Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information: Ab initio Investigation of the Role of the d-states Occupation on the Adsorption Properties of H_2, CO, CH_4 and CH_3OH on the Fe_{13}, Co_{13}, Ni_{13} and Cu_{13} Clusters

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Contents

S1 Introduction

A large number of calculations and analyses were done along with the present study. However, several results and analyses, which can be considered complementary to the main manuscript, were not reported within the manuscript due to the space limitation. Additionally, we report in this document all the results employed to build up the figures. Thus, the present file contains the following information:

1. Additional technical computational parameters and convergence tests.
2. Additional technical analyses.
3. Additional structural, energetic and electronic properties of the gas-phase molecules and clusters.
4. Additional structural, energetic and electronic properties of the adsorbed systems.

S2 Computational Convergence Tests for the Electron-density Self-consistency and Geometric Optimization Parameters

As mentioned in the manuscript, the *ab initio* investigation of weak interacting systems such as CH_4-TM_{13} is a challenge for electronic structure calculations, in particular, due to the small magnitude of the adsorption energy, which requires tight computational parameters to reduce the errors in the self-consistency process to obtain the electron density. Thus, to obtain accurate results, we performed several computational convergence tests employing the CH_4/Co_{13} system as a model as the remaining systems have higher adsorption energy, and hence, less sensitive to the computational parameters. In the FHI-aims package, the most important computational parameters, which control the self-consistency process,

are the following flags: sc_accuracy_etot (total energy), sc_accuracy_rho (electron density), sc_accuracy_eev (sum of the eigenvalues), and sc_accuracy_forces. Furthermore, we performed several tests using several values for the flags that control the magnitude of the residual forces required to reach the equilibrium structures. All results obtained from those computational convergence tests are reported within the Figure S1 and Table S1.

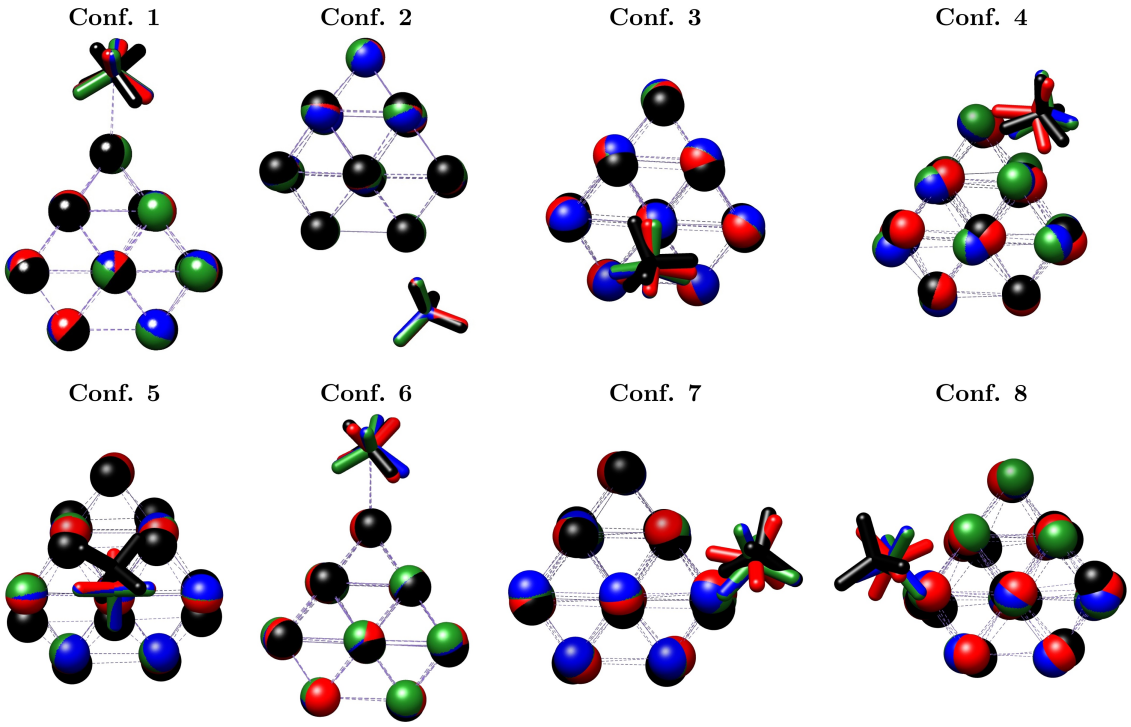

Figure S1: Optimized CH_4/Co_{13} structures for the computational convergence tests for the electron-density self-consistency and geometric optimization parameters at the PBE+vdw-TS/light-tier2 level. Each color in the molecular figures represents one level of accuracy for the evaluated parameters, i.e., from first (black), second (red), third (blue) to fourth (green) level, see Table S1.

Our results showed that the optimal values for the electron density self-consistency parameters are 2.5×10^{-6} eV and 2.5×10^{-5} eV Å^{-1} for total energy (sc_accuracy_etot) and atomic forces (sc_accuracy_forces) respectively, while 2.5×10^{-4} eV Å^{-1} is for the atomic forces (relax_geometry trm) for the geometric optimization. Those values are enough to obtain accurate results for the adsorbed CH_4/Co_{13} system, and hence, correctly describe the weak nature of the CH_4-Co interactions. Therefore, this level of accuracy was employed for all Mol/TM_{13} systems.

Table S1: Computational convergence tests for the electron-density self-consistency and geometric optimization parameters at the PBE+vdW-TS/light-tier2 level. The following parameters were considered: sc_accuracy_etot (total energy), sc_accuracy_rho (electron density), sc_accuracy_forces (atomic forces), and relax_geometry trm (forces for relaxation). Thus, the following properties were investigated in function of the evaluated parameters: relative total energy, ΔE_{tot}, (meV), HOMO energy, $\epsilon_{\mathbf{H}}$ (eV), LUMO energy, $\epsilon_{\mathbf{L}}$ (eV), HOMO-LUMO energy separation, E_g (eV), smallest distance between the H and the TM atoms, $d_{min}^{\mathrm{H-TM}}$ (Å), smallest distance between the C and TM atoms, $d_{min}^{\mathrm{C-TM}}$ (Å), and average H−C−H angle, HCH (°).

	Conf.	ΔE (meV)	ϵ_{H} (eV)	ϵ_{L} (eV)	E_g (eV)	$d_{min}^{\mathrm{H-TM}}$ (Å)	$d_{min}^{\mathrm{C-TM}}$ (Å)	HCH (^{o})
First test (black)	8	122	−3.90	−3.59	0.31	3.39	4.48	109.47
	7	115	−3.84	−3.54	0.31	2.39	3.25	109.47
sc_accuracy_etot 2.5×10^{-5}	5	96	−3.90	−3.59	0.31	2.81	3.72	109.47
sc_accuracy_rho 2.5×10^{-3}	4	87	−3.90	−3.59	0.31	3.14	3.72	109.47
sc_accuracy_forces 2.5×10^{-3}	3	87	−3.90	−3.58	0.31	3.02	3.74	109.47
relax_geometry trm 2.5×10^{-2}	6	22	−3.66	−3.43	0.23	2.00	2.39	109.47
	1	21	−3.67	−3.43	0.24	2.00	2.39	109.48
	2	0	−3.72	−3.47	0.25	2.03	2.42	109.48
Second test (red)	4	80	−3.90	−3.59	0.31	3.06	3.64	109.47
	3	70	−3.90	−3.59	0.31	3.37	3.82	109.47
sc_accuracy_etot 2.5×10^{-6}	5	51	−3.85	−3.53	0.32	2.39	2.89	109.47
sc_accuracy_rho 2.5×10^{-3}	8	24	−3.67	−3.43	0.24	2.01	2.42	109.48
sc_accuracy_forces 2.5×10^{-4}	7	22	−3.68	−3.43	0.25	2.01	2.42	109.48
relax_geometry trm 2.5×10^{-3}	6	17	−3.68	−3.43	0.25	2.01	2.40	109.48
	1	16	−3.69	−3.43	0.26	2.02	2.40	109.48
	2	0	−3.73	−3.48	0.25	2.02	2.42	109.48
Third test (blue)	3	69	−3.90	−3.59	0.31	3.41	3.80	109.47
	5	50	−3.85	−3.53	0.32	2.40	2.88	109.47
sc_accuracy_etot 2.5×10^{-6}	4	49	−3.85	−3.53	0.32	2.38	2.89	109.47
sc_accuracy_rho 2.5×10^{-3}	7	15	−3.69	−3.43	0.26	2.03	2.41	109.48
sc_accuracy_forces 2.5×10^{-5}	1	14	−3.69	−3.43	0.26	2.03	2.41	109.48
relax_geometry trm 2.5×10^{-4}	6	14	−3.69	−3.43	0.26	2.03	2.41	109.48
	8	13	−3.69	−3.43	0.26	2.03	2.41	109.48
	2	0	−3.73	−3.48	0.25	2.01	2.43	109.48
Fourth test (green)	3	69	−3.90	−3.59	0.31	3.41	3.81	109.47
	5	50	−3.85	−3.53	0.32	2.40	2.88	109.47
sc_accuracy_etot 2.5×10^{-6}	4	49	−3.85	−3.53	0.32	2.38	2.89	109.47
sc_accuracy_rho 2.5×10^{-3}	7	15	−3.69	−3.43	0.26	2.03	2.41	109.48
sc_accuracy_forces 2.5×10^{-6}	1	14	−3.69	−3.43	0.26	2.03	2.41	109.48
relax_geometry trm 2.5×10^{-5}	6	14	−3.69	−3.43	0.26	2.03	2.41	109.48
	8	12	−3.69	−3.43	0.26	2.03	2.41	109.48
	2	0	−3.73	−3.48	0.25	2.02	2.43	109.48

S3 Analyses: Structural and Energetic Parameters

S3.1 Effective Coordination Concept

To characterize the changes induced by the molecules in the TM_{13} clusters, we employed the effective coordination concept,[1,2] which yields the weighted bond length, d_{av}^{i}, and the effective coordination number, ECN^{i}, for each atom in the cluster. In this framework, the d_{av}^{i} values are calculated using a self-consistent approach based on weighted obtained via an exponential function.

Thus, d_{av}^{i} is obtained using the following equation,

$$d_{av}^{i,new} = \frac{\sum_i d_{ij} exp\left[1 - \left(\frac{d_{ij}}{d_{av}^{i,old}}\right)^6\right]}{\sum_j exp\left[1 - \left(\frac{d_{ij}}{d_{av}^{i,old}}\right)^6\right]} \ , \tag{1}$$

where d_{av}^{i} is obtained in a self-consistent manner. In the QTNano implementation, the shortest distance between the i and j atoms are employed as the starting value for the $d_{av}^{i,old}$ parameters. The convergence is achieved once the condition, $\mid d_{av}^{i,new} - d_{av}^{i,old} \mid \ < 10^{-4}$ Å is reached for every atom i within the molecular system. For complicated systems with lower symmetry, the self-consistent scheme reaches its convergence in less than 10 steps.

Once the d_{av}^{i} results are calculated, the ECN^{i} results can be obtained using the following equation,

$$\mathrm{ECN}^{i} = \sum_j exp\left[1 - \left(\frac{d_{ij}}{d_{av}^{i}}\right)^6\right] \ . \tag{2}$$

Thus, the average values, i.e., ECN_{av} and d_{av}, are obtained by the following equations,

$$\mathrm{ECN}_{av} = \frac{1}{N}\sum_i \mathrm{ECN}_i \ , \tag{3}$$

and

$$d_{av} = \frac{1}{N}\sum_i d_{av}^{i} \ , \tag{4}$$

where N is the number of atoms in the system. This framework is suitable for transition-metal clusters with lower symmetry as it takes into account tiny differences among the bond lengths. Thus, it can capture small changes in the cluster structure upon the adsorption of molecular systems.

S3.2 Energetic Analyses: Relative Total Energy, Binding Energy, Adsorption and Interaction Energies

The energetic analyses is a key point in our investigation, and hence, we provided below the definition for several energetic quantities.

1. Relative total energy, ΔE^i_{tot}, is given by the following equation,

$$\Delta E^i_{tot} = E^i_{tot} - E^{lowest}_{tot} \ , \tag{5}$$

   where E^i_{tot} is the total energy of the configuration i, while E^{lowest}_{tot} is the total energy of the lowest energy configuration. Thus, this quantity is useful as only the relative energies (small numbers) are represented and not large total energy values.

2. Binding energy, E_b, which are given by the following equations for the different molecules,

$$E_b^{\mathrm{TM_{13}}} = (E_{tot}^{\mathrm{TM_{13}}} - 13E_{tot}^{\mathrm{TM}\ atom})/13 \ , \tag{6}$$

$$E_b^{\mathrm{CH_4}} = [E_{tot}^{\mathrm{CH_4}} - (E_{tot}^{\mathrm{C}\ atom} + 4E_{tot}^{\mathrm{H}\ atom})]/5 \ , \tag{7}$$

$$E_b^{\mathrm{CO}} = [E_{tot}^{\mathrm{CO}} - (E_{tot}^{\mathrm{C}\ atom} + E_{tot}^{\mathrm{O}\ atom})]/2 \ , \tag{8}$$

$$E_b^{\mathrm{H_2}} = (E_{tot}^{\mathrm{H_2}} - 2E_{tot}^{\mathrm{H}\ atom})/2 \ , \tag{9}$$

$$E_b^{\mathrm{CH_3OH}} = [E_{tot}^{\mathrm{CH_3OH}} - (E_{tot}^{\mathrm{C}\ atom} + E_{tot}^{\mathrm{O}\ atom} + 4E_{tot}^{\mathrm{H}\ atom})]/6 \ , \tag{10}$$

   where E^{Mol}_{tot} (Mol = CH_4, CO, H_2, and CH_3OH) is the total energy of the molecules,

while $E_{tot}^{X\ atom}$ (X = TM, C, O, and H) are the total energies of the free-atoms obtained from spin-polarized calculations.

3. To evaluate the strength of the Mol-TM_{13} interactions, we calculated the adsorption energy, E_{ad}, as follows,

$$E_{ad} = E_{tot}^{\mathrm{Mol/TM_{13}}} - (E_{tot}^{\mathrm{TM_{13}}\ lowest} + E_{tot}^{\mathrm{Mol}\ lowest}) \ , \tag{11}$$

where, $E_{tot}^{\mathrm{Mol/TM_{13}}}$ is the total energy of the adsorbed system in the lowest energy configuration, while $E_{tot}^{\mathrm{TM_{13}}\ lowest}$ and $E_{tot}^{\mathrm{Mol}\ lowest}$ are the total energies of the gas-phase cluster and molecule upon relaxation, respectively.

4. Furthermore, we calculated the interaction energy, E_{int}, using the following equation:

$$E_{int} = E_{tot}^{\mathrm{Mol/TM_{13}}} - (E_{tot}^{\mathrm{TM_{13}}\ frozen} + E_{tot}^{\mathrm{Mol}\ lowest}) \ , \tag{12}$$

where, $E_{tot}^{\mathrm{TM_{13}}\ frozen}$ and $E_{tot}^{\mathrm{Mol}\ frozen}$ are the total energies of the cluster and molecule in their frozen geometry of the adsorbed system, respectively. Thus, E_{ad} and E_{int} are related as follows:

$$E_{ad} = E_{int} + \Delta E_{tot}^{\mathrm{TM_{13}}} + \Delta E_{tot}^{\mathrm{Mol}} \ , \tag{13}$$

where, $\Delta E_{tot}^{\mathrm{TM_{13}}}$ and $\Delta E_{tot}^{\mathrm{Mol}}$ are the deformation energies, i.e., the energy differences between the gas-phase frozen and lowest energy configurations,

$$\Delta E_{tot}^{\mathrm{Mol}} = E_{tot}^{\mathrm{Mol}\ frozen} - E_{tot}^{\mathrm{Mol}\ lowest} \ , \tag{14}$$

$$\Delta E_{tot}^{\mathrm{TM_{13}}} = E_{tot}^{\mathrm{TM_{13}}\ frozen} - E_{tot}^{\mathrm{TM_{13}}\ lowest} \ . \tag{15}$$

S4 Structural, Energetic and Electronic Properties of the Gas-phase Molecules

All complementary information for the gas-phase molecules, i.e., CH_4, CO, H_2 and CH_3OH, are presented here. Thus, we separated this section into two main subsections: (A) structural and energetic properties, i.e., binding energy, average bond lengths, and average bond angles; and (B) electronic properties, i.e., molecular orbital diagram, project density of states, and dipole moment.

