Supporting Information

Can Machine Learning predict the reaction paths in catalytic CO_2 reduction on small Cu/Ni clusters?

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S.1 Notation and markings used

A special notation was developed for the project, which facilitated the entire task. Its basis is the transfomation of three-dimensional metallic clusters into a one-dimensional list of elements (see Figure 1)
This one-dimensional representation of the cluster is possible due to the omission of geometric changes in the clusters.
The complexes we studied consist of metallic clusters and small carbon reactants (CO2, HCOO, COOH). A special description of the attachment of these small structures to the clusters was also developed for this work:

1. binding mode "to the corner" meaning that the molecule is concentrated around one metal of the cluster. It is possible to uniquely identify an attachment site of this type by specifying just the atom to which the molecule is attached. However, we decided to take into account the close proximity of these atoms in addition to the atoms to which the attachment occurs, in view of which the following notation:

   [2, 3, Cu]

   means that the molecule is bound to such a copper atom in the cluster, which in its first coordination sphere has 2 nickel atoms and 3 copper atoms.

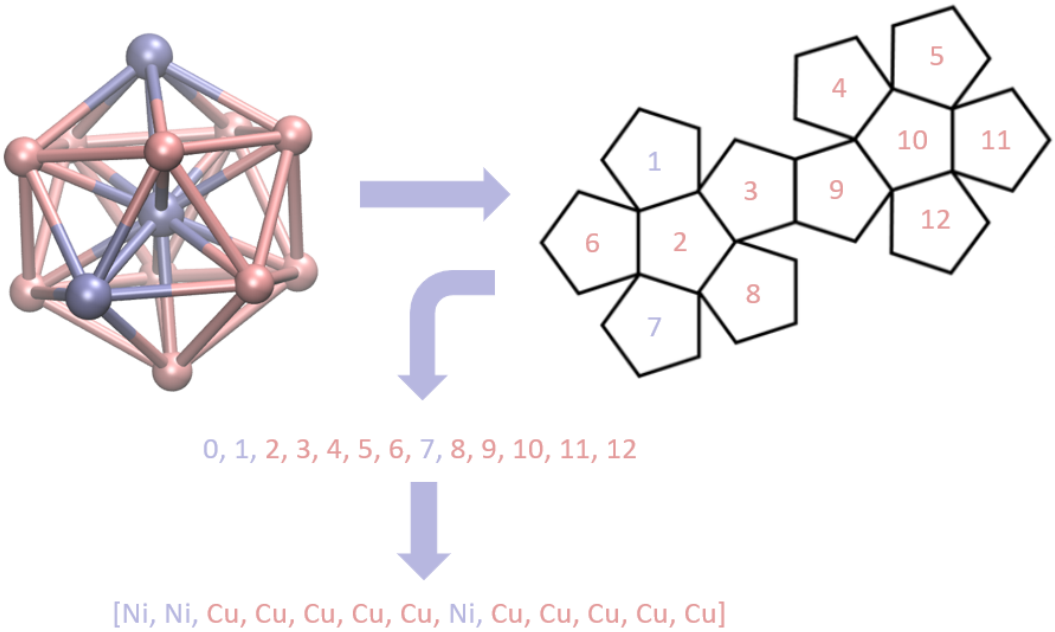

Figure S.1: Diagram for creating notation. The position of "0", where the atom that is in the center of the molecule is located, has not been plotted on the drawing on the right.

