Electronic Supplementary Material (ESI) for Energy Advances.

Supplementary Materials for

Machine Learning Assisted Binary Alloy Catalyst Design for the Electroreduction of CO_2 to C_2 Products

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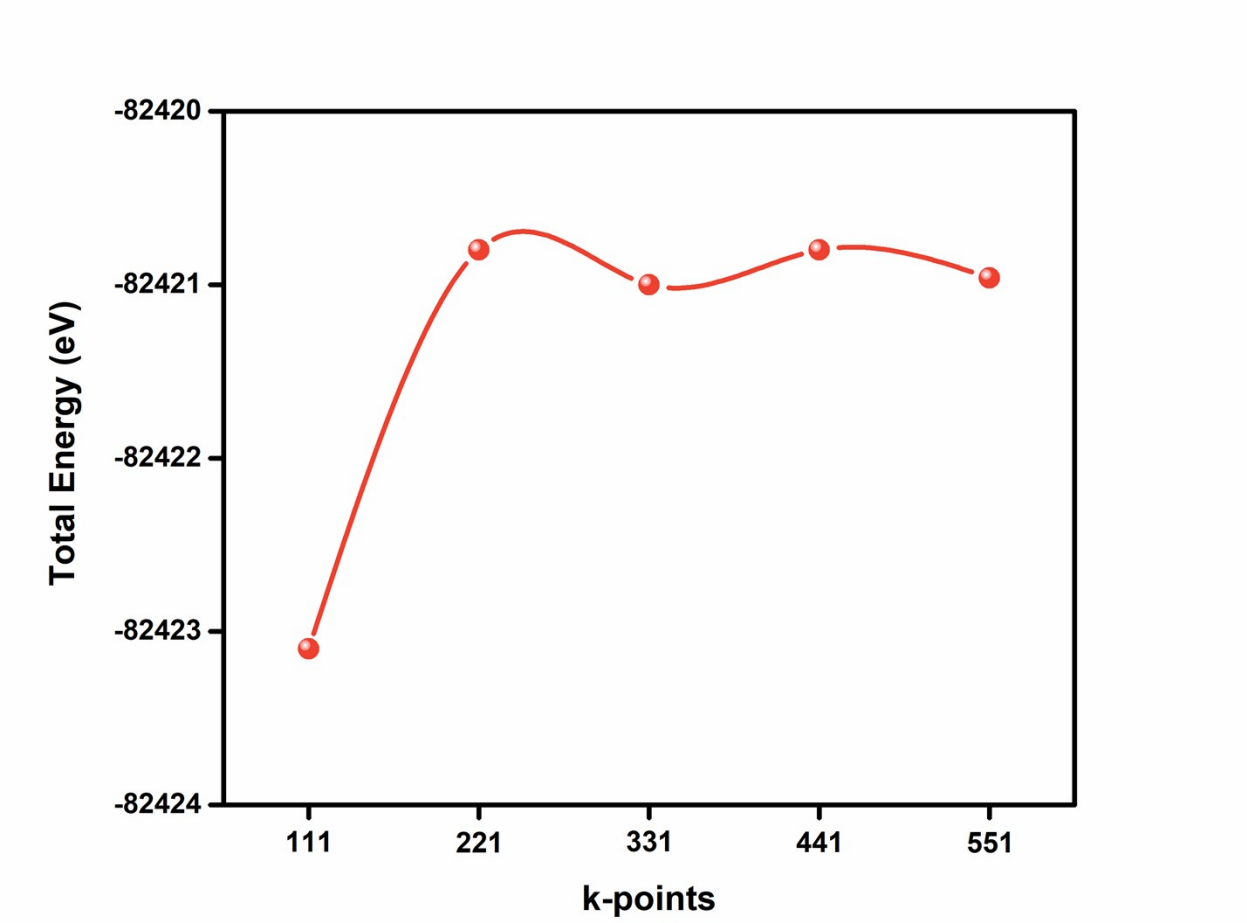

Figure S1. KPOINTS convergence test ranging from 1x1x1 gamma centered k-points mesh up to 5x5x1 k-points mesh.