S4.1 Structural and Energetic Properties

The results for the gas-phase molecules summarized in Fig. S2 are in good agreement with the literature. The average deviation from the experimental values for the structural properties is about $\leq \ |2.33\,\%|$ whereas for the energetic is $\leq 4.48\,\%$.

Table S2: Structural and energetic parameters for CH_4, CO, H_2 and CH_3OH at DFT-PBE+TS level, where d_{av} is the average bond length (Å), θ_{av} is the average bond angle (°) and E_b is the binding energy per atom (eV). The numbers in parentheses are the deviation (in %) with respect to the experimental data.

		CH_4		CO		H_2		CH_3OH	
d_{av} (Å)	DFT-PBE+TS	1.09		1.13		0.75	(1.35)	1.09^{C-H}	
								1.39^{C-O}	(−2.33)
								0.95^{O-H}	(1.06)
	DFT-PBE[3]			1.14		0.75			
	Expt.[4]	1.09		1.13		0.74		1.09	
								1.42	
								0.94	
θ (°)	DFT-PBE+TS	109.5						109.3^{HCH}	(0.64)
								107.5^{HOC}	(−0.92)
	Expt.[4]	109.5						108.6^{HCH}	
								108.5^{HOC}	
E_b (eV)	DFT-PBE+TS	−3.65	(3.99)	−5.83	(4.48)	−2.27	(0.44)	−3.76	
	DFT-PBE[3]			−5.83		−2.28			
	Expt.[5]	−3.51		−5.58		−2.26			

S4.2 Electronic Properties

Below, we provide the molecular orbital diagram (MO) and the project density of states per atom (PDOS) for each gas-phase molecule. For both analyses, we focus only on the valence states. Thus, at the end of this subsection, the resultant dipole moment vector (μ), i.e., magnitude and direction, for each investigated molecule is shown.

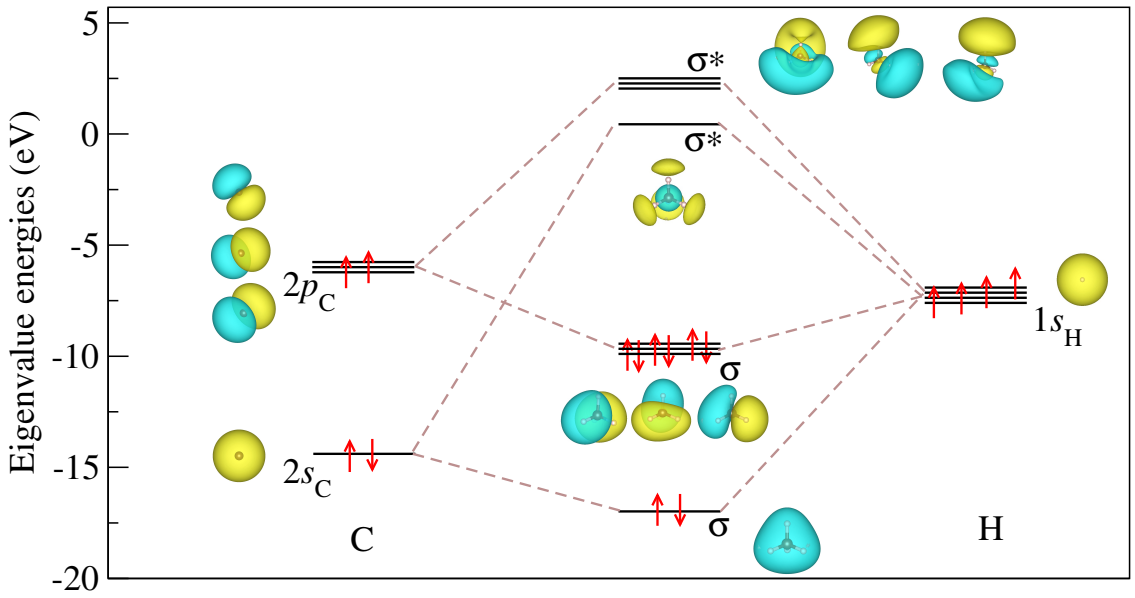

Figure S2: Molecular orbital diagram for gas-phase CH_4, where degenerated states are depicted by closer lines and their respective orbitals are placed linearly. The blue (negative) and yellow (positive) regions are the isosurfaces plots with a cutoff of $0.05\,e\text{Å}^{-3}$.

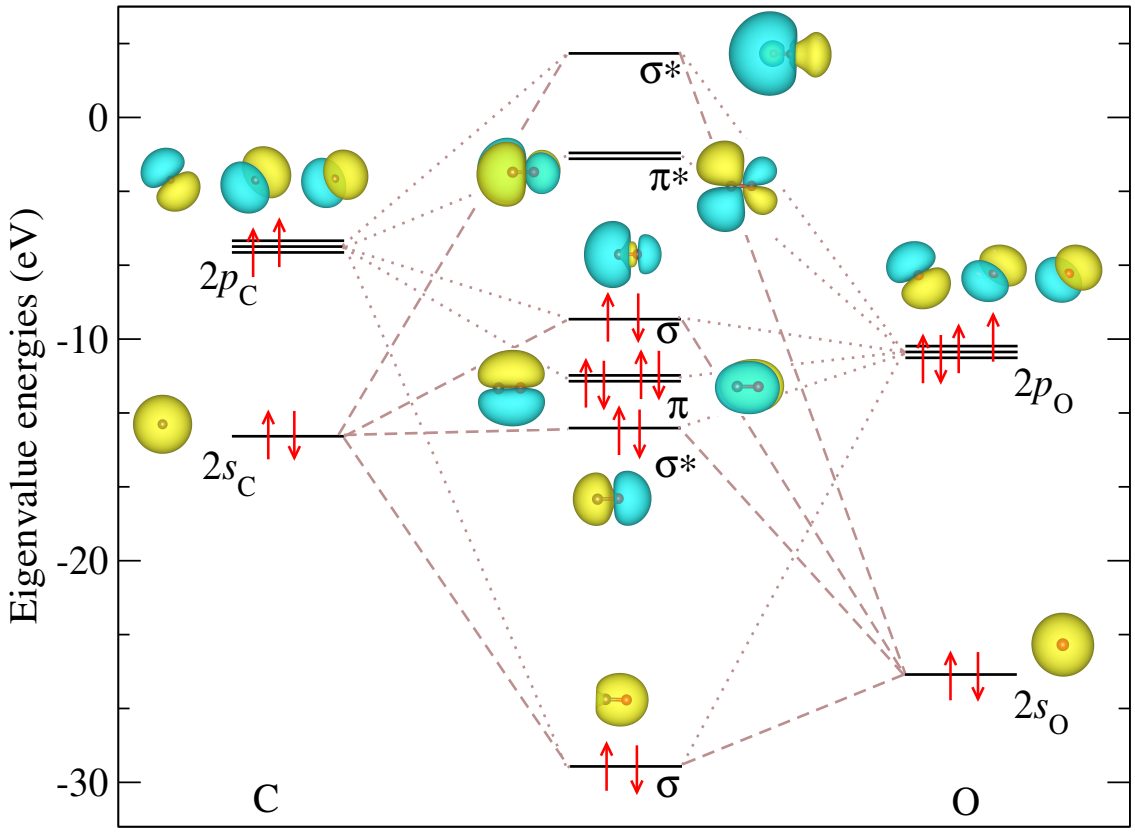

Figure S3: Molecular orbital diagram for gas-phase CO, where degenerated states are depicted by closer lines and their respective orbitals are placed aside. The blue (negative) and yellow (positive) regions are the isosurfaces plots with a cutoff of $0.05\,e\text{Å}^{-3}$.

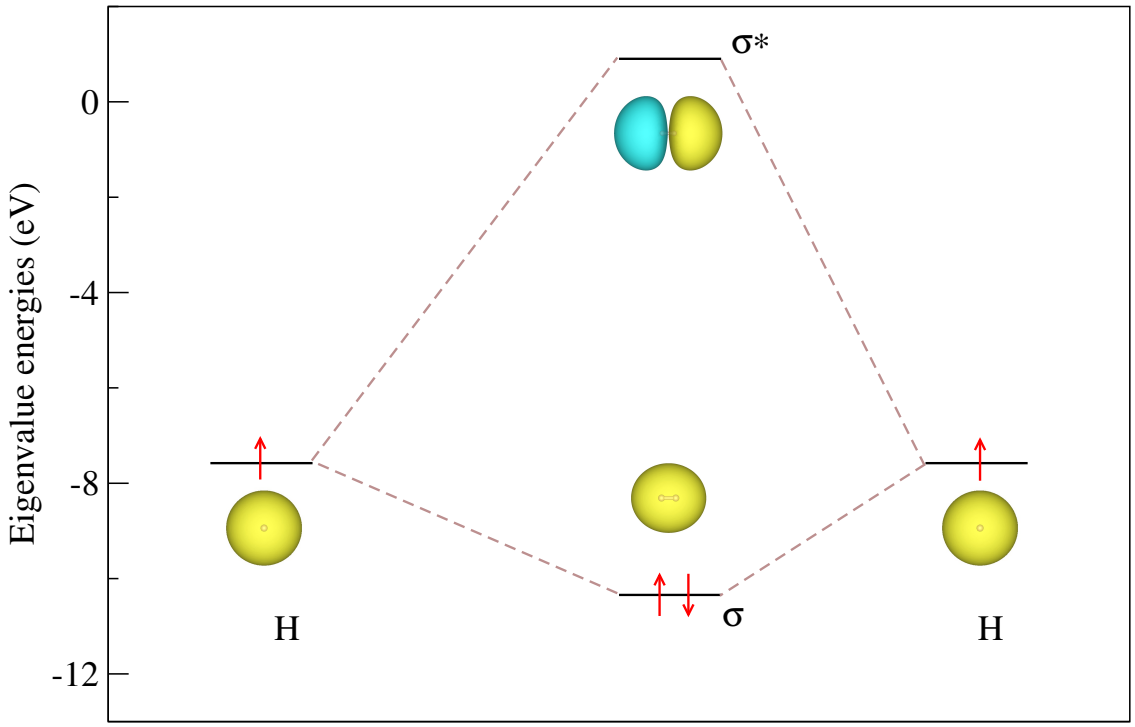

Figure S4: Molecular orbital diagram for gas-phase H_2, where degenerated states are depicted by closer lines and their respective orbitals are placed aside. The blue (negative) and yellow (positive) regions are the isosurfaces plots with a cutoff of $0.05\,e\text{Å}^{-3}$.

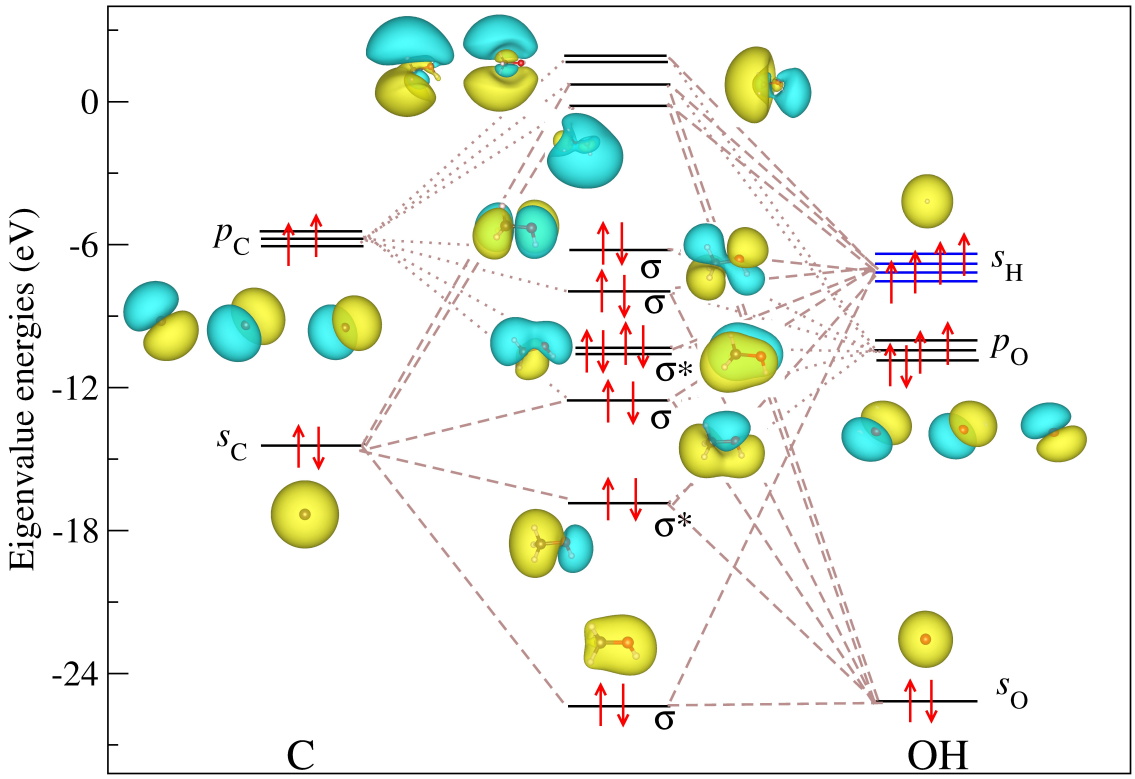

Figure S5: Molecular orbital diagram for gas-phase CH_3OH, where degenerated states are depicted by closer lines and their respective orbitals are placed aside. The blue (negative) and yellow (positive) regions are the isosurfaces plots with a cutoff of $0.05\,e\text{Å}^{-3}$.

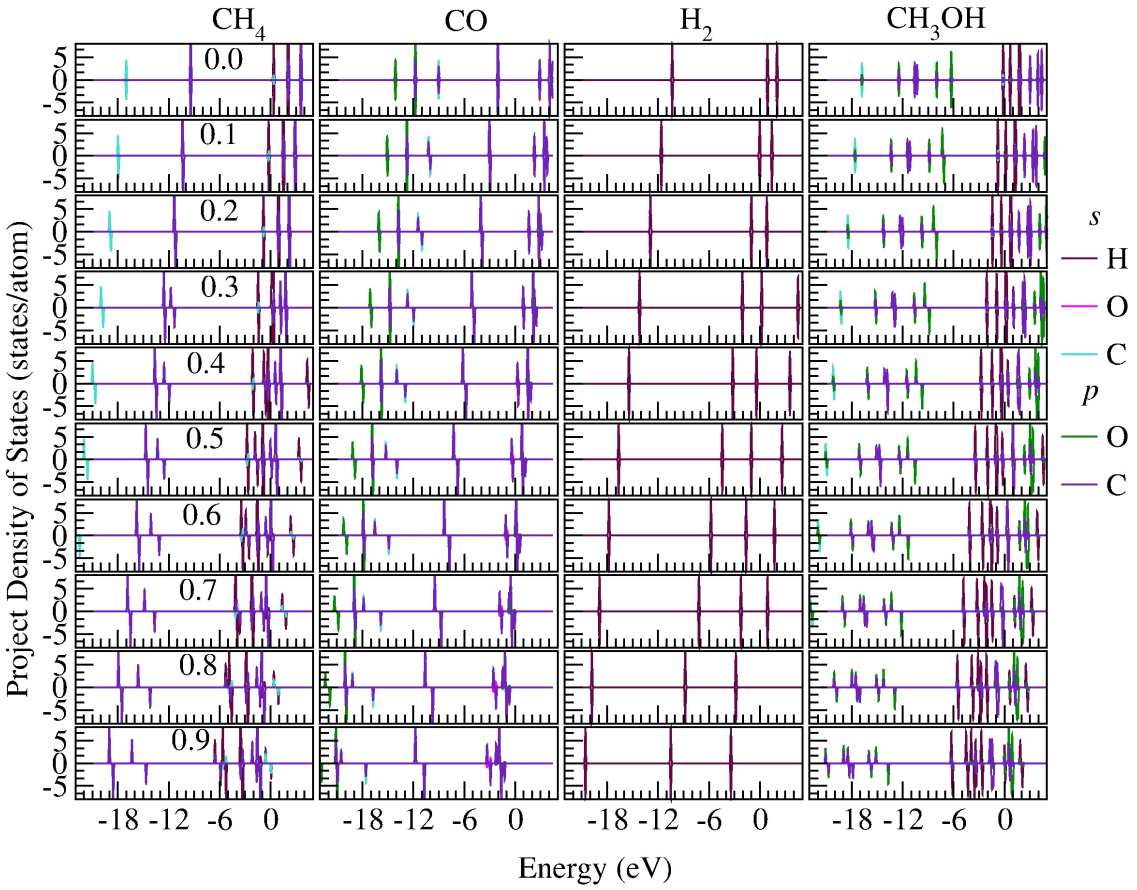

Figure S6: Project density of states per atom for the gas-phase molecules, i.e., methane, carbon monoxide, hydrogen molecule, and methanol, respectively. To improve our atomistic understanding of the charge influence on the energetic distribution of the molecule electronic states, we evaluated the PDOS in function of charge, in which ranges from 0.0 e to 0.9 e. The electronic states are represented by colored lines as follows: C s- (turquoise), C p- (violet), O s- (magenta), O p- (green), and H s- (purple) states.

