation coeficients are presented in Figure 9 of the manuscript.

Elements	Correlation coefficient	MAE of adds. Model vs. DFT	d BC correlation coefficient	MAE d BC of Model vs. DFT	Bader charge correlation coefficient	MAE Bader charge Model vs. DFT	Correlation coeficient of d BC vs. Badder
Mo	0.62	0.07	0.54	0.1	0.96	0.02	0.035
Cr	0.66	0.11	0.78	0.2	0.95	0.03	0.638
Mn	0.05	0.23	0.51	0.3	0.8	0.06	0.583
Fe	0.57	0.1	0.68	0.06	0.98	0.02	-0.21
Co	0.55	0.07	0.44	0.05	0.99	0.02	-0.261
Ni	0.77	0.07	0.92	0.04	0.99	0.01	0.732
Cu	0.6	0.04	0.91	0.05	0.97	0.02	0.826
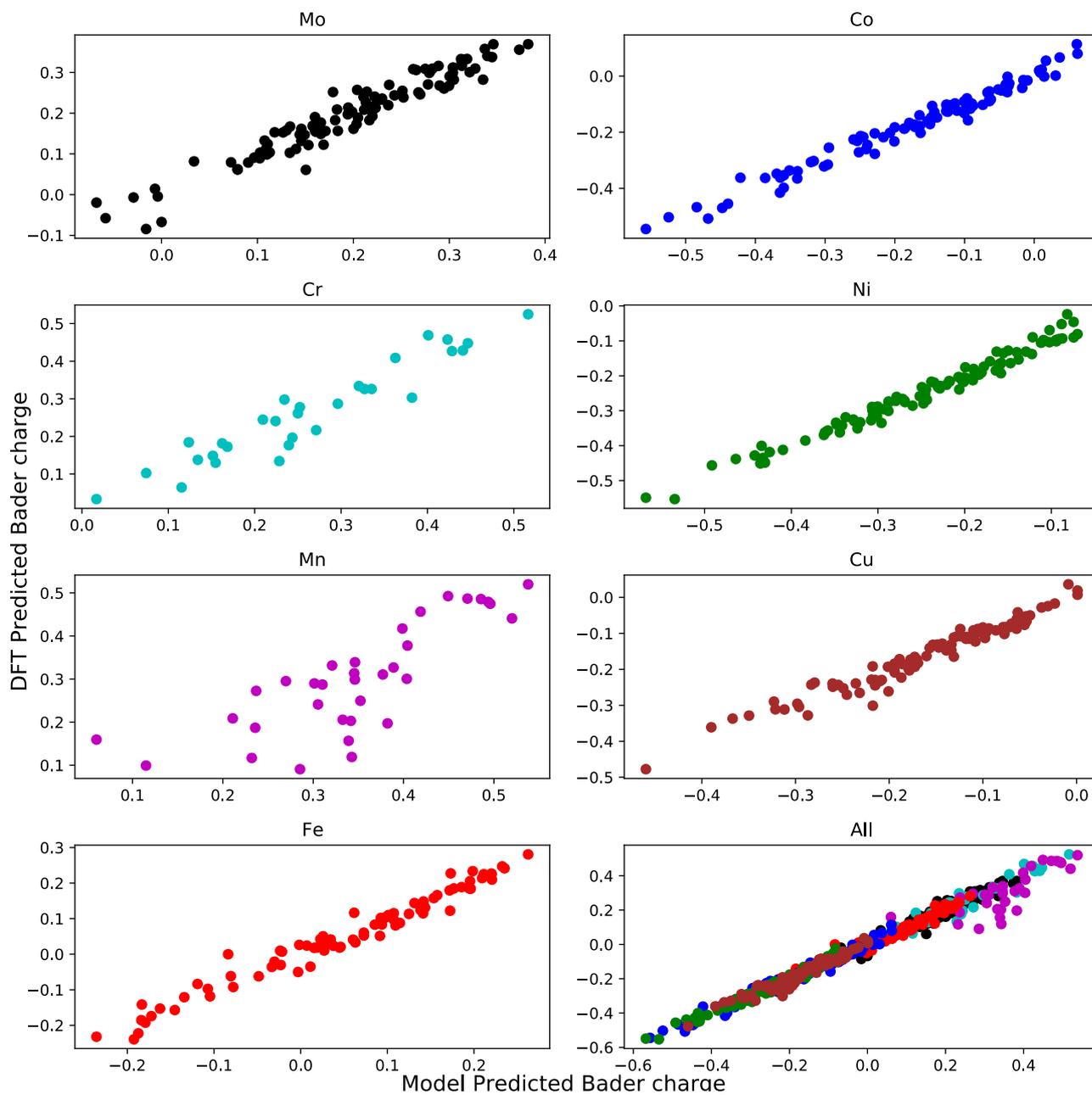
Figure S1: Multilinear models to predict Bader charges based on the number of elements in the first solvation shell of the adsorbing element. Here, N_2 adsorbing on Mo, Cr, Mn, Fe, Ni and Cu elements are plotted with distinct colors and also plotted all together.
