Supporting Information for

The Roles of Various Fe-Cu Bimetallic Nanoclusters in Controlling the C2 Selectivity for CO Reduction Reaction - A DFT Study

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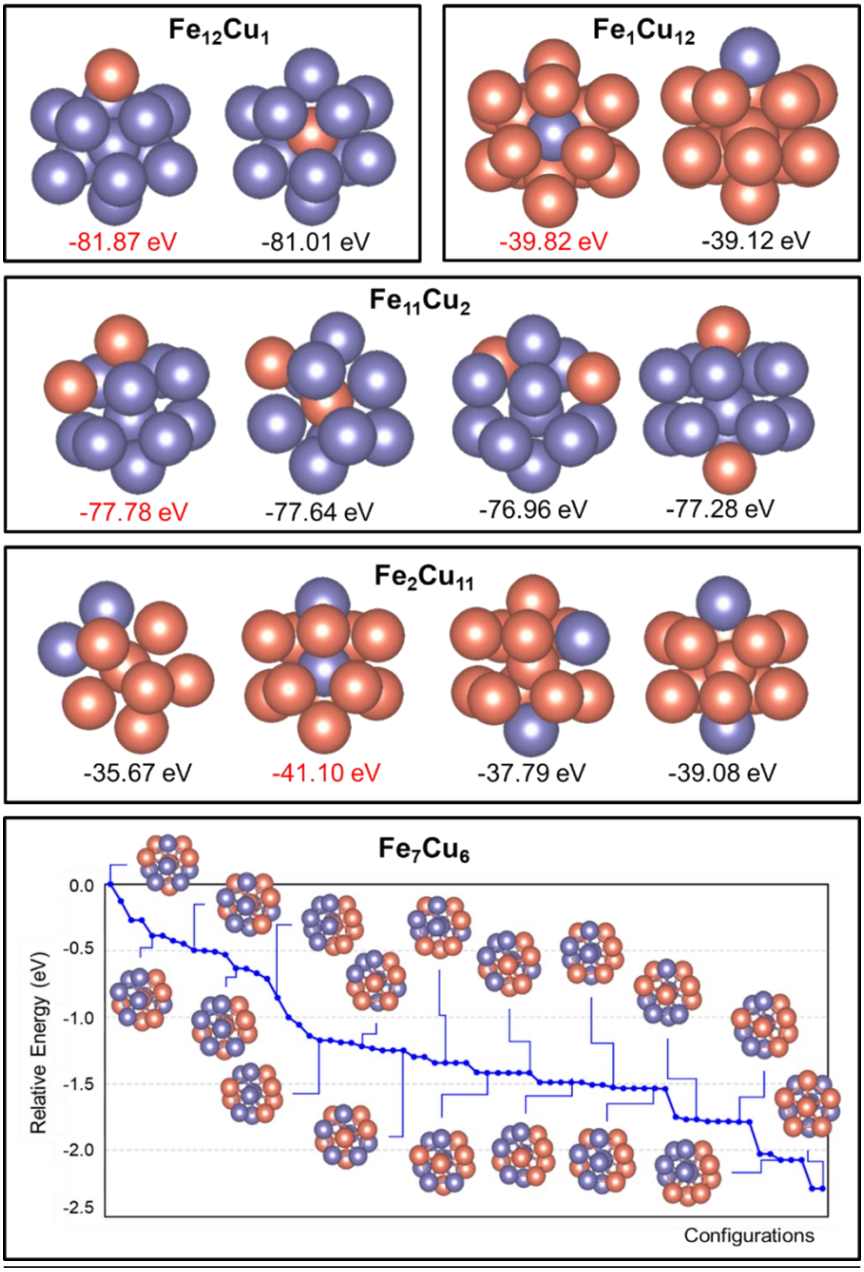


Figure S1. Relative energy (eV) of different Fe_nCu_{13-n} (n = 1, 2, 7, 11, 12) nanocluster configurations.