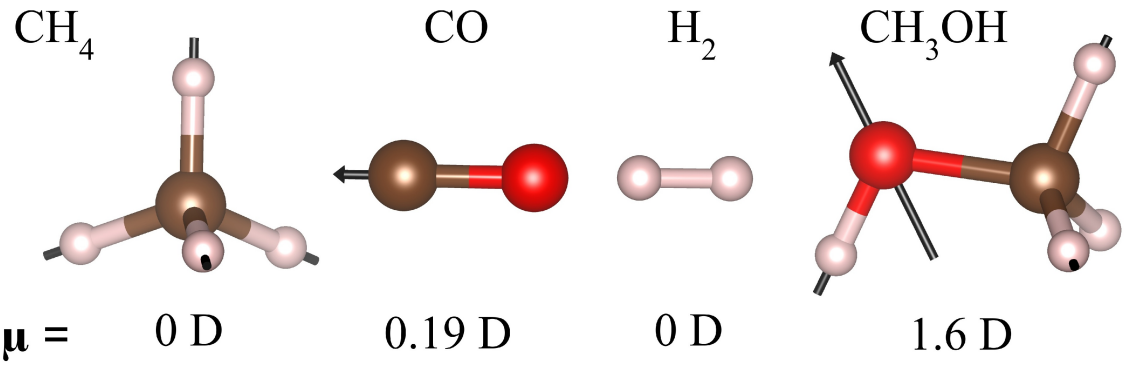

Figure S7: Dipole moment for the gas-phase molecules, i.e., methane, carbon monoxide, hydrogen molecule, and methanol, respectively. The arrows (black) indicated the magnitude and direction of the resultant dipole moment vector.

S5 Vibration Frequency of the Gas-phase Molecules

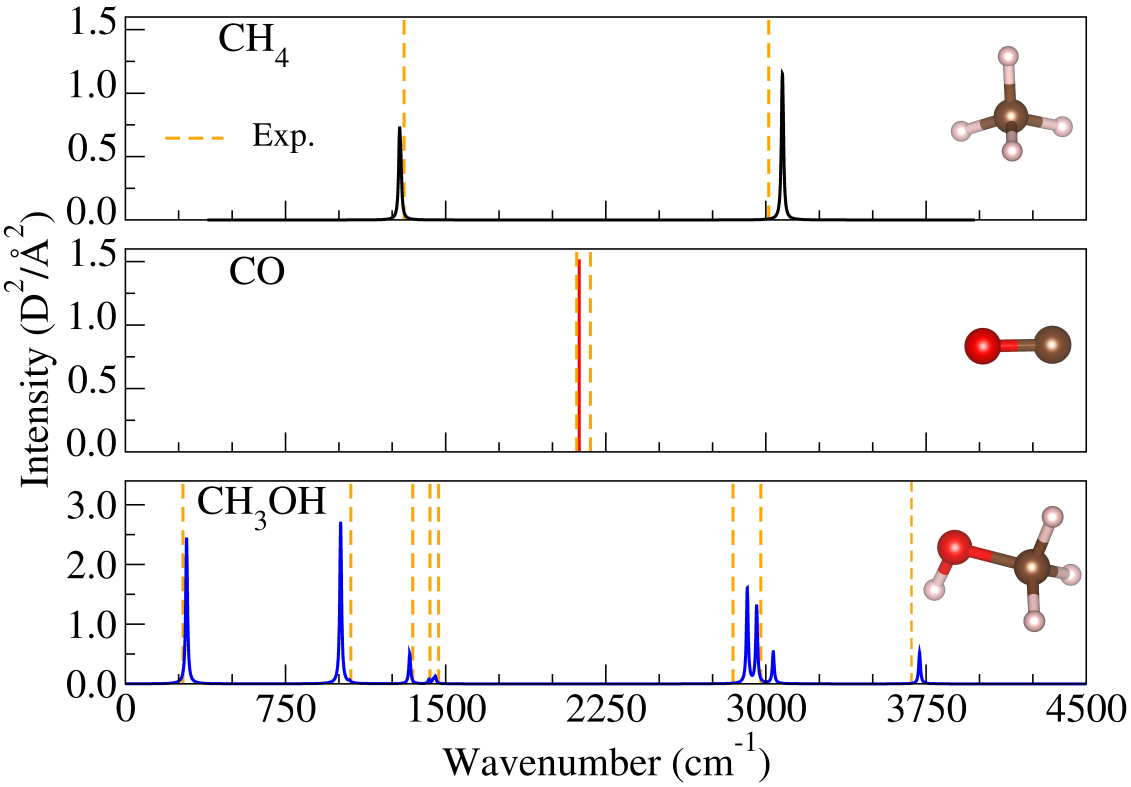

Figure S8: Infra-red spectra for the gas-phase molecules, i.e., methane (black), carbon monoxide (red), and methanol (blue), respectively. As observed, the calculated spectra for the gas-phase molecules are in good agreement with the experimental available data (yellow dashed line) for methane,[6] carbon monoxide,[6] and methanol.[7]

S6 Structural, Energetic, and Electronic Properties of Gas-phase 13-atom Transition-metal Clusters

Accordingly, the electronic self-consistency was achieved once the total energy and atomic forces criteria were smaller than 2.5×10^{-5} eV and 2.5×10^{-3} eV Å^{-1}, respectively. The modified Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm[8,9] was used to optimize the atomic forces on each atom, and the equilibrium geometry was obtained once the atomic forces on every atom were smaller than 2.5×10^{-2} eV Å^{-1}. Furthermore, we re-optimized all TM_{13} putative global minimum configurations (pGMCs) with the same level of theory defined

at the Theoretical Approach and Computational Details section of the main manuscript's text. Thus, the present section was separated as follows: (A) energetic properties, i.e., relative total energy and binding energy; (B) structural and magnetic properties, i.e., effective coordination number, average weighted bond length, and total magnetic moment per atom; and (C) electronic properties, i.e., Hirshfeld charges, HOMO-LUMO plots and projected density of states per atom.

S6.1 Energetic Properties

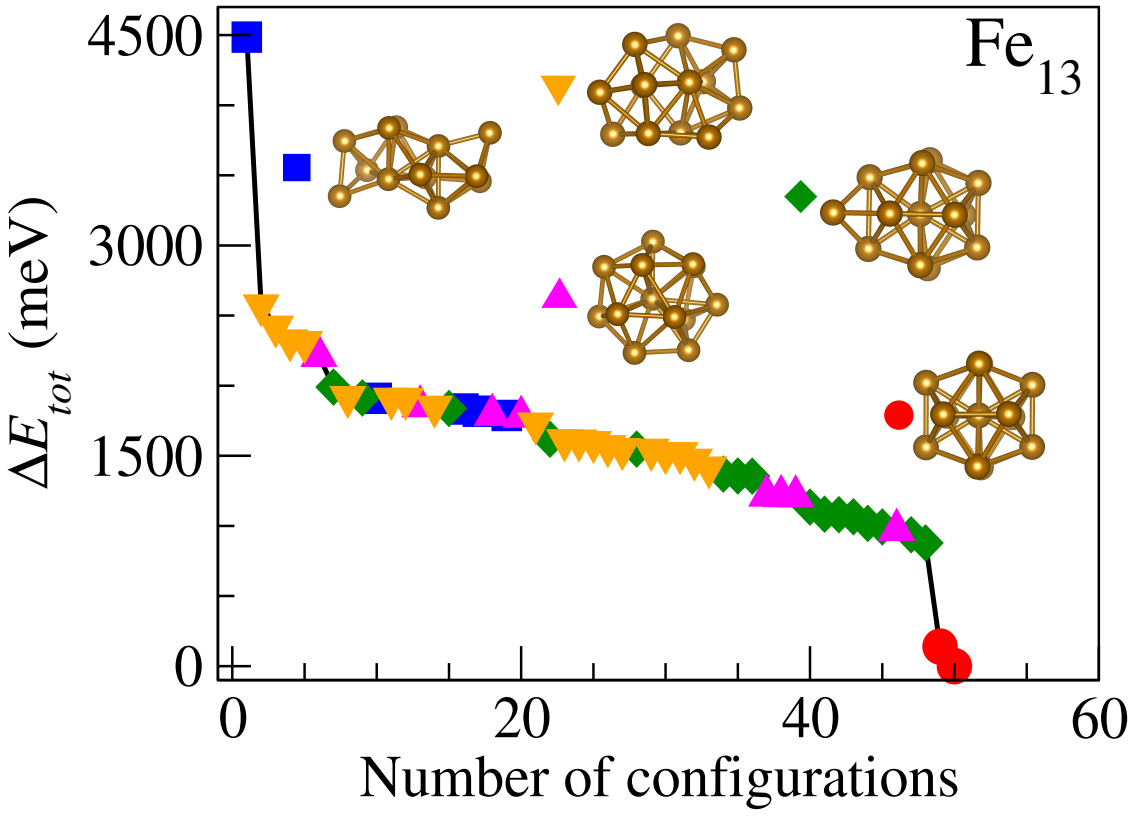

Figure S9: Relative total energy (meV) for Fe_{13} configurations set. The five representative adsorbed structures selected by the *k-means* clustering algorithm are inserted within the graphics, where each selected structure is the lowest energy configuration within its group.

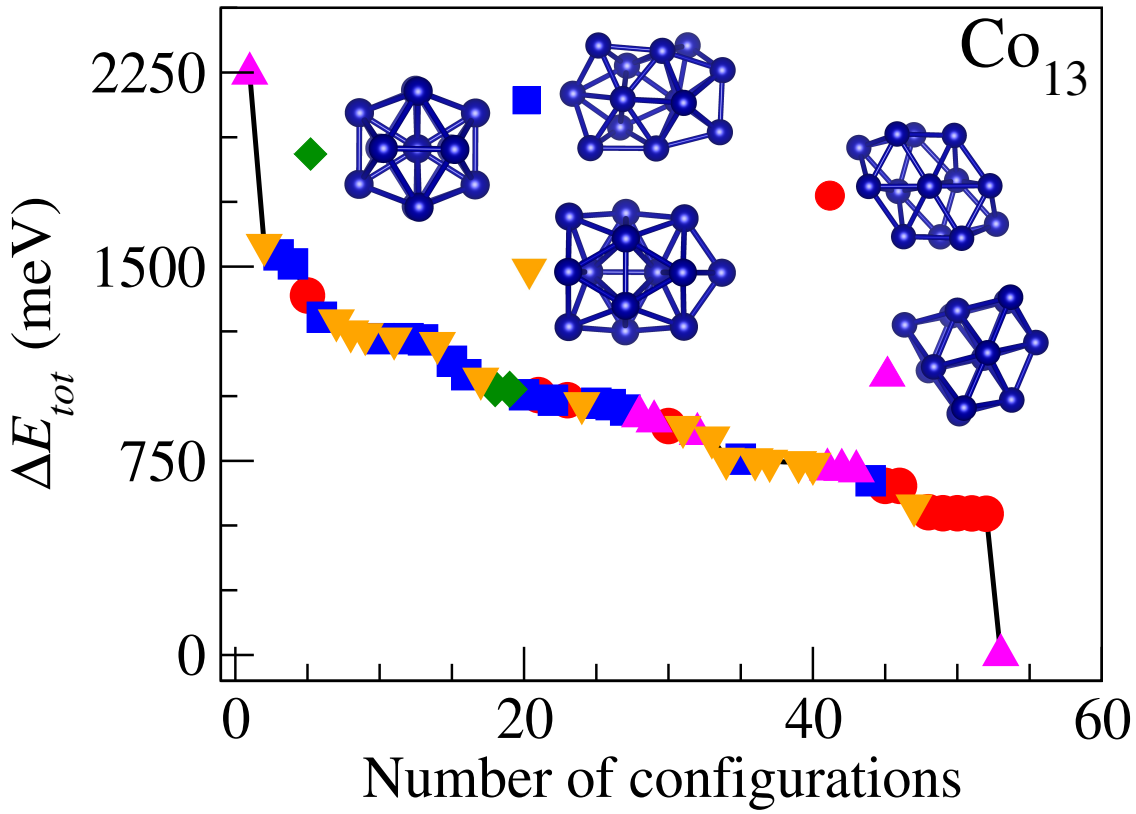

Figure S10: Relative total energy (meV) for Co_{13} configurations set. The five representative adsorbed structures selected by the *k-means* clustering algorithm are inserted within the graphics, where each selected structure is the lowest energy configuration within its group.

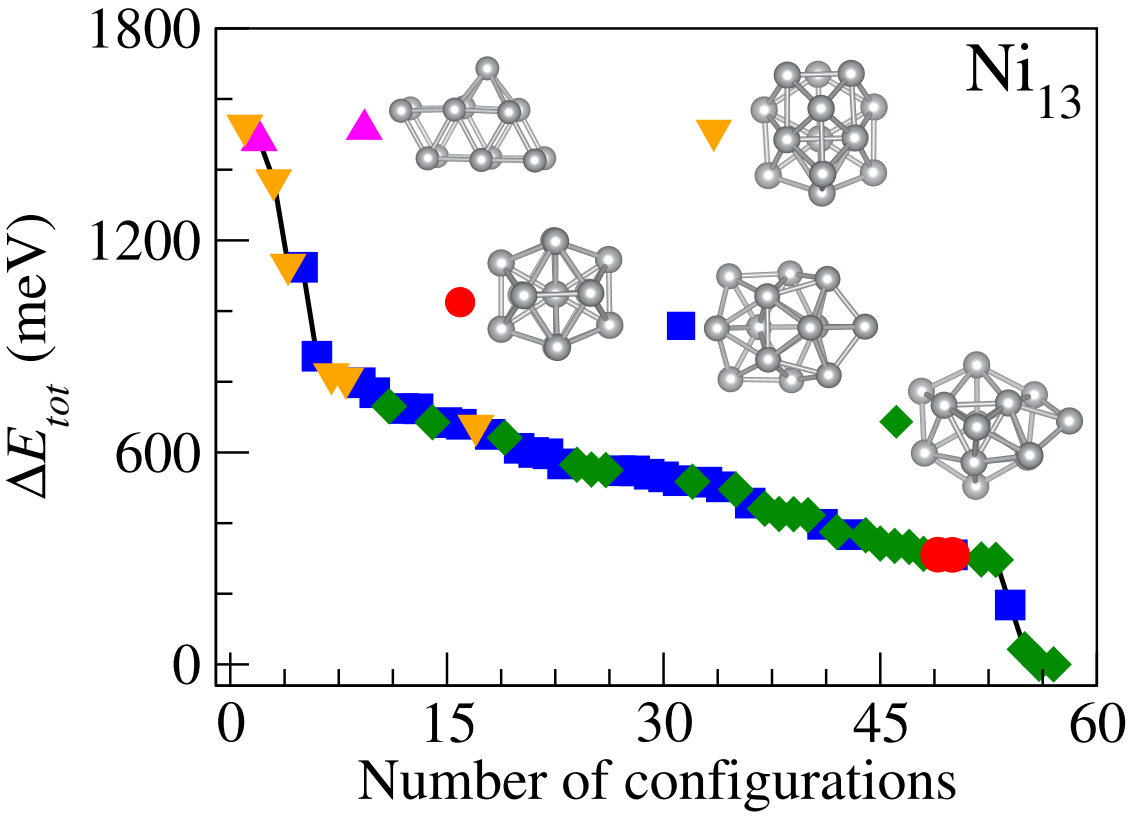

Figure S11: Relative total energy (meV) for Ni_{13} configurations set. The five representative adsorbed structures selected by the *k-means* clustering algorithm are inserted within the graphics, where each selected structure is the lowest energy configuration within its group.