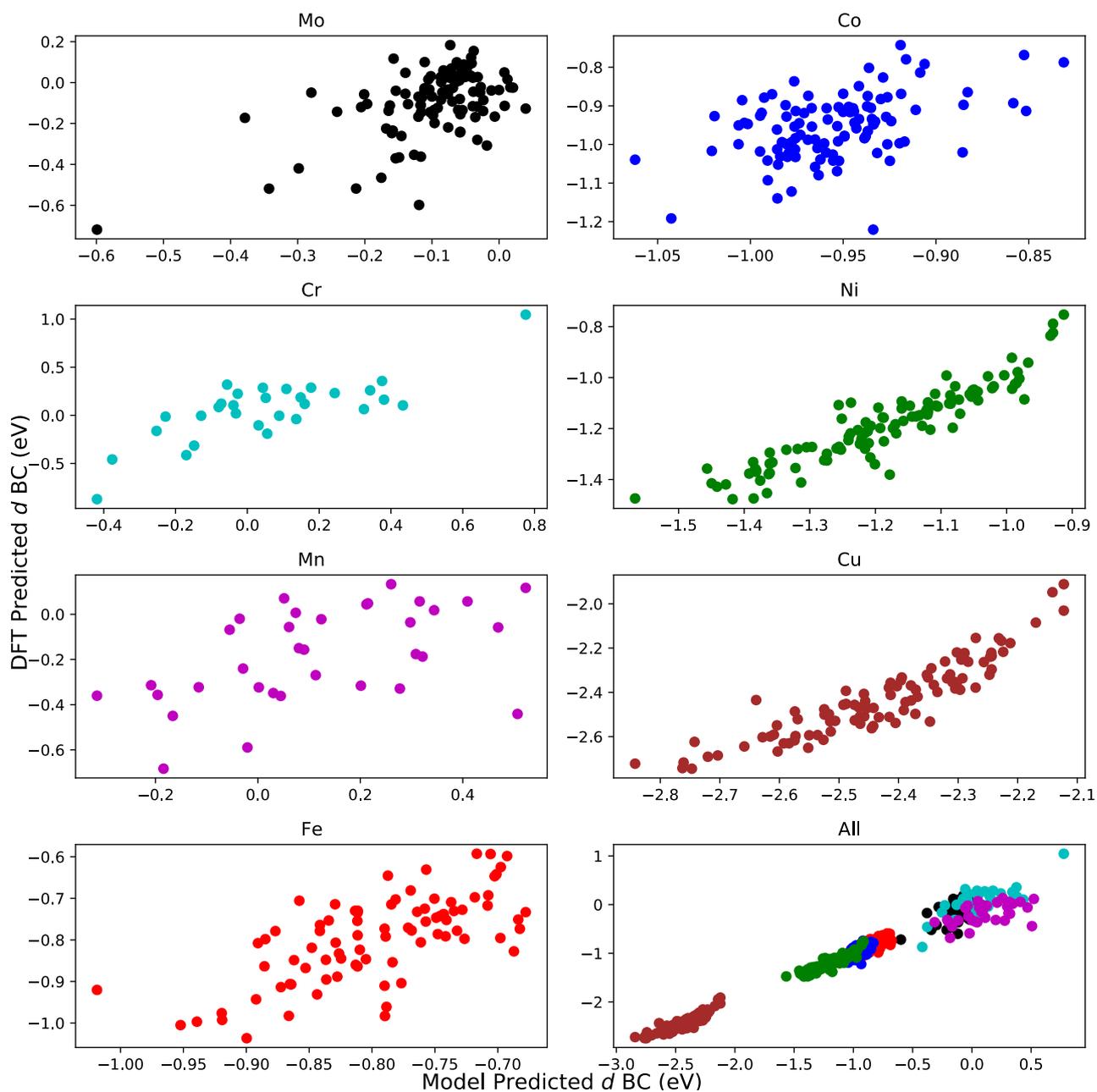
Figure S2: Multilinear models to predict d BCs based on the number of elements in the first solvation shell of the adsorbing element. Here, N₂ adsorbing on Mo, Cr, Mn, Fe, Ni and Cu elements are plotted with distinct colors and also plotted all together.