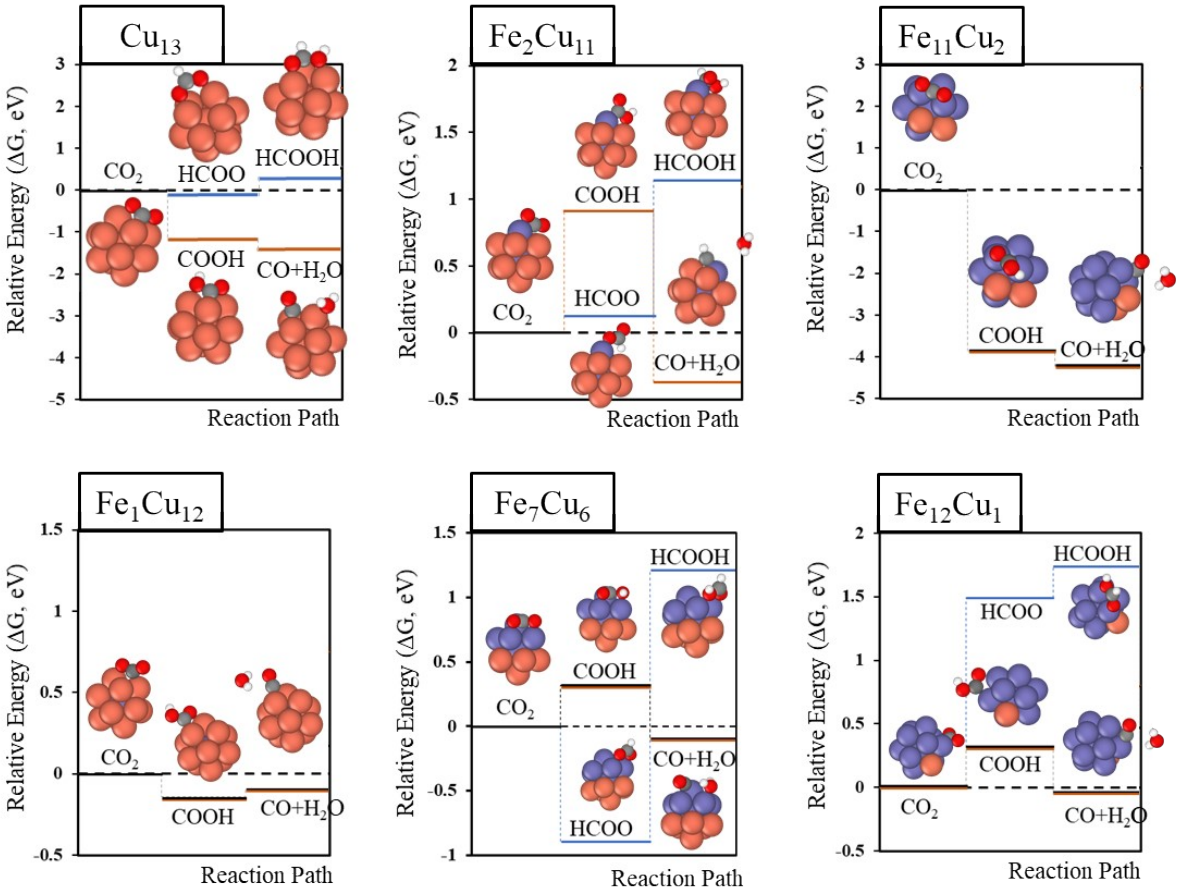