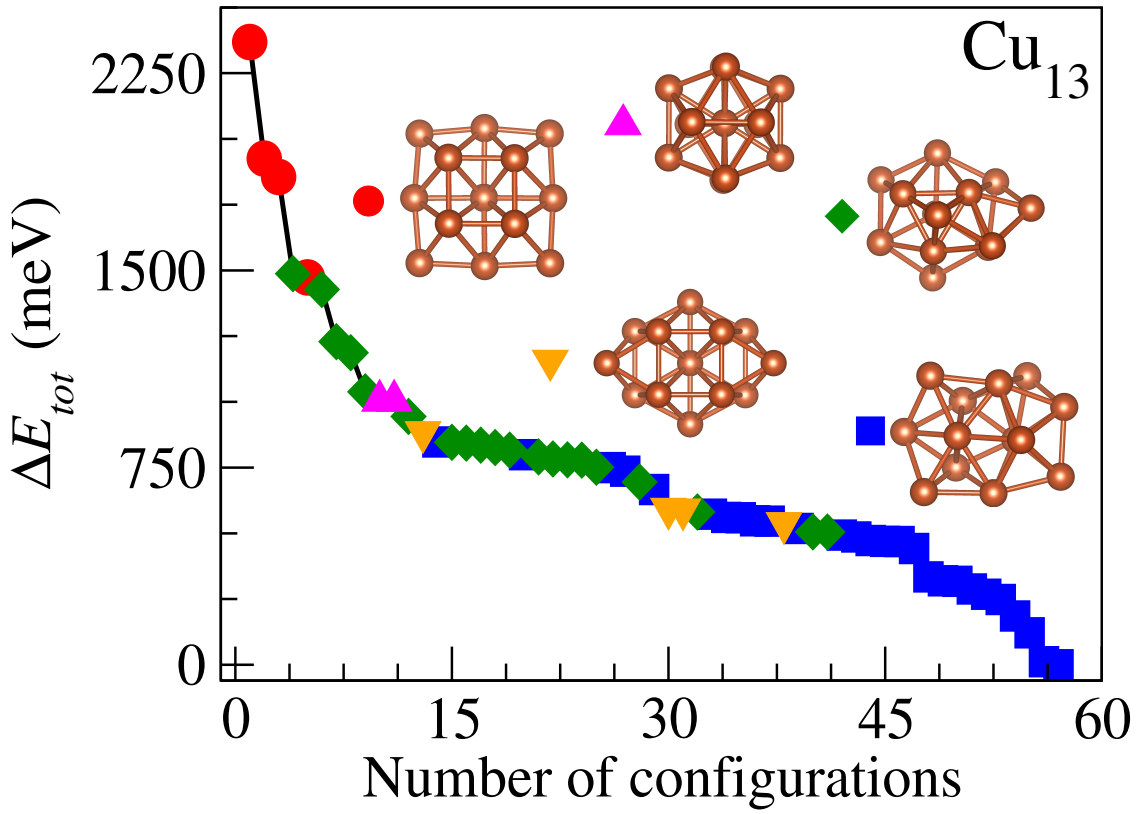

Figure S12: Relative total energy (meV) for Cu_{13} configurations set. The five representative adsorbed structures selected by the *k-means* clustering algorithm are inserted within the graphics, where each selected structure is the lowest energy configuration within its group.

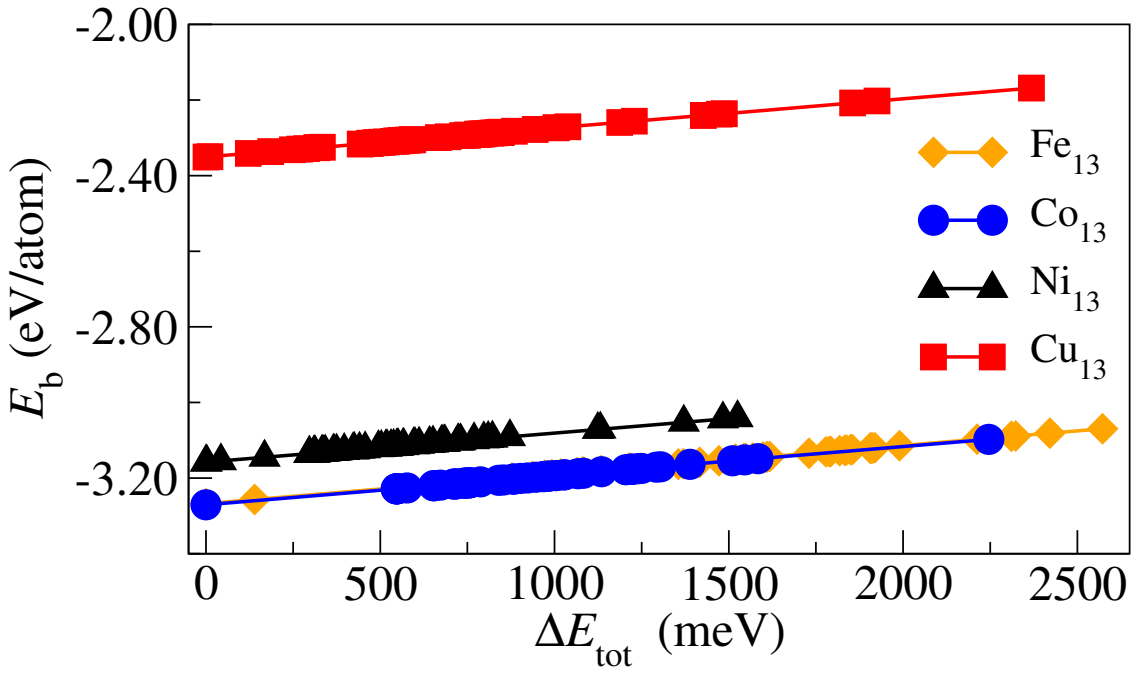

Figure S13: Binding energy per atom for all sets of Fe_{13} (orange), Co_{13} (blue), Ni_{13} (black), and Cu_{13} (red) gas-phase clusters in relation to the relative total energy.

S6.2 Structural and Magnetic Properties

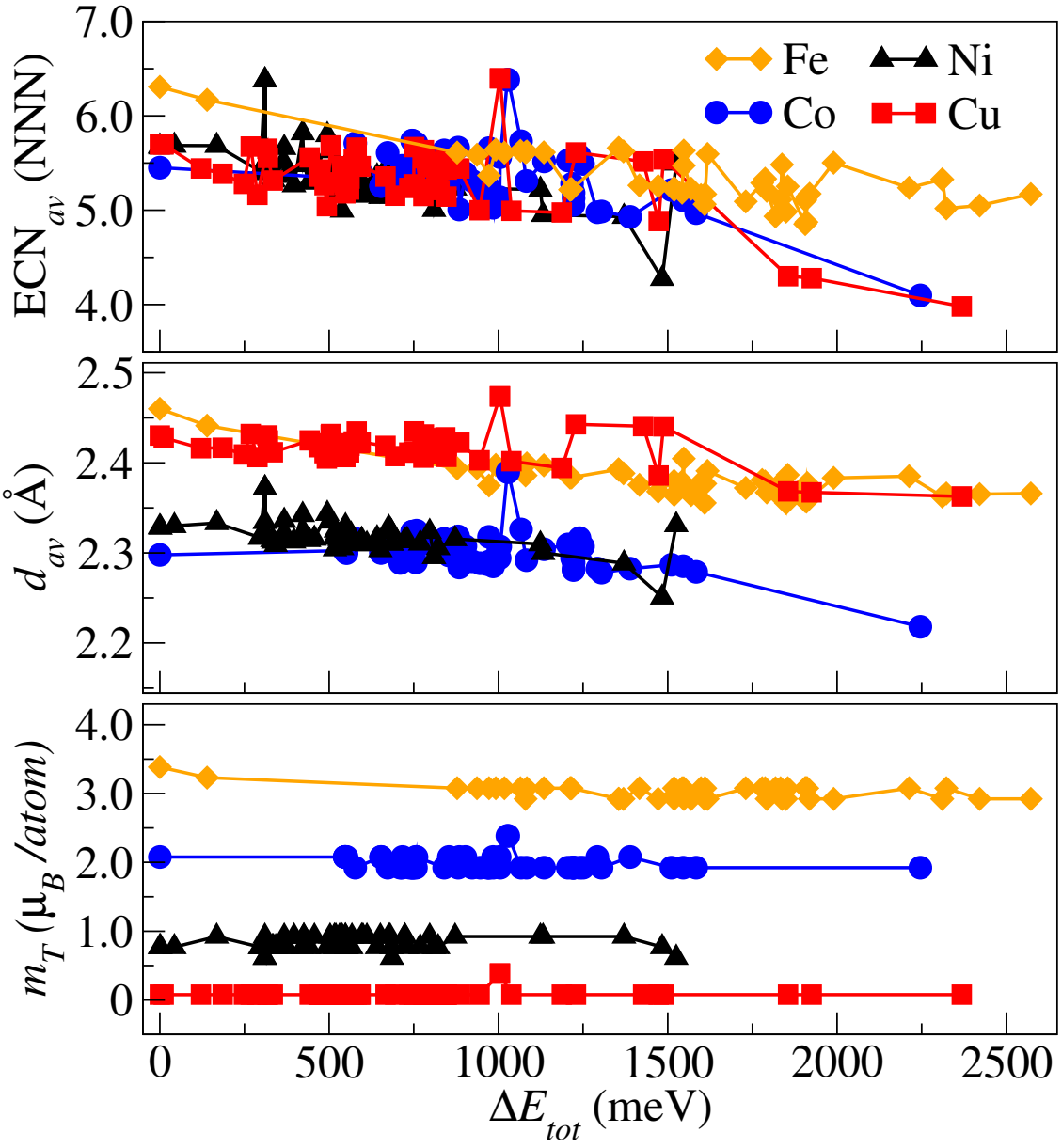

Figure S14: Structural properties for all sets of Fe_{13} (orange), Co_{13} (blue), Ni_{13} (black), and Cu_{13} (red) gas-phase clusters in relation to the relative total energy. Average effective coordination number ECN_{av}, average weighted bond length d_{av}, and total magnetic moment per atom m_T.

Additional properties for the TM_{13} clusters, as LUMO-HOMO energy gap, are given in Table S3.

Table S3: Energetic, structural and electronic properties for the representative set of the TM_{13} clusters, where TM = Fe, Co, Ni, and Cu; ΔE_{tot} - Relative total energy per atom, m_{av} - Average magnetic moment per atom, E_g - LUMO-HOMO energy gap, E_b - Binding energy, ECN_{av} - Average effective coordination number per atom, d_{av} - Average weighted bond lengths, and N_b - Number of bonds.

	ΔE_{tot} (meV)	m_{av} (μ_B/atom)	E_g (eV)	E_b (eV/atom)	ECN_{av} (NNN)	d_{av} (Å)	N_b
Fe_{13}	1787	3.07	0.19	−3.13	5.33	2.41	36
	1416	3.07	0.25	−3.16	5.26	2.41	37
	972	3.07	0.17	−3.19	5.37	2.41	38
	878	3.07	0.22	−3.20	5.61	2.42	39
	0	3.38	0.28	−3.27	6.31	2.48	42
Co_{13}	1026	2.38	0.15	−3.19	6.38	2.42	42
	673	1.92	0.18	−3.22	5.61	2.35	38
	577	1.92	0.18	−3.23	5.71	2.35	38
	546	2.08	0.14	−3.23	5.34	2.34	39
	0	2.08	0.31	−3.27	5.45	2.34	36
Ni_{13}	1483	0.78	0.07	−3.04	4.27	2.29	28
	676	0.92	0.06	−3.10	5.45	2.36	36
	310	0.61	0.10	−3.13	6.38	2.40	42
	168	0.92	0.11	−3.14	5.68	2.37	38
	0	0.78	0.10	−3.16	5.67	2.36	38
Cu_{13}	1473	0.08	0.17	−2.24	4.88	2.41	33
	1004	0.38	0.48	−2.27	6.40	2.50	42
	538	0.08	0.21	−2.31	5.46	2.45	36
	505	0.08	0.21	−2.31	5.69	2.46	38
	0	0.08	0.20	−2.35	5.70	2.46	38

S6.3 Electronic Properties

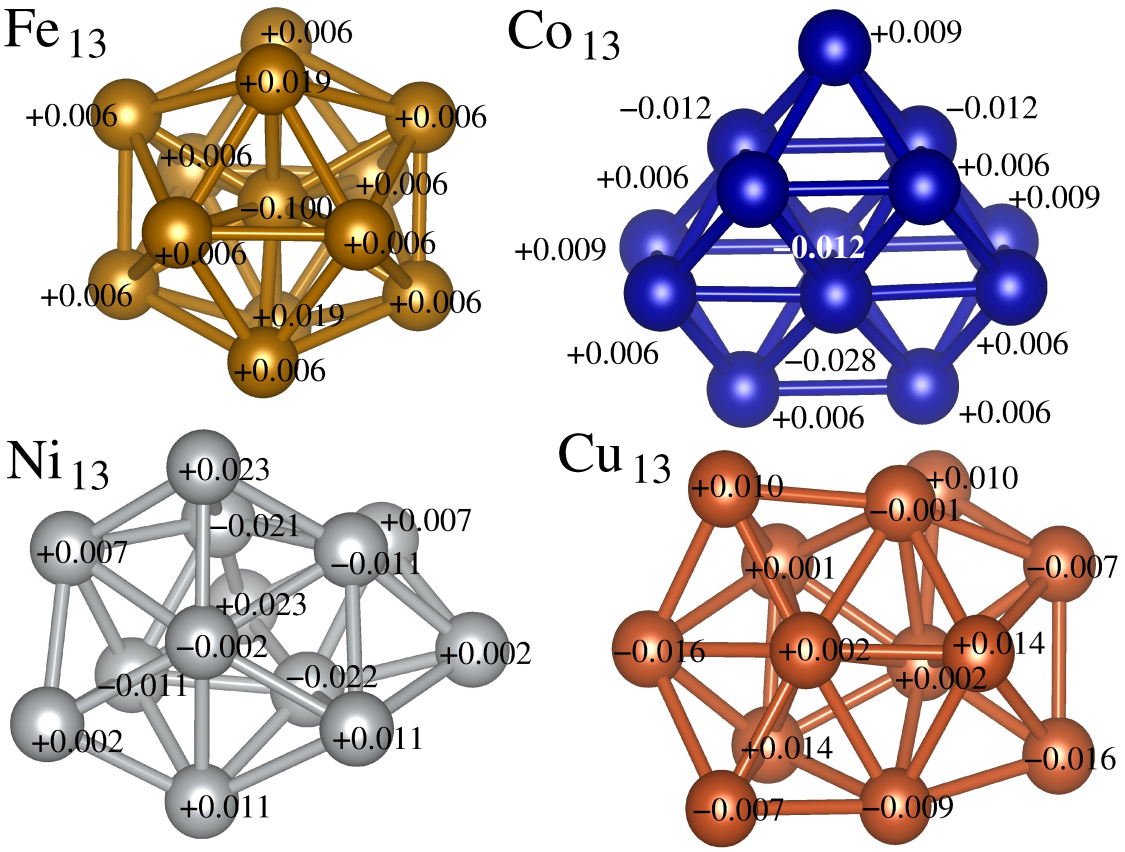

Figure S15: Hirshfeld charge analysis (in e) for the Fe_{13} (orange), Co_{13} (blue), Ni_{13} (black), and Cu_{13} (red) pGMCs.