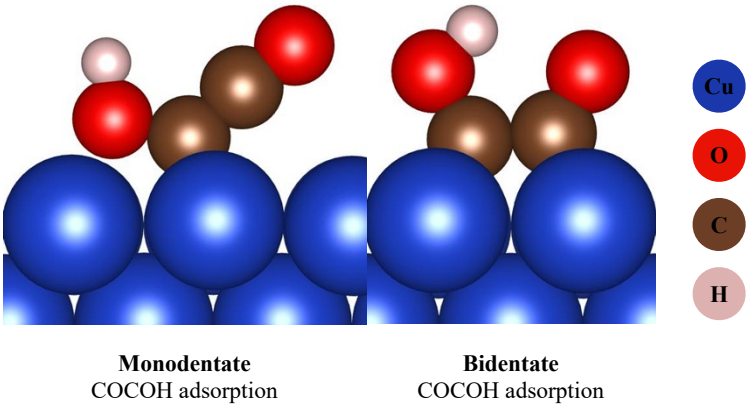

Figure S2. Visualization of 2 possible COCOH adsorption configurations on a Cu (100) surface. The monodentate adsorption favors a single bridge site adsorption whereas the bidentate adsorption favors dual bridge site adsorption.

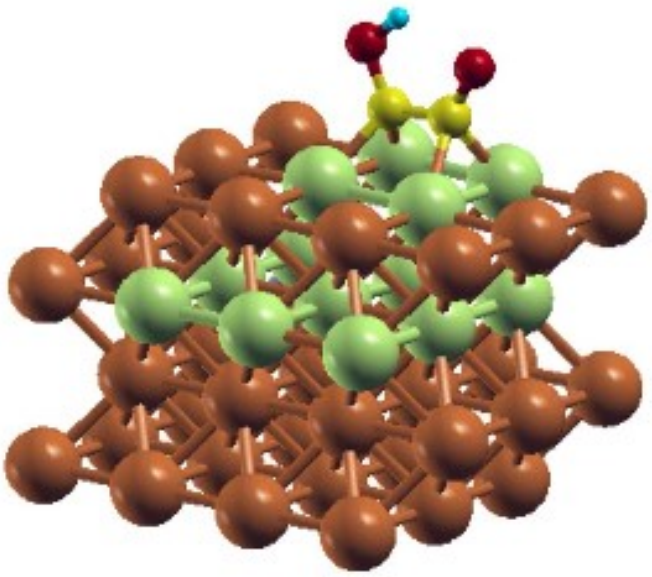

Figure S3. Visualization of 13 atoms in top two layers that influence adsorption properties the most (Green: 13 selected positions Brown: Copper Purple: Platinum Yellow: Carbon Red: Oxygen Blue: Hydrogen)