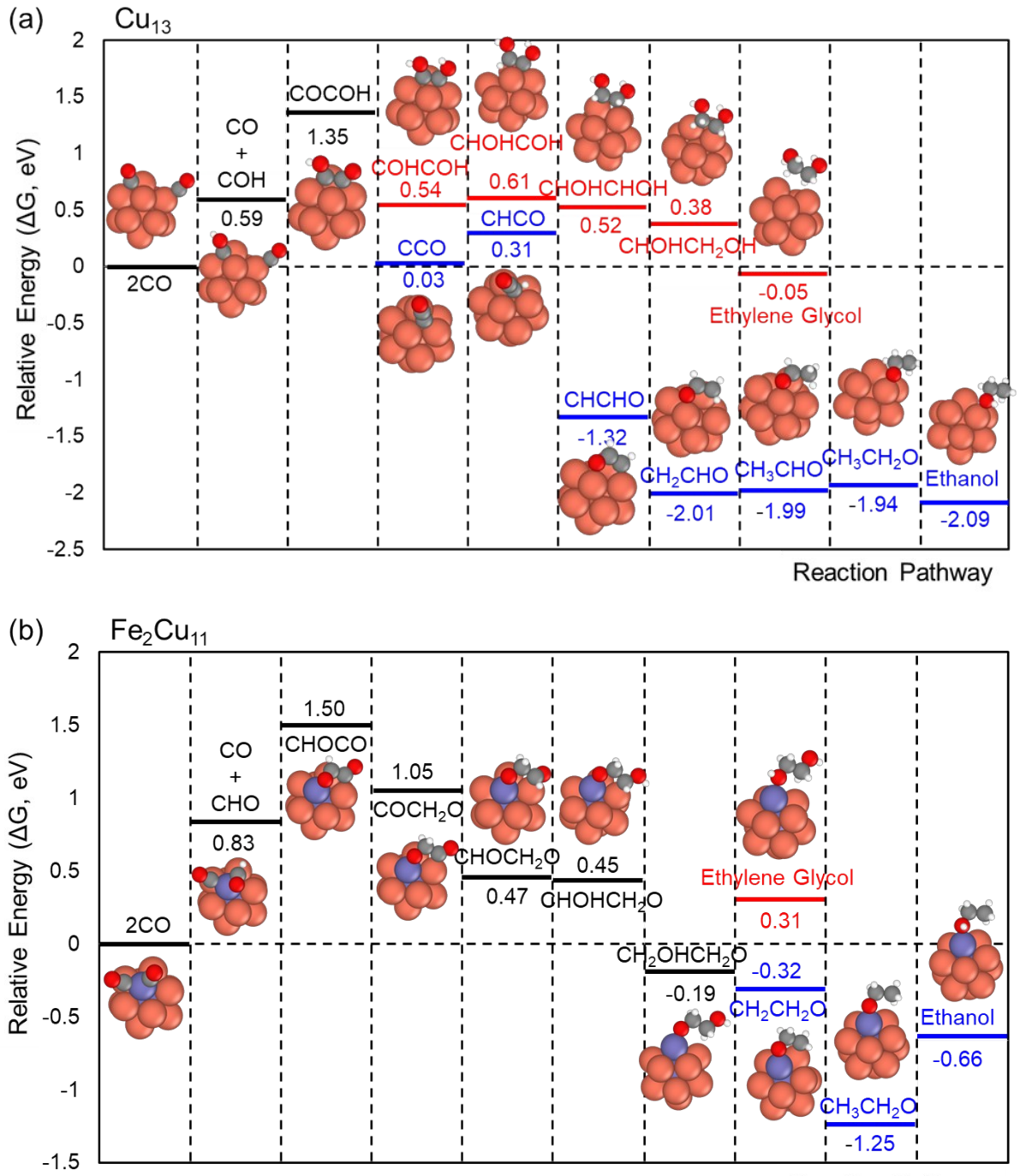