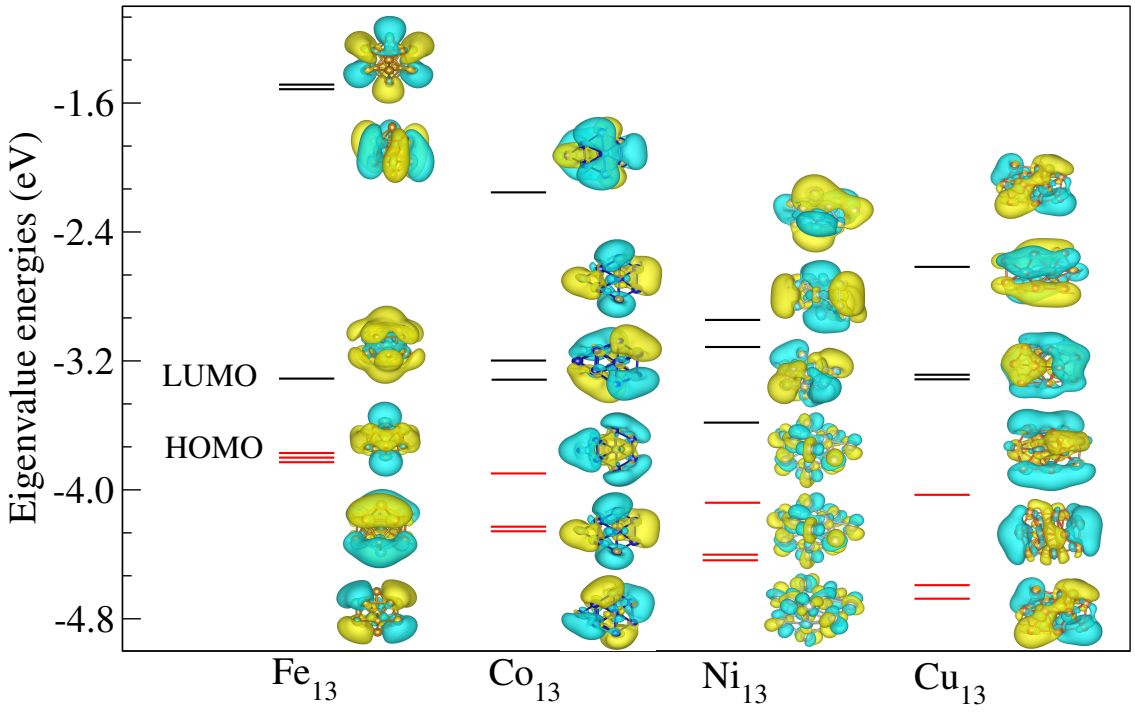

Figure S16: HOMO and LUMO plots for the Fe_{13}, Co_{13}, Ni_{13}, and Cu_{13} pGMCs. The blue (negative) and yellow (positive) regions are the isosurfaces plots with a cutoff of $0.05\,e\text{Å}^{-3}$.

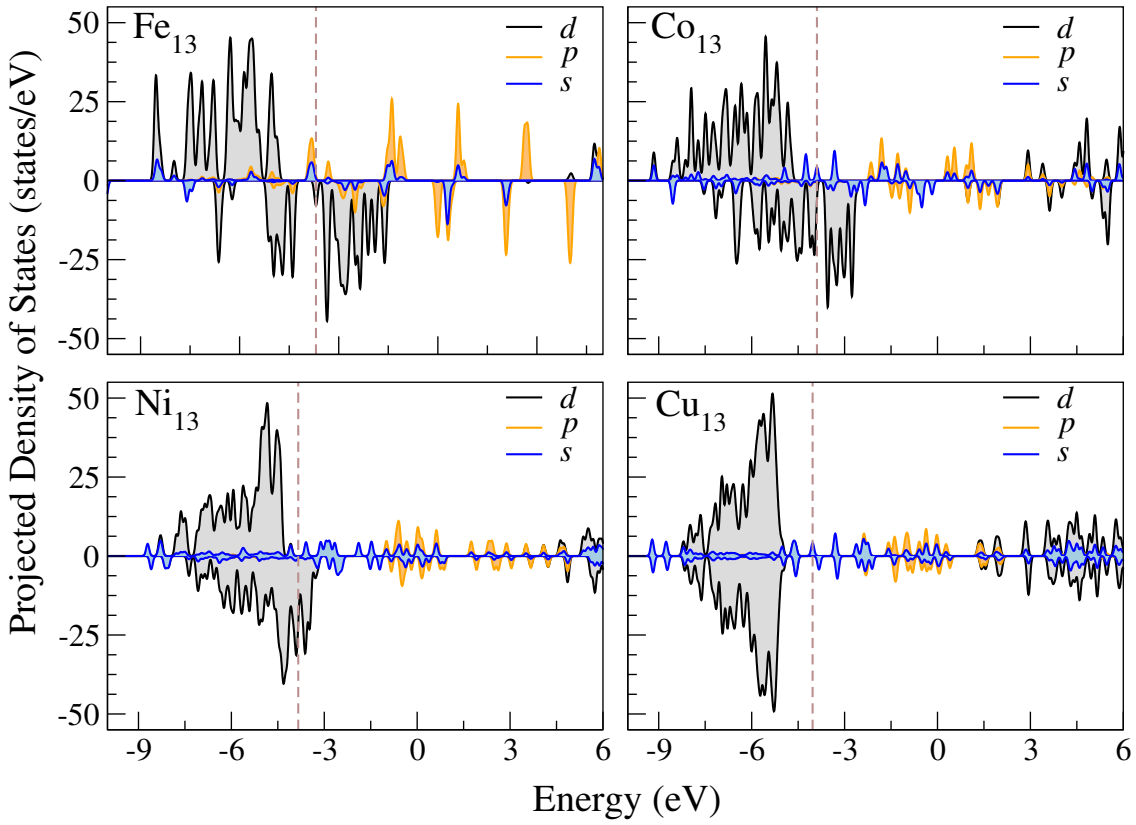

Figure S17: Project density of states per atom for the Fe_{13}, Co_{13}, Ni_{13}, and Cu_{13} pGMCs. The states are represented by *s*-TM (green), *p*-TM (orange), *d*-TM (black) lines.

S7 Vibrational Frequency of the Gas-phase 13-atom Transition-metal Clusters

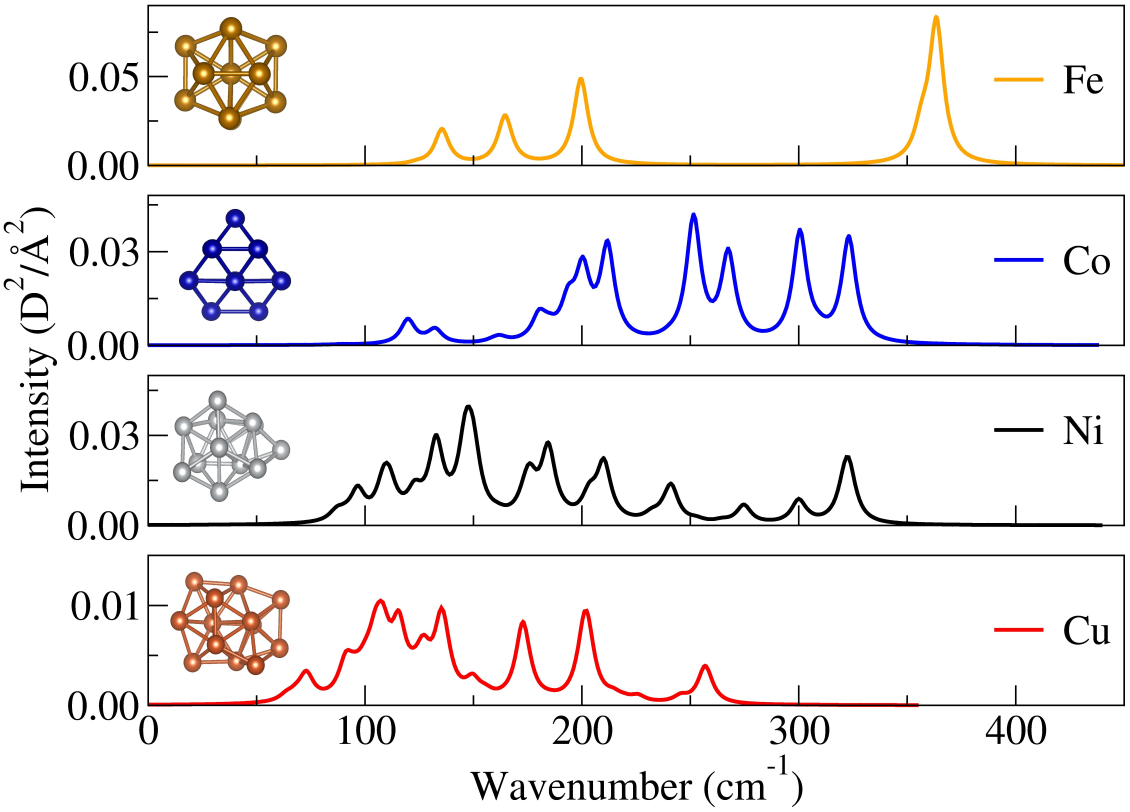

Figure S18: Infra-red spectra for Fe_{13} (orange), Co_{13} (blue), Ni_{13} (black), and Cu_{13} (red) pGMCs.

S8 Structural, Energetic, and Electronic Properties of the Mol/TM_{13} Systems

In this section, we provide all the raw data for the representative set of the adsorbed Mol/TM_{13} systems used for generating the manuscript main figures. Thus, we also provide additional analyses for the higher-energy configurations, e.g., electron density difference.

S8.1 Structural and Energetic Properties

Table S4: Energetic and structural properties for representative set of the CH_4/TM_{13} system. ΔE_{tot} - Relative total energy, E_{ad} - Adsorption energy, E_{int} - Interaction energy, $d^{\text{Mol-TM}_{13}}$ - Minimum distance between Mol and TM_{13}, Δd_0 - Relative changes in the average weighted bond length of Mol, ΔECN_{av} - Relative changes in the TM_{13} average effective coordination number after adsorption, Δd_{av} - Relative changes in the average weighted bond lengths of TM_{13} after adsorption, m_T - Total magnetic moments per structure.

CH_4	ΔE_{tot} (meV)	E_{ad} (eV)	E_{int} (eV)	$d^{\text{Mol-TM}_{13}}$ (Å)	Δd_0 (%)	ΔECN_{av} (%)	Δd_{av} (%)	m_T (μ_B)
Fe_{13}	15	−0.26	−0.46	2.02	0.92	−1.95	−0.69	42
	3	−0.28	−0.32	2.06	0.79	−0.73	−0.08	44
	2	−0.28	−0.32	2.06	0.79	−0.72	−0.08	44
	0	−0.28	−0.32	2.06	0.80	−0.71	−0.08	44
	0	−0.28	−0.32	2.06	0.79	−0.70	−0.08	44
Co_{13}	98	−0.16	−0.24	1.92	1.10	0.06	−0.05	27
	14	−0.24	−0.28	2.03	0.81	−0.02	0.05	27
	13	−0.24	−0.27	2.03	0.81	−0.02	0.05	27
	1	−0.25	−0.29	2.02	0.78	−0.09	0.04	27
	0	−0.26	−0.29	2.02	0.78	−0.09	0.04	27
Ni_{13}	138	−0.30	−0.36	1.99	0.83	0.11	0.13	10
	118	−0.32	−0.44	1.76	1.71	0.34	0.02	10
	61	−0.38	−0.48	1.81	1.52	0.26	0.16	10
	45	−0.39	−0.46	1.86	1.20	0.28	0.11	10
	0	−0.44	−0.51	1.83	1.30	0.11	0.10	10
Cu_{13}	119	−0.11	−0.13	2.10	0.53	−0.02	0.06	1
	113	−0.12	−0.13	2.26	0.33	−0.01	0.00	1
	73	−0.16	−0.17	2.33	0.29	0.06	0.01	1
	59	−0.17	−0.20	2.03	0.66	0.17	0.05	1
	0	−0.23	−0.26	2.06	0.57	0.46	0.08	1

Table S5: Energetic and structural properties for representative set of the CO/TM_{13} system. ΔE_{tot} - Relative total energy, E_{ad} - Adsorption energy, E_{int} - Interaction energy, $d^{\text{Mol-TM}_{13}}$ - Minimum distance between Mol and TM_{13}, Δd_0 - Relative changes in the average weighted bond length of Mol, ΔECN_{av} - Relative changes in the TM_{13} average effective coordination number after adsorption, Δd_{av} - Relative changes in the average weighted bond lengths of TM_{13} after adsorption, m_T - Total magnetic moments per structure.

CO	ΔE_{tot} (meV)	E_{ad} (eV)	E_{int} (eV)	$d^{\text{Mol-TM}_{13}}$ (Å)	Δd_0 (%)	ΔECN_{av} (%)	Δd_{av} (%)	m_T (μ_B)
Fe_{13}	197	−1.66	−2.40	1.91	9.85	−0.57	−1.95	40
	137	−1.72	−2.28	1.78	6.81	−0.90	−3.39	40
	25	−1.83	−2.03	1.80	3.80	−0.31	−1.01	42
	18	−1.84	−2.32	1.99	7.05	−0.05	−1.09	42
	0	−1.86	−2.10	1.81	4.29	−0.43	−1.79	42
Co_{13}	814	−1.21	−1.50	1.71	2.67	0.20	−1.65	25
	268	−1.75	−1.89	1.75	2.47	0.37	−0.07	27
	237	−1.78	−1.98	1.90	4.42	0.50	0.11	27
	131	−1.89	−2.03	1.76	2.51	0.26	−0.34	27
	0	−2.02	−2.22	1.90	4.29	0.03	−0.10	25
Ni_{13}	528	−1.78	−2.03	1.73	2.17	0.01	−3.82	10
	424	−1.89	−1.97	1.74	2.08	0.31	0.31	10
	192	−2.12	−2.35	1.83	4.06	0.29	−1.22	10
	111	−2.20	−2.29	1.73	2.22	0.19	−0.14	10
	0	−2.31	−2.49	1.84	4.30	0.12	−0.27	8
Cu_{13}	548	−0.81	−1.06	1.92	2.70	−0.04	−5.00	1
	211	−1.14	−1.21	1.82	1.35	0.17	0.15	1
	197	−1.16	−1.28	1.88	2.66	0.20	−0.19	1
	154	−1.20	−1.27	1.82	1.31	0.20	0.01	1
	0	−1.36	−1.42	1.81	1.20	0.21	0.57	1

Table S6: Energetic and structural properties for representative set of the H_2/TM_{13} system. ΔE_{tot} - Relative total energy, E_{ad} - Adsorption energy, E_{int} - Interaction energy, $d^{\text{Mol-TM}_{13}}$ - Minimum distance between Mol and TM_{13}, Δd_0 - Relative changes in the average weighted bond length of Mol, ΔECN_{av} - Relative changes in the TM_{13} average effective coordination number after adsorption, Δd_{av} - Relative changes in the average weighted bond lengths of TM_{13} after adsorption, m_T - Total magnetic moments per structure.