2. In the case of an "edge" binding mode , i.e. one in which the molecule bound at an area between two atoms in the cluster, we must describe the two metals in an analogous way, e.g:

   [5, 0, Cu, 4, 1, Ni]

   This notation means that the molecule attaches to the space between a copper atom adjacent only to nickel atoms and a nickel atom adjacent to 4 nickel atoms and one copper atom

The last boundary condition for using this notation remains. In the case where there are 2 atoms of one type and 3 atoms of the second type, we can distinguish two possibilities:

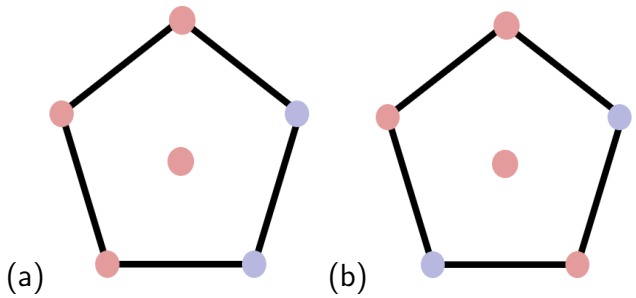

Figure S.2: A pictorial representation of the notation when there are two metals of one kind in the first coordination sphere of an atom (shown as a circle in the center of the pentagon) (atoms in the first coordination sphere are shown as circles on the vertices of the pentagon

In this case situation from Figure S.2(a) is described as:

[2, 3, Cu]

while situation from Figure S.2(b) is described as:

[2.1, 3, Cu]

The final element that we have described is the rotation of clusters. Rotations of a cluster always take place around its own axis. A rotation written in the form *n_m* means that the cluster has been rotated in such a way that the atom that was initially at position *n* is at position 1, and the cluster that was initially at position *m* is at position 2 (Figure S.1).
Finally, to fully describe the cluster-agent carbon system we use the following notation:

7_MOCMHnbond_2_1

Where *7* is the number describing the position of the cluster in the list of all possible cluster combinations, *MOCMHnbond* is the type of attachment of the carbon reactant to the cluster (see Figure S.1, and *2_1* is the rotation of the cluster relative to that molecule.