Figure S2. The profiles of the potential energy surface (ΔG, eV) of CO_2 molecules reduction on Cu_{13} and Fe_nCu_{13-n} (n = 1, 2, 7, 11, 12) nanoclusters, illustrating the relative energies of various intermediates and products in the reaction pathway.


(a)
Cu13
Relative Energy (ΔG, eV)
Reaction Pathway
2CO
CO + COH
0.59
COCOH
1.35
COHCOH
0.54
CHOHCOH
0.61
CCO
0.03
CHCO
0.31
CHOHCHOH
0.52
CHOHCH2OH
0.38
-0.05
Ethylene Glycol
CHCHO
-1.32
CH2CHO
-2.01
CH3CHO
-1.99
CH3CH2O
-1.94
Ethanol
-2.09
(b)
Fe2Cu11
Relative Energy (ΔG, eV)
2CO
CO + CHO
0.83
1.50
CHOCO
1.05
COCH2O
CHOCH2O
0.47
0.45
CHOHCH2O
CH2OHCH2O
-0.19
Ethylene Glycol
0.31
-0.32
CH2CH2O
CH3CH2O
-1.25
Ethanol
-0.66

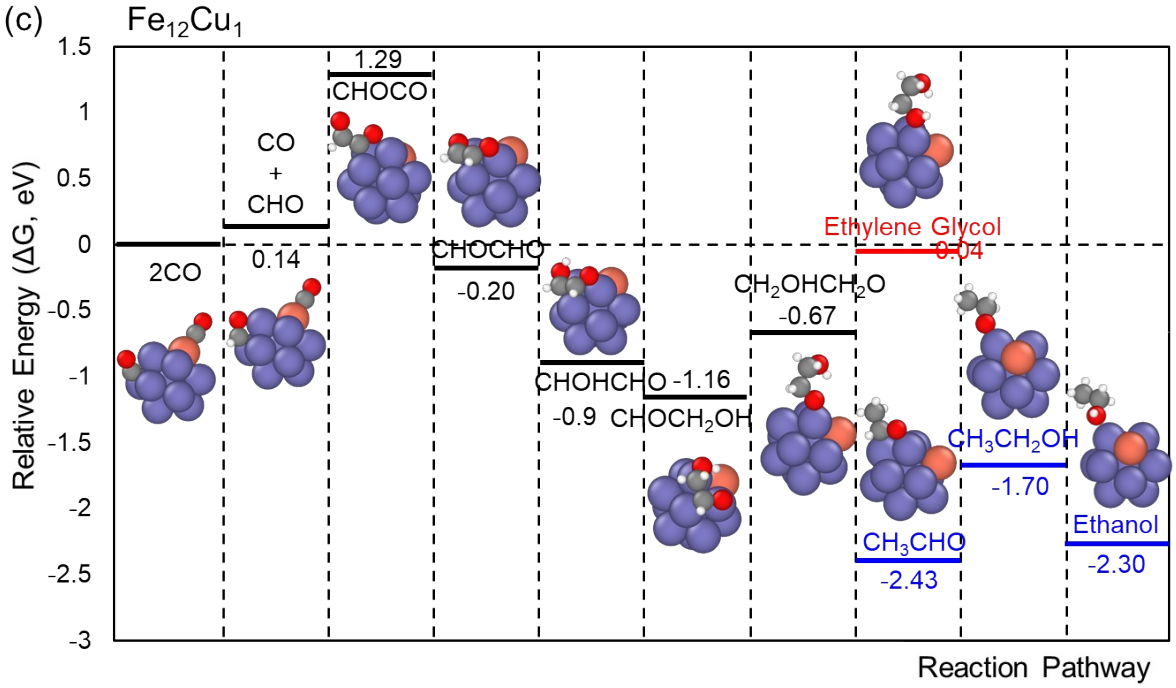


Figure S3. The profiles of the potential energy surface (ΔG, eV) of 2CO molecules reduction towards C2 products on (a) Cu_{13}, (b) Fe_2Cu_{11}, and (c) $Fe_{12}Cu_1$ nanoclusters, illustrating the relative energies of various intermediates and products in the reaction pathway.

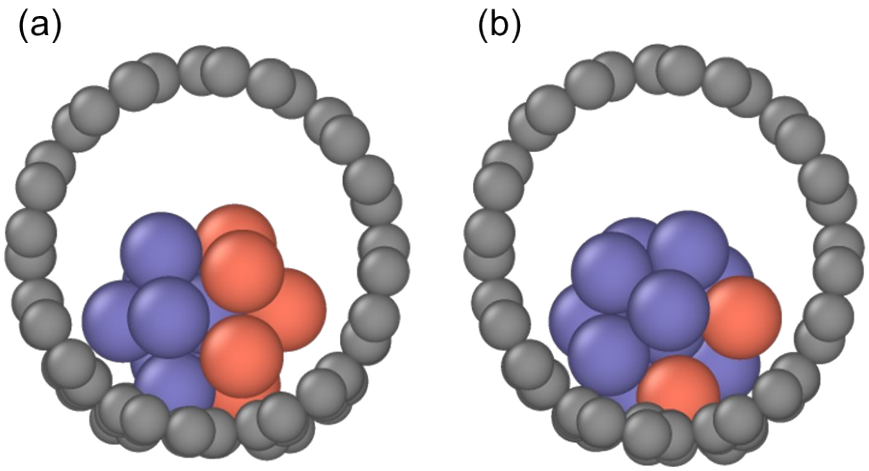


Figure S4. Optimized geometries of (a) Fe_7Cu_6/CNT and (b) $Fe_{11}Cu_2$/CNT.