H_2	ΔE_{tot} (meV)	E_{ad} (eV)	E_{int} (eV)	$d^{\text{Mol-TM}_{13}}$ (Å)	Δd_0 (%)	ΔECN_{av} (%)	Δd_{av} (%)	m_T (μ_B)
Fe_{13}	66	−0.31	−0.42	1.76	10.88	−0.02	−0.82	44
	4	−0.38	−0.67	1.71	14.16	−0.56	−1.60	42
	2	−0.38	−0.74	1.67	18.45	−0.51	−1.40	42
	1	−0.38	−0.73	1.69	16.87	−0.58	−1.87	42
	0	−0.38	−0.72	1.70	15.71	−0.57	−1.76	42
Co_{13}	238	−0.34	−0.62	1.63	16.96	0.02	0.31	25
	208	−0.37	−0.55	1.65	14.21	0.16	0.00	27
	97	−0.49	−0.72	1.64	16.71	0.14	−0.03	27
	67	−0.52	−0.79	1.64	17.81	0.13	−0.09	27
	0	−0.58	−1.10	1.57	27.11	0.00	0.16	25
Ni_{13}	358	−0.42	−0.84	1.58	18.48	0.02	−3.12	10
	119	−0.66	−0.95	1.58	17.56	0.16	0.35	10
	80	−0.70	−1.00	1.58	18.35	0.17	0.19	10
	68	−0.71	−1.04	1.57	18.91	0.20	−0.05	10
	0	−0.78	−1.05	1.57	17.57	0.16	0.02	10
Cu_{13}	192	−0.16	−0.22	1.77	6.15	0.18	0.01	1
	185	−0.17	−0.22	1.75	6.76	0.14	−0.03	1
	109	−0.25	−0.33	1.74	7.71	0.16	0.09	1
	106	−0.25	−0.31	1.73	7.27	0.10	0.22	1
	0	−0.35	−0.43	1.71	7.71	0.13	0.55	1

Table S7: Energetic and structural properties for representative set of the CH_3OH/TM_{13} system. ΔE_{tot} - Relative total energy, E_{ad} - Adsorption energy, E_{int} - Interaction energy, $d^{\text{Mol-TM}_{13}}$ - Minimum distance between Mol and TM_{13}, Δd_0 - Relative changes in the average weighted bond length of Mol, ΔECN_{av} - Relative changes in the TM_{13} average effective coordination number after adsorption, Δd_{av} - Relative changes in the average weighted bond lengths of TM_{13} after adsorption, m_T - Total magnetic moments per structure.

CH_3OH	ΔE_{tot} (meV)	E_{ad} (eV)	E_{int} (eV)	$d^{\text{Mol-TM}_{13}}$ (Å)	Δd_0 (%)	ΔECN_{av} (%)	Δd_{av} (%)	m_T (μ_B)
Fe_{13}	13	−0.79	−0.96	2.07	−0.07	−0.68	−1.89	42
	5	−0.80	−0.82	2.09	−0.13	−0.09	−0.69	44
	3	−0.80	−0.82	2.09	−0.11	−0.09	−0.69	44
	1	−0.80	−0.82	2.08	−0.12	−0.08	−0.67	44
	0	−0.80	−0.82	2.09	−0.11	−0.09	−0.67	44
Co_{13}	153	−0.62	−0.67	2.15	0.05	0.05	−0.23	27
	63	−0.71	−0.73	2.06	0.15	0.05	−0.04	27
	59	−0.71	−0.73	2.08	0.13	0.06	−0.06	27
	31	−0.74	−0.77	2.09	0.14	0.04	−0.14	27
	0	−0.77	−0.79	2.07	0.13	0.06	−0.04	27
Ni_{13}	402	−0.46	−0.55	2.16	−0.04	0.08	−1.24	10
	36	−0.82	−0.86	2.04	0.09	0.09	0.14	10
	4	−0.86	−0.89	2.02	0.10	0.05	−0.14	10
	3	−0.86	−0.90	2.02	0.10	0.06	−0.12	10
	0	−0.86	−0.90	2.02	0.10	0.06	−0.08	10
Cu_{13}	322	−0.35	−0.37	2.42	−0.09	0.00	−0.92	1
	145	−0.52	−0.57	2.12	0.02	0.12	0.13	1
	118	−0.55	−0.58	2.12	0.12	0.01	−0.01	1
	39	−0.63	−0.65	2.09	0.14	0.03	0.11	1
	0	−0.67	−0.70	2.10	0.08	0.09	0.56	1

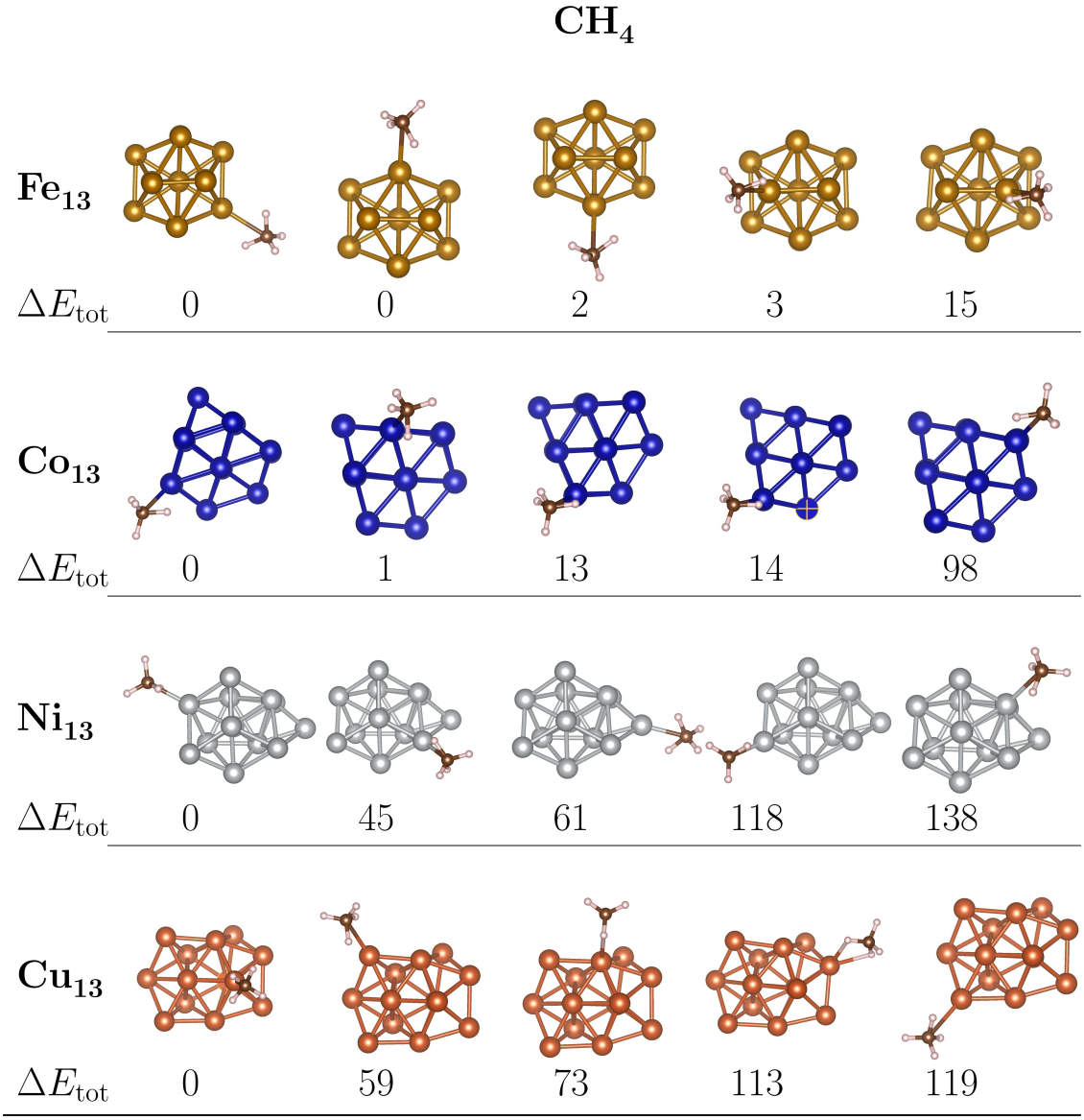

Figure S19: Representative set of the CH_4/TM_{13} systems, in relation to the relative total energy (in meV), where TM = Fe (orange), Co (blue), Ni (silver), and Cu (red).

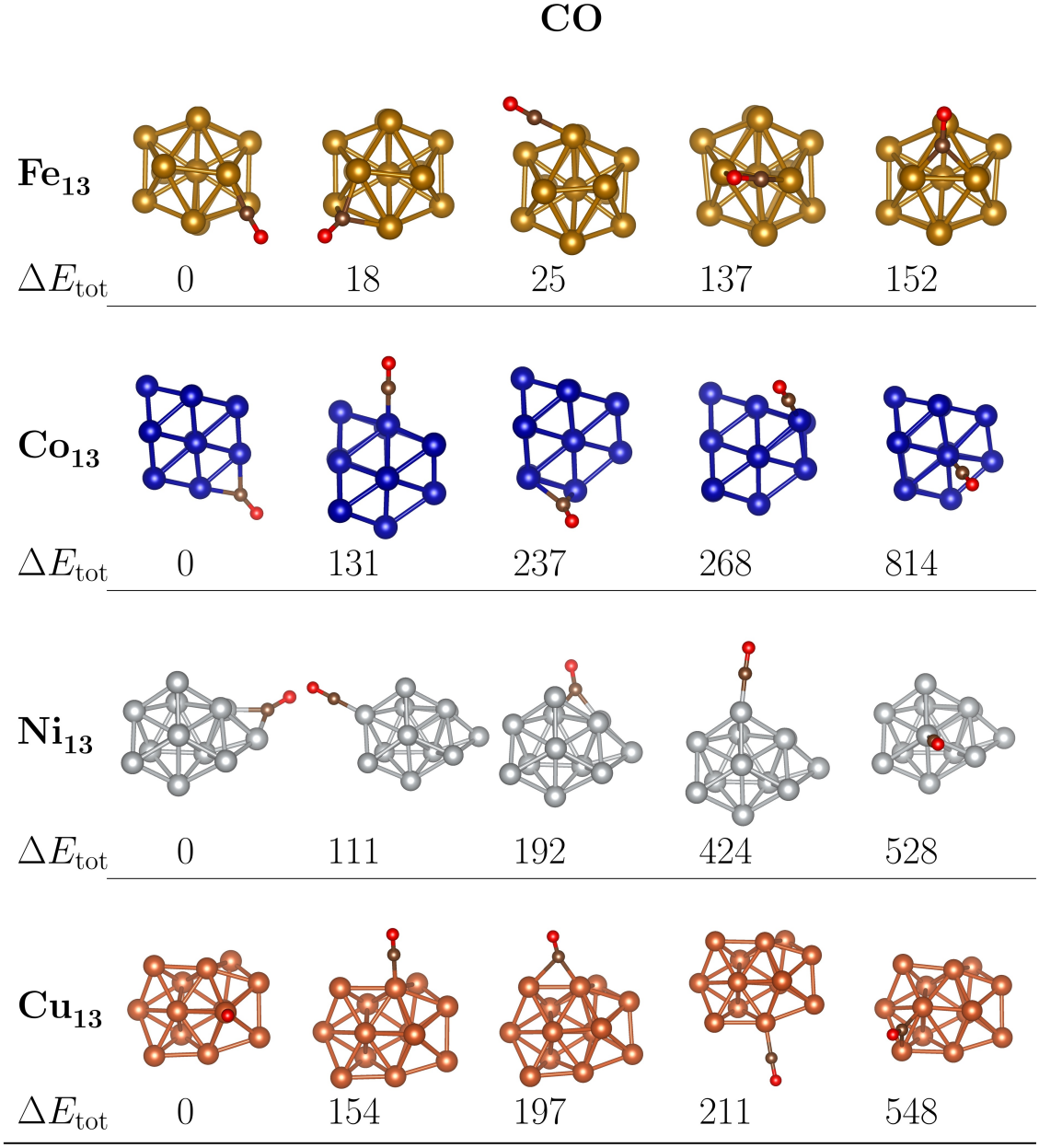

Figure S20: Representative set of the CO/TM_{13} systems, in relation to the relative total energy (in meV), where TM = Fe (orange), Co (blue), Ni (silver), and Cu (red).

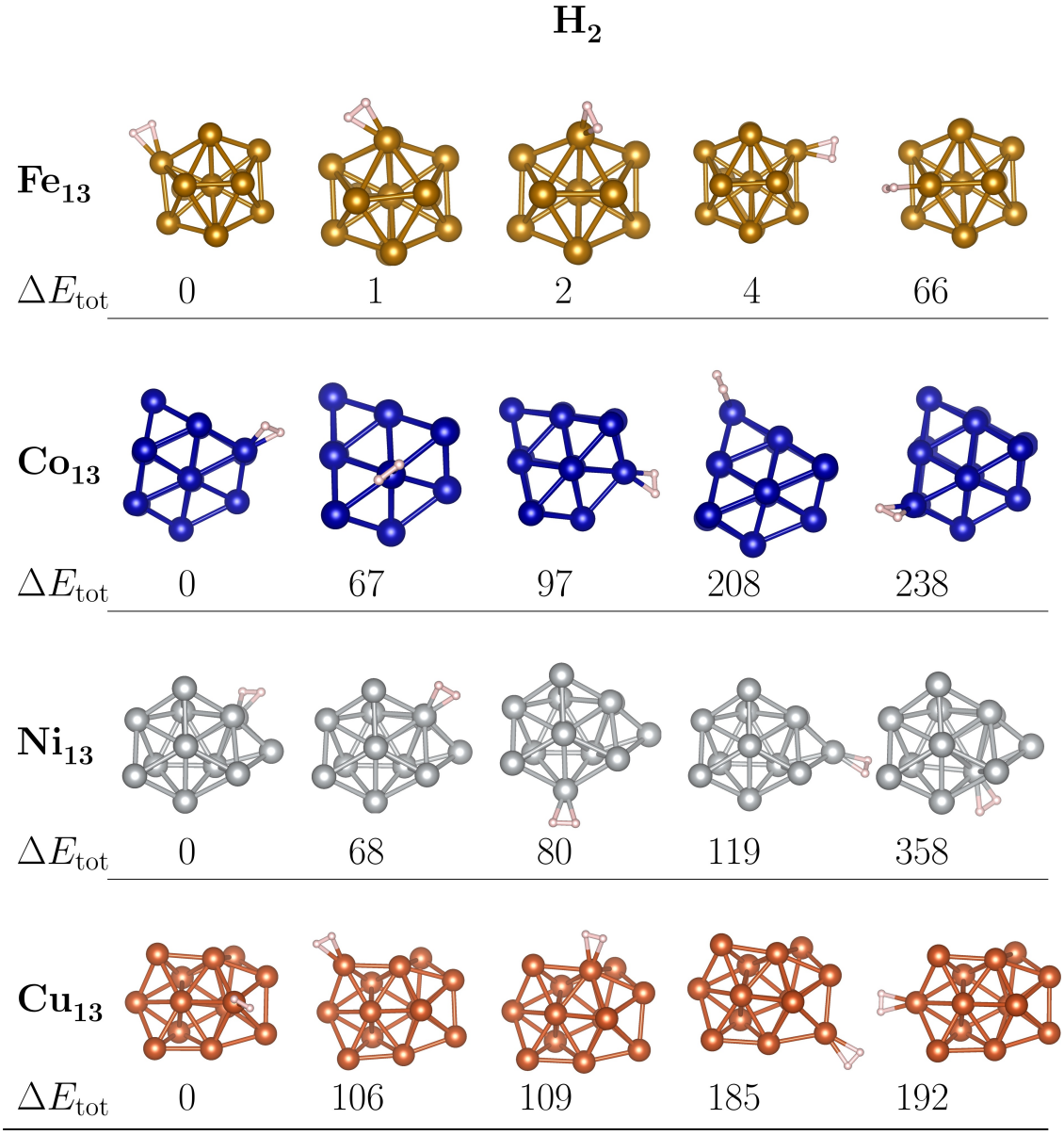

Figure S21: Representative set of the H_2/TM_{13} systems, in relation to the relative total energy (in meV), where TM = Fe (orange), Co (blue), Ni (silver), and Cu (red).