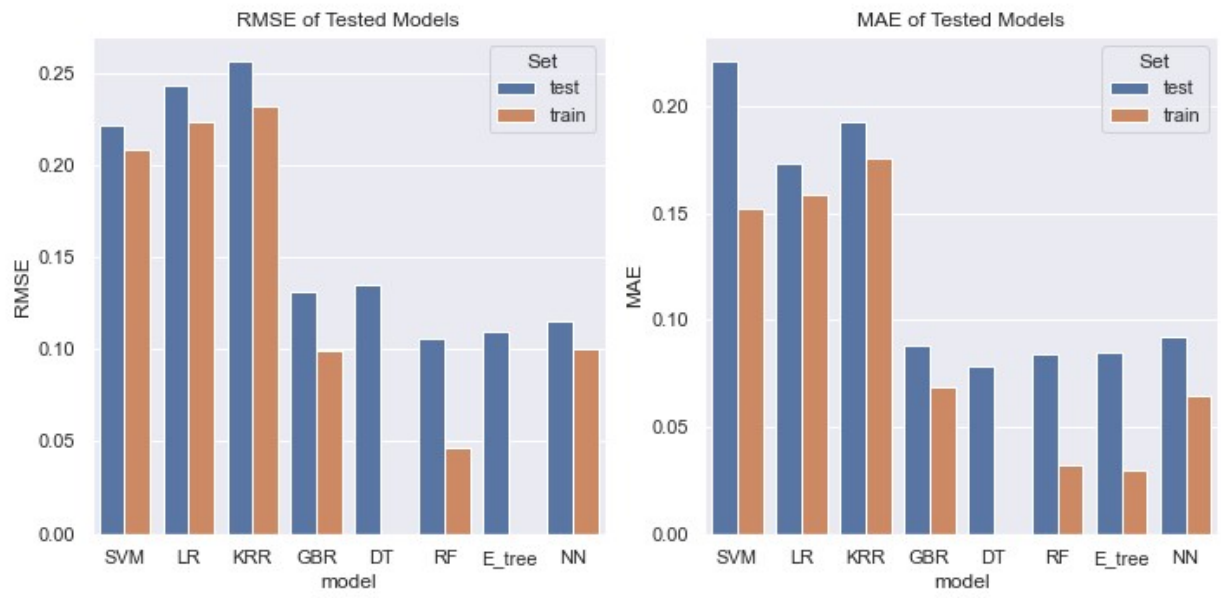

Figure S4. Comparison of the Root mean square error and mean absolute error of 8 commonly used regression models for electrocatalyst adsorption energy modeling.