S.2 Heatmap

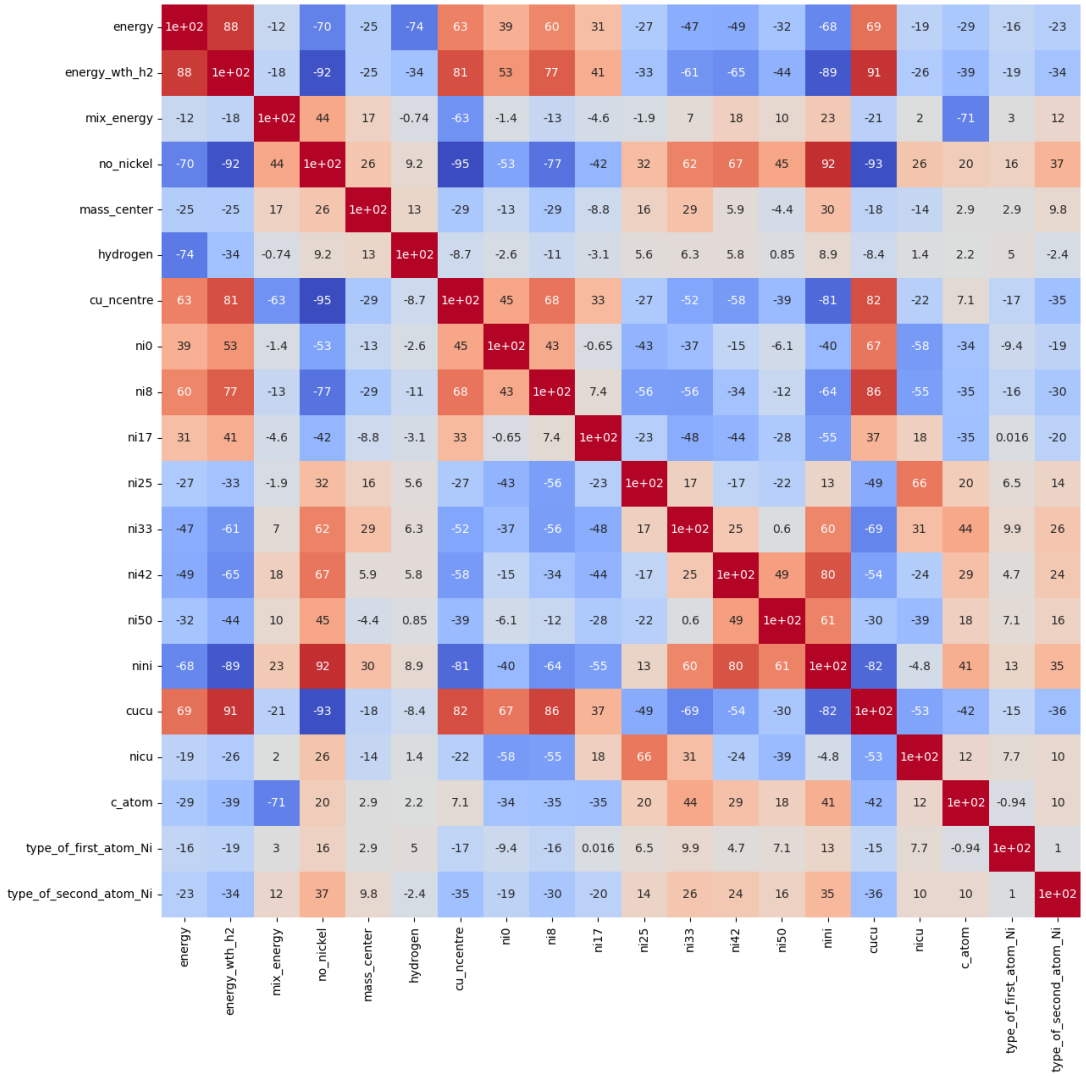

Figure S.3: Heatmap of the importance of all descriptors and all predicted values

S.3 Predicted energy values

Table S.1: Most stable CuNi clusters for each Cu:Ni ratio and binding mode category

number of nickel	cluster id	binding mode	predicted energy [eV]
1	1	MC	-62.725282
		MO	-58.350873
		MOCM	-59.369437
		MOCMHnbond	-63.215742
		MOCOM	-63.431317
2	3	MC	-64.039012
		MO	-60.352587
		MOCM	-60.722803
		MOCMHnbond	-64.540771
		MOCOM	-65.396034
3	9	MC	-65.375948
		MO	-61.675259
		MOCM	-62.094551
		MOCMHnbond	-65.889005
		MOCOM	-66.753495
4	19	MC	-66.710465
		MO	-62.995032
		MOCM	-63.463400
		MOCMHnbond	-67.234821
		MOCOM	-68.099854
5	43	MC	-68.048102
		MO	-64.320317
		MOCM	-64.837761
		MOCMHnbond	-68.583757
		MOCOM	-69.474332
6	71	MC	-69.360779
		MO	-65.618978
		MOCM	-66.185498
		MOCMHnbond	-69.907733
		MOCOM	-70.793287
7	128	MC	-70.741304
		MO	-66.986708
		MOCM	-67.602305
		MOCMHnbond	-71.299557
		MOCOM	-72.180089

8	159	MC	-72.032674
		MO	-68.264374
		MOCM	-68.929047
		MOCMHnbond	-72.602226
		MOCOM	-73.477737
9	176	MC	-73.395011
		MO	-69.614372
		MOCM	-70.328121
		MOCMHnbond	-73.975862
		MOCOM	-74.846352
10	184	MC	-74.702397
		MO	-70.90847
		MOCM	-71.671295
		MOCMHnbond	-75.294547
		MOCOM	-76.160016
11	188	MC	-76.040516
		MO	-72.233638
		MOCM	-73.045539
		MOCMHnbond	-76.643964
		MOCOM	-77.504412
12	190	MC	-77.297111
		MO	-73.472551
		MOCM	-74.333528
		MOCMHnbond	-77.911858
		MOCOM	-78.767285