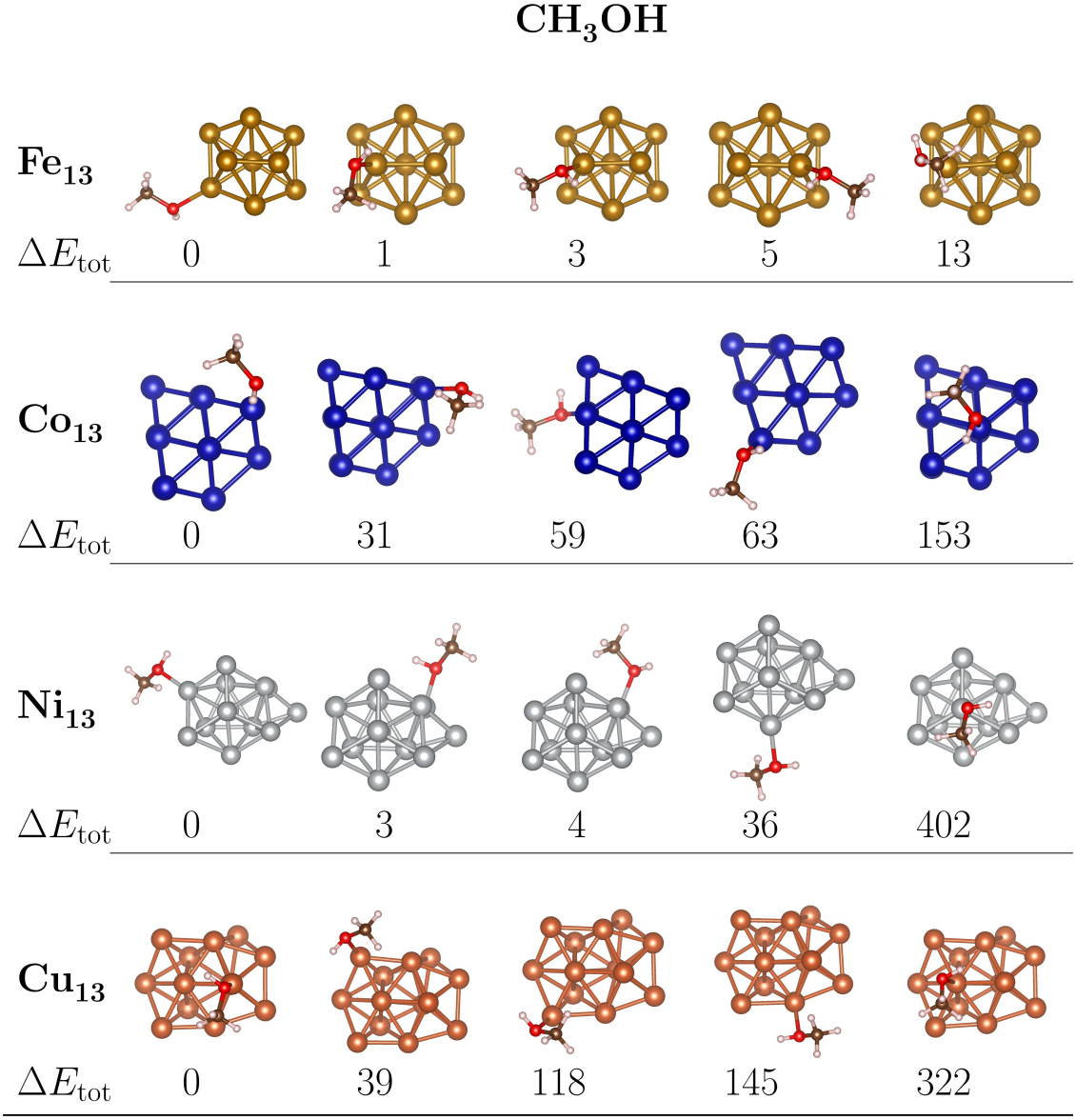

Figure S22: Representative set of the CH_3OH/TM_{13} systems, in relation to the relative total energy (in meV), where TM = Fe (orange), Co (blue), Ni (silver), and Cu (red).

S8.2 Electronic Properties

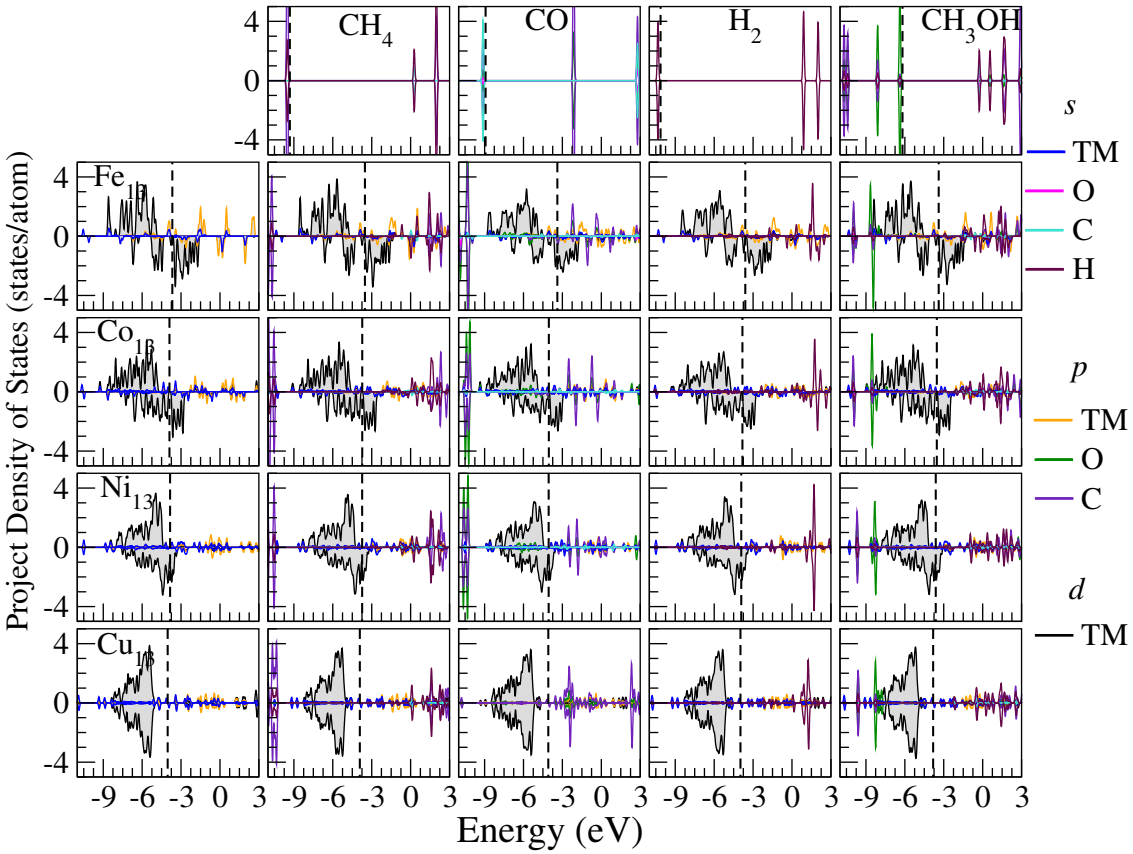

Figure S23: Project density of states per atom for the lowest energy configurations for the adsorption of CH_4, CO, H_2, CH_3OH on the TM_{13} clusters, where TM = Fe, Co, Ni and Cu. For comparison, the projected density of states for the gas-phase molecules and clusters are indicated as pink and blue dashed lines, respectively.

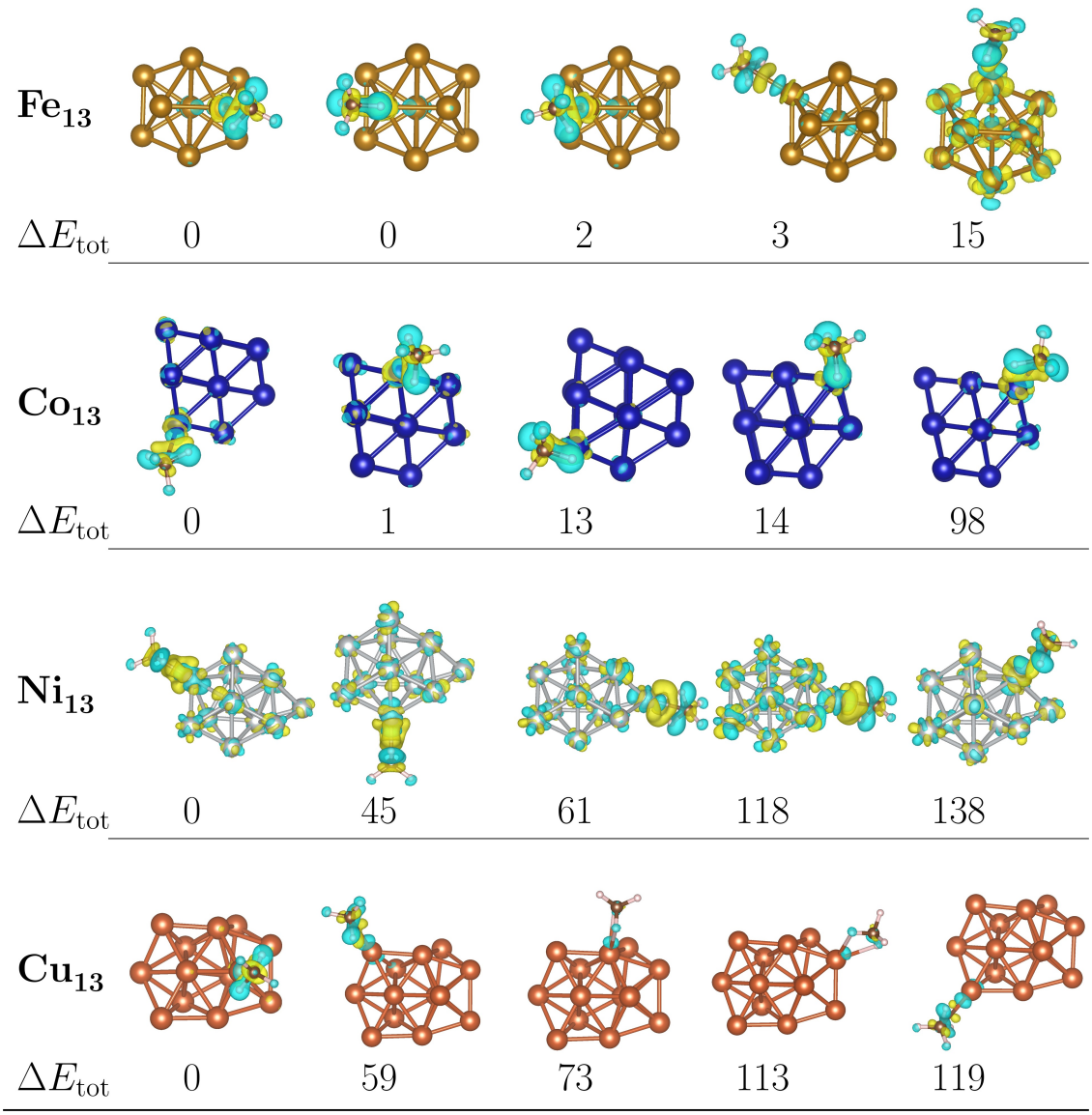

Figure S24: Electron density difference for the representative set of the CH_4/TM_{13} systems, in relation to the relative total energy (in meV), where TM = Fe (orange), Co (blue), Ni (silver), and Cu (red). The blue (yellow) isosurfaces ($0.015\,e\text{Å}^{-3}$ cutoff) indicate accumulation (depletion) of the charge.

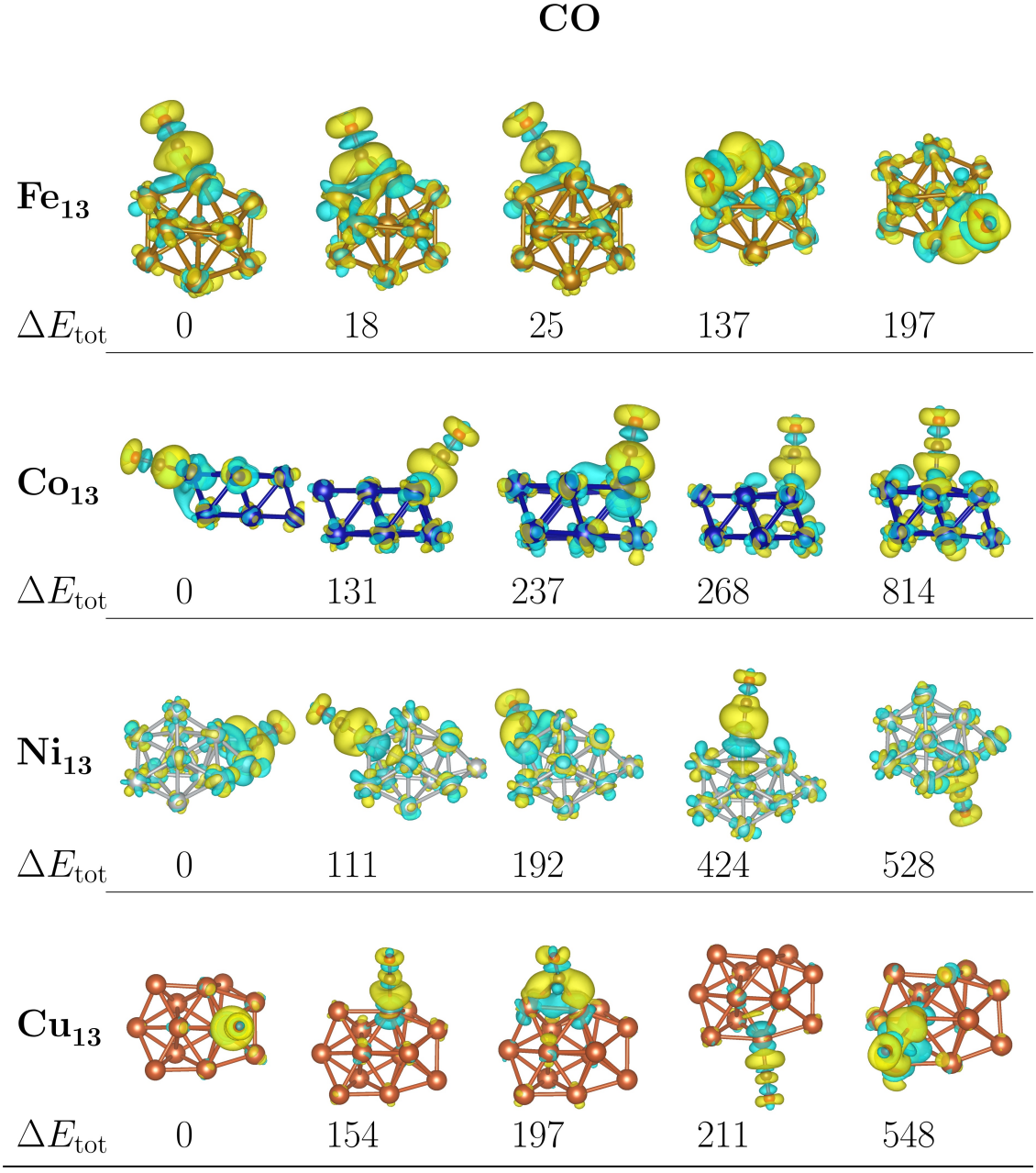

Figure S25: Electron density difference for the representative set of the CO/TM_{13} systems, in relation to the relative total energy (in meV), where TM = Fe (orange), Co (blue), Ni (silver), and Cu (red). The blue (yellow) isosurfaces ($0.015\,e\text{Å}^{-3}$ cutoff) indicate accumulation (depletion) of the charge.