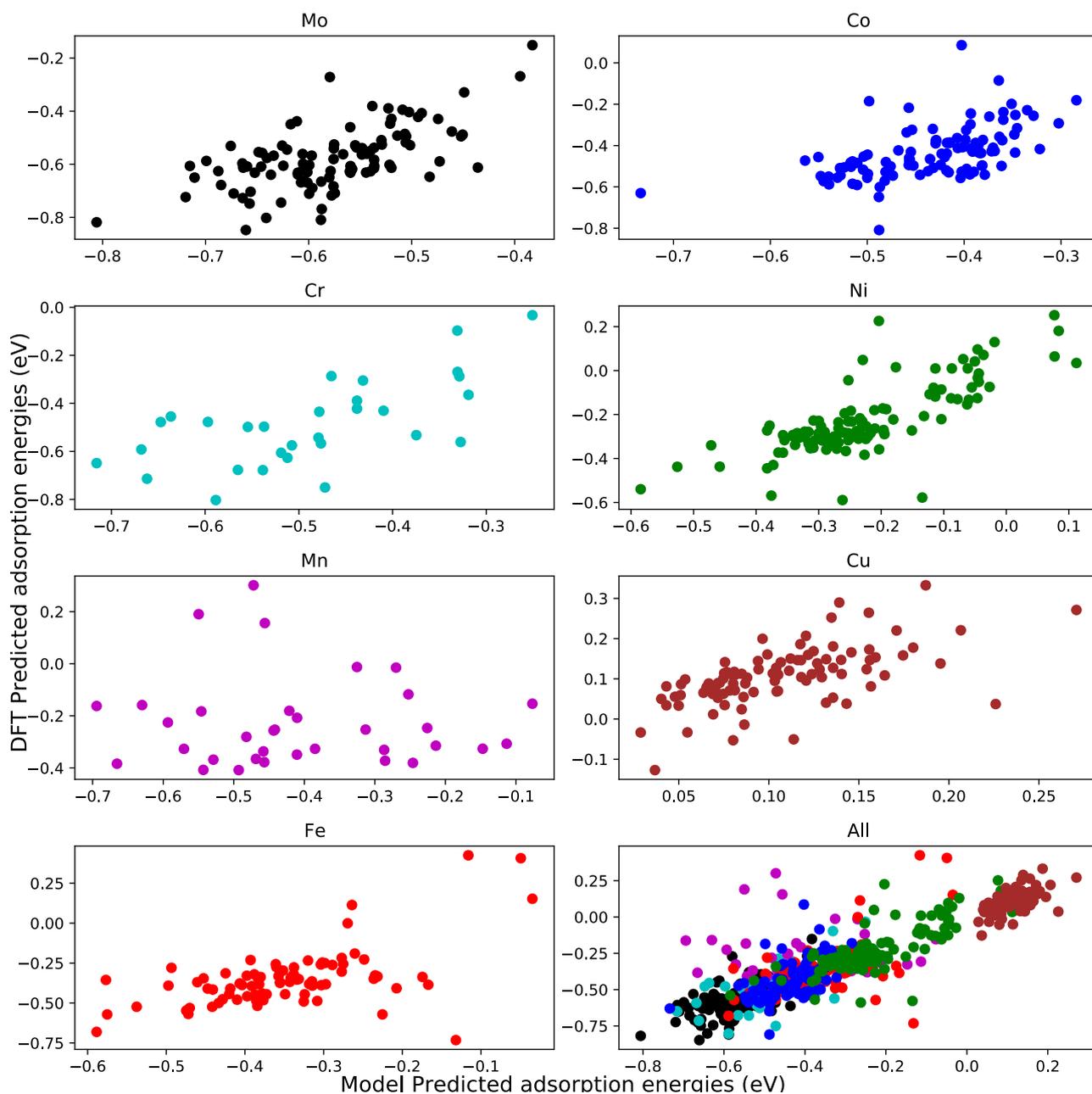
Figure S3: Multilinear models to predict DFT adsorption energies based on the number of elements in the first solvation shell of the adsorbing element. Here, N_2 adsorbing on Mo, Cr, Mn, Fe, Ni and Cu elements are plotted with distinct colors and also plotted all together.