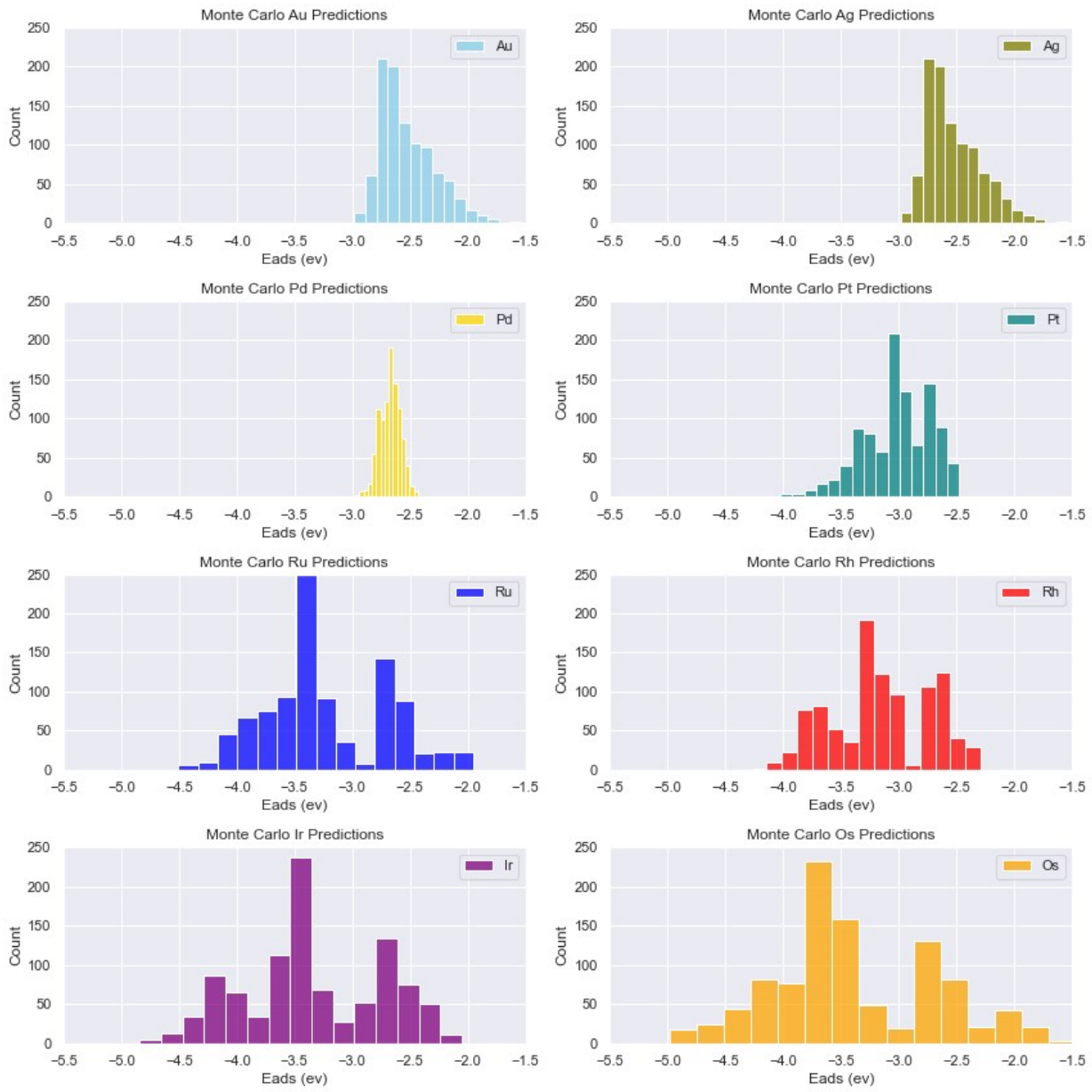

Figure S5. Eads distribution of 8 SAC elemental combinations. Each histogram contains the Eads of 1000 randomly generated surface structures predicted by a multilayer perceptron NN.

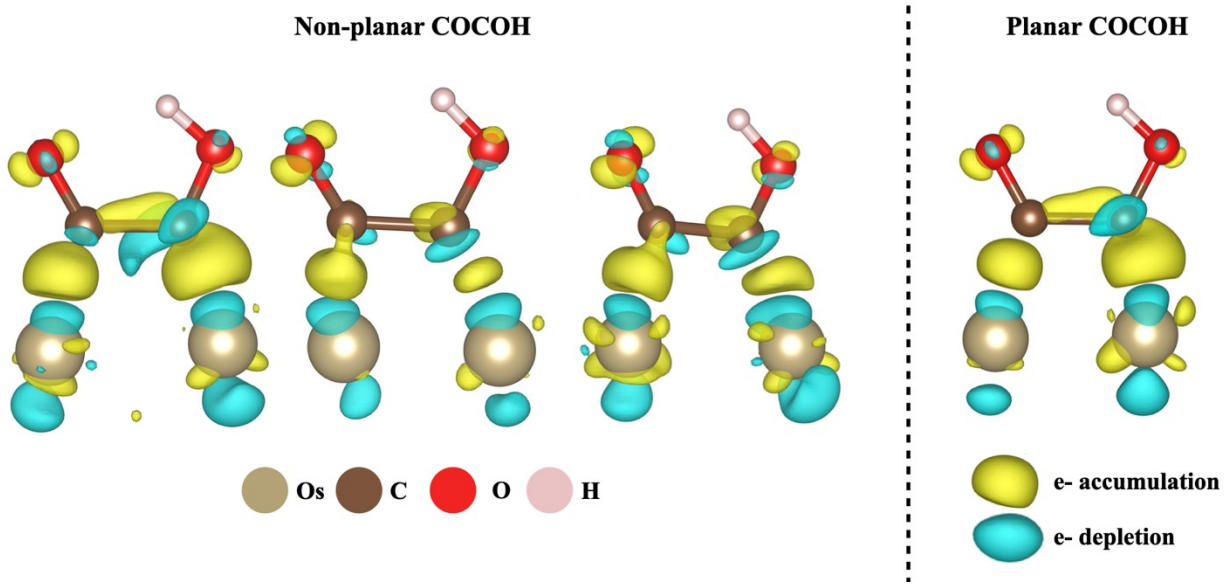

Figure S6. a,b,c) Charge Density Difference of 3 nonplanar COCOH adsorbates at low, medium, high adsorption energies. d) Typical planar COCOH adsorbate at medium adsorption energy.

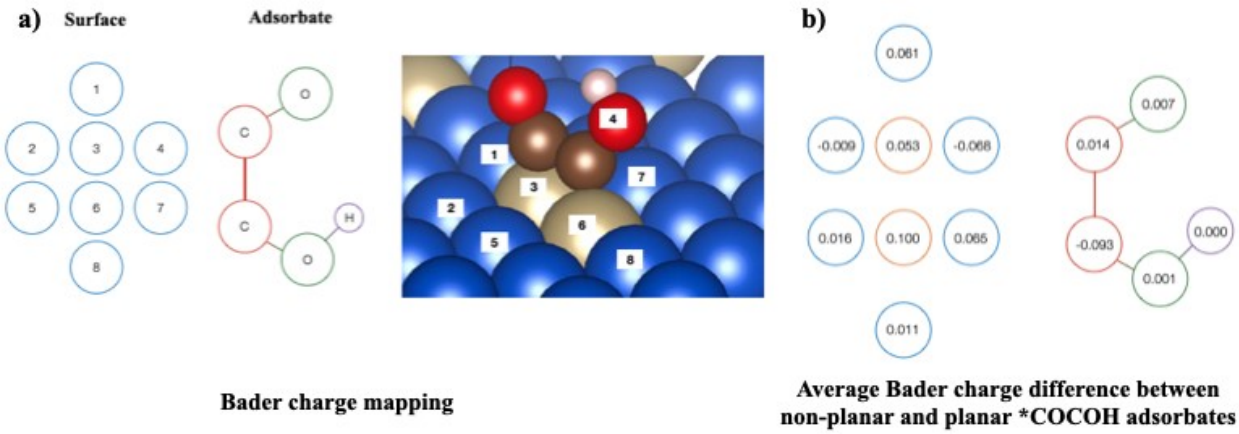

Figure S7. a) Bader charge mapping of substrate and adsorbate. b) average Bader charge difference between 3 non-planar COCOH datapoints and a reference planar COCOH adsorbate.

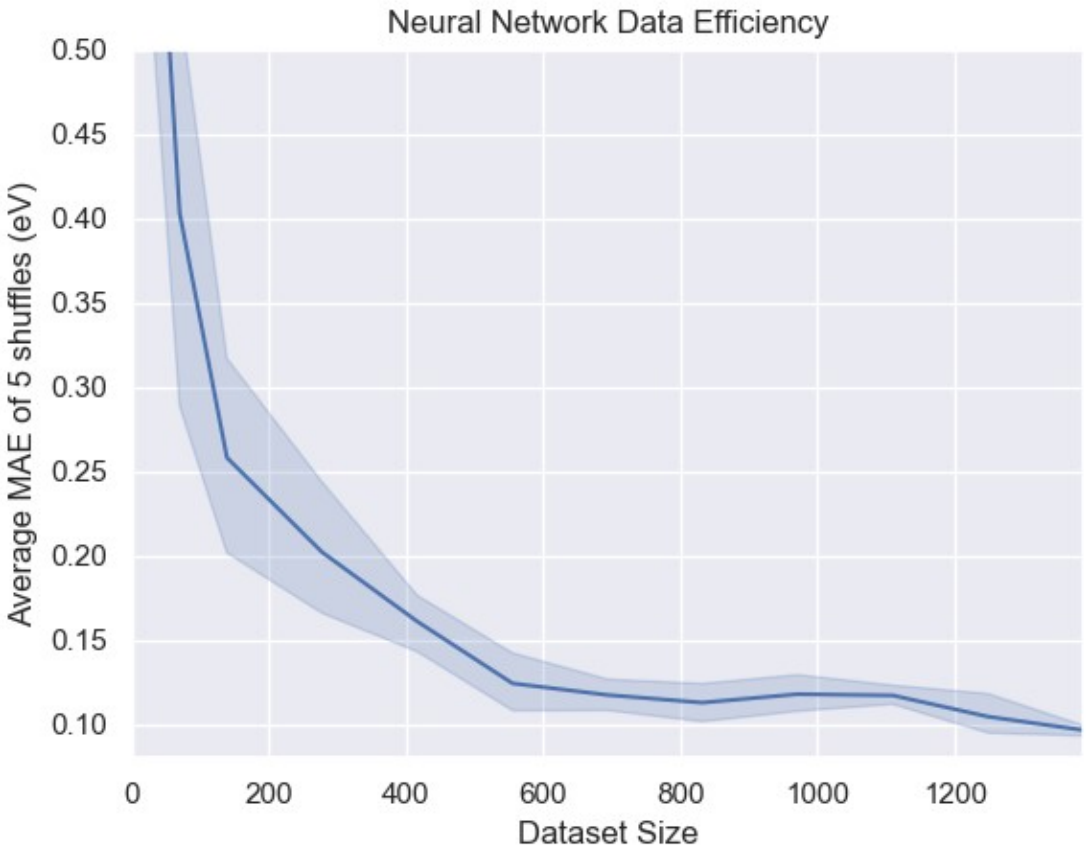

Figure S8. Data efficiency of the Neural Network model. The y axis is the average MAE value of 5 dataset reshuffles in eV with uncertainties visible and the x axis is the dataset size used to train the model.