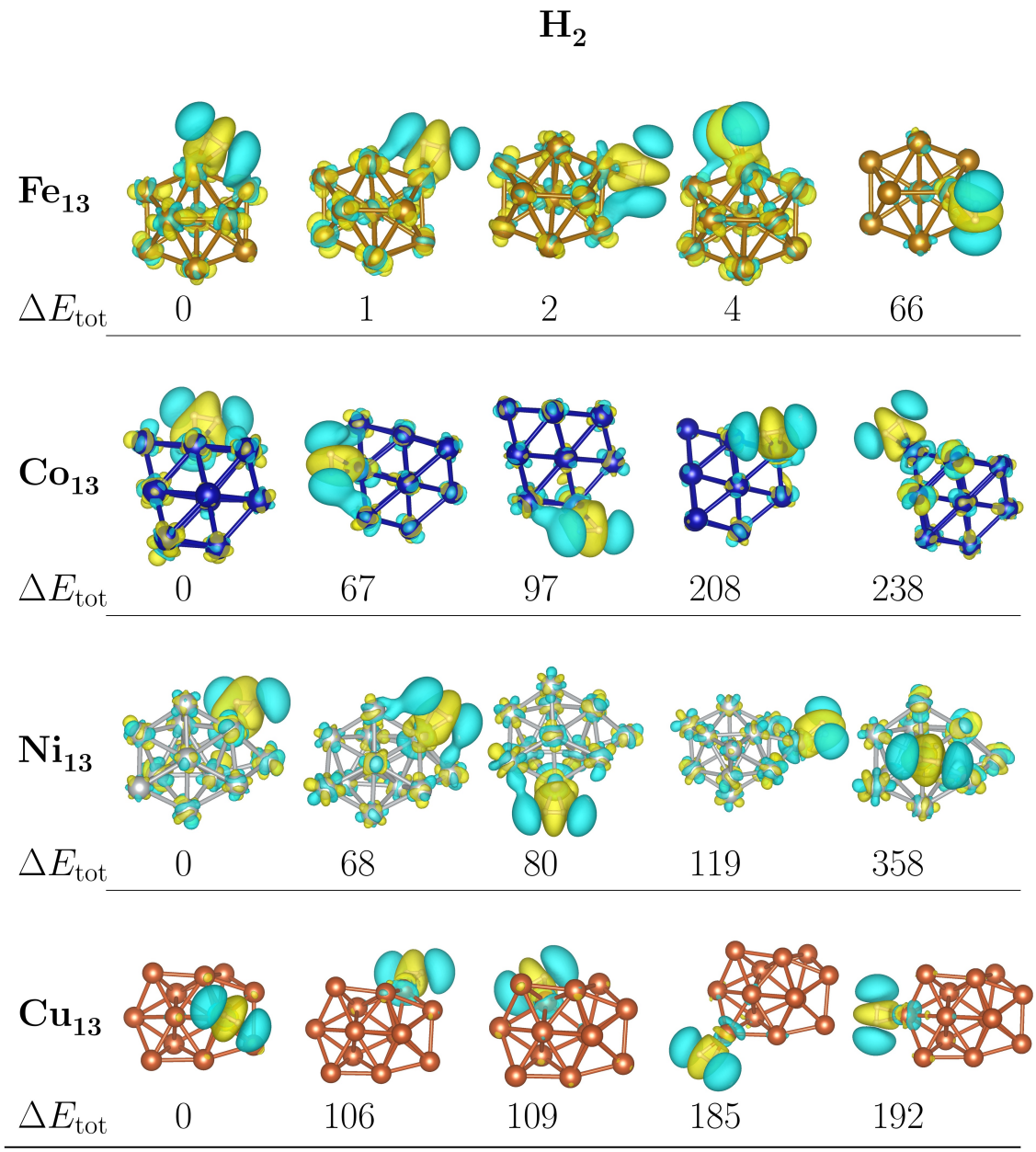

Figure S26: Electron density difference for the representative set of the H_2/TM_{13} systems, in relation to the relative total energy (in meV), where TM = Fe (orange), Co (blue), Ni (silver), and Cu (red). The blue (yellow) isosurfaces ($0.015\,e\text{Å}^{-3}$ cutoff) indicate accumulation (depletion) of the charge.

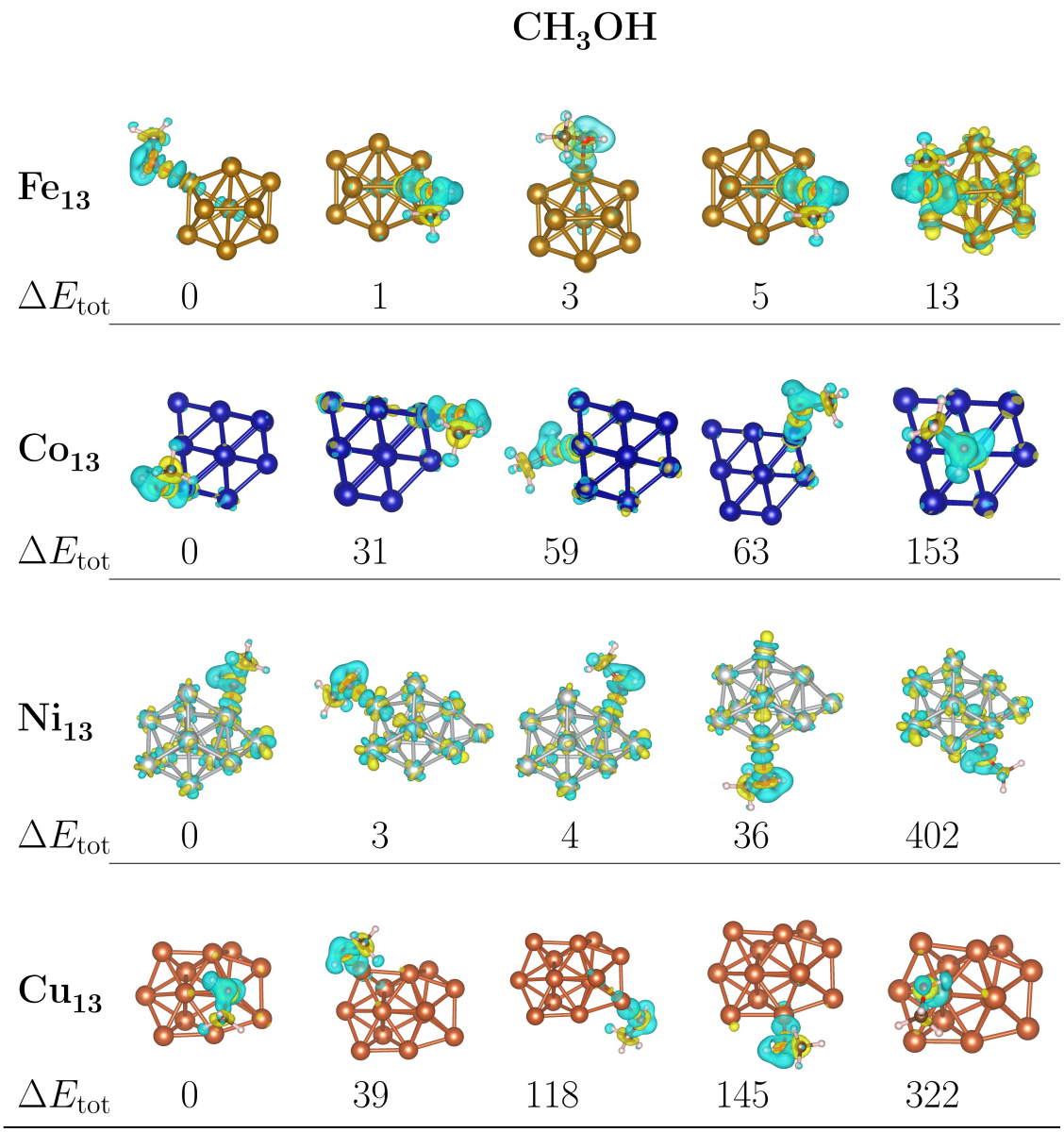

Figure S27: Electron density difference for the representative set of the CH_3OH/TM_{13} systems, in relation to the relative total energy (in meV), where TM = Fe (orange), Co (blue), Ni (silver), and Cu (red). The blue (yellow) isosurfaces ($0.015\,e\text{Å}^{-3}$ cutoff) indicate accumulation (depletion) of the charge.

S9 Cartesian Coordinates for the Representative Sets

Below, we provide the atomic positions (x, y, z) for the five representative adsorbed structures selected by the *k-means* clustering algorithm. Additional structures can be provided upon request. All Cartesian coordinates are given in Å.

S9.1 Unary TM_{13} Clusters

S9.1.1 Fe_{13}

Fe_{13}	$E_{tot} = -451\,949.93\,\mathrm{eV}$		$\Delta E_{tot} = 0.00\,\mathrm{meV}$
Fe	−0.548 078	−1.978 221	1.104 587
Fe	2.357 369	0.321 025	−0.399 694
Fe	−1.579 547	0.715 156	−1.679 012
Fe	−2.362 189	−0.372 210	0.318 252
Fe	1.412 792	−1.893 116	−0.511 303
Fe	1.073 862	1.676 761	1.369 412
Fe	0.000 164	−0.000 168	0.000 200
Fe	0.710 295	−0.273 266	−2.287 372
Fe	−0.993 281	−1.713 445	−1.384 572
Fe	1.535 046	−0.659 807	1.742 347
Fe	−1.355 488	1.916 367	0.574 438
Fe	0.553 821	1.977 958	−1.102 313
Fe	−0.804 766	0.282 964	2.255 030

Fe_{13}	$E_{tot} = -451\,949.05\,\mathrm{eV}$	$\Delta E_{tot} = 878.13\,\mathrm{meV}$	
Fe	1.330 984	1.726 773	−1.268 179
Fe	−1.416 506	0.517 546	1.505 280
Fe	1.986 759	−0.729 926	−1.786 935
Fe	−0.828 880	−1.792 437	0.962 023
Fe	−0.118 884	−2.160 368	−1.296 278
Fe	−2.222 032	−0.636 396	−0.612 987
Fe	0.120 224	−0.041 107	−0.479 325
Fe	2.533 162	0.375 379	0.244 944
Fe	1.667 090	−1.945 587	0.229 384
Fe	−1.259 847	1.944 878	−0.591 710
Fe	0.903 030	−0.349 736	1.881 763
Fe	−3.239 094	1.205 653	0.223 256
Fe	0.543 997	1.885 328	0.988 765

Fe_{13}	$E_{tot} = -451\,948.95\,\mathrm{eV}$	$\Delta E_{tot} = 972.08\,\mathrm{meV}$	
Fe	2.284 927	−1.004 248	0.815 373
Fe	0.234 010	0.379 324	0.346 487
Fe	0.310 373	−2.230 289	−0.230 264
Fe	−1.050 198	2.209 197	1.207 796
Fe	−0.831 500	2.105 317	−1.121 828
Fe	0.949 259	1.008 728	−2.160 241
Fe	−0.797 779	−0.541 308	−1.658 737
Fe	−1.732 536	−1.472 968	0.582 624
Fe	−2.350 746	0.637 683	−0.208 299
Fe	1.823 122	−0.982 572	−1.479 728
Fe	−1.500 288	0.198 440	2.178 586
Fe	2.368 637	1.084 981	−0.273 653
Fe	0.292 718	−1.392 285	2.001 885

Fe_{13}	$E_{tot} = -451\,948.51\,\mathrm{eV}$	$\Delta E_{tot} = 1416.37\,\mathrm{meV}$	
Fe	−0.198 837	2.349 675	−1.726 315
Fe	−1.612 791	−0.410 886	1.815 944
Fe	2.394 681	−0.731 069	−0.531 353
Fe	0.250 000	−1.654 855	2.555 525
Fe	−0.754 647	−1.456 940	−1.992 838
Fe	−2.335 632	−0.745 200	−0.480 133
Fe	0.769 440	0.307 117	−1.977 217
Fe	2.177 589	−0.592 165	1.768 067
Fe	0.189 064	−1.009 372	0.251 531
Fe	−1.732 980	0.679 999	−2.264 384
Fe	0.369 183	0.772 513	2.306 945
Fe	−0.957 663	1.200 132	0.115 955
Fe	1.442 593	1.291 051	0.158 271

Fe_{13}	$E_{tot} = -451\,948.14\,\mathrm{eV}$	$\Delta E_{tot} = 1787.56\,\mathrm{meV}$	
Fe	−1.473 875	−0.713 380	−2.438 248
Fe	−1.363 209	−1.147 434	0.061 543
Fe	−0.769 118	−1.238 940	2.532 703
Fe	0.570 051	−1.422 099	−1.494 390
Fe	0.848 663	−0.576 666	0.801 195
Fe	1.534 564	−1.610 721	2.702 574
Fe	−1.525 245	1.610 563	−2.699 583
Fe	−0.482 665	0.894 108	−0.814 528
Fe	−1.232 026	0.864 255	1.535 448
Fe	0.479 752	0.454 399	−3.108 978
Fe	0.862 564	1.795 848	0.958 322
Fe	0.705 939	0.567 913	3.047 320
Fe	1.844 603	0.522 155	−1.083 379

S9.1.2 Co_{13}

Co_{13}	$E_{tot} = -494\,936.86\,\mathrm{eV}$		$\Delta E_{tot} = 0.00\,\mathrm{meV}$
Co	−0.656 876	2.391 203	0.518 481
Co	−0.656 884	−2.391 202	0.518 484
Co	−0.718 923	0.000 008	0.612 762
Co	1.208 072	−1.203 912	−0.116 326
Co	1.208 079	1.203 913	−0.116 333
Co	−1.969 329	−1.222 781	−1.022 325
Co	−1.969 328	1.222 787	−1.022 322
Co	0.717 307	−1.168 480	2.130 298
Co	0.717 315	1.168 456	2.130 298
Co	−0.144 521	0.000 011	−1.703 426
Co	−0.128 954	2.360 633	−1.680 404
Co	−0.128 956	−2.360 619	−1.680 406
Co	2.522 996	−0.000 015	1.431 217

Co_{13}	$E_{tot} = -494\,936.31\,\text{eV}$	$\Delta E_{tot} = 545.80\,\text{meV}$	
Co	−0.140 435	−0.372 381	3.177 380
Co	1.178 857	−1.658 813	−1.254 723
Co	0.507 060	−1.055 875	1.031 163
Co	−1.717 601	−0.659 918	1.527 752
Co	−0.198 287	−1.087 159	−3.004 586
Co	−0.901 992	1.459 397	1.962 822
Co	0.248 897	1.070 083	−0.127 168
Co	1.363 242	0.856 101	1.999 018
Co	1.345 621	0.450 059	−2.188 014
Co	−0.954 616	0.900 483	−2.206 835
Co	−2.045 977	1.020 837	−0.015 555
Co	2.284 044	0.003 768	−0.104 170
Co	−0.968 812	−0.926 581	−0.797 084

Co_{13}	$E_{tot} = -494\,936.28\,\mathrm{eV}$	$\Delta E_{tot} = 577.18\,\mathrm{meV}$	
Co	−2.230 160	−1.487 854	1.356 941
Co	−0.121 667	0.511 120	−1.111 822
Co	−0.300 809	−0.761 220	2.520 102
Co	1.947 203	1.497 389	−0.994 293
Co	1.822 252	−0.892 362	−0.949 178
Co	−0.141 779	−1.530 349	−2.159 619
Co	−0.103 846	1.599 304	2.542 617
Co	1.118 247	0.382 619	0.960 746
Co	−0.176 434	−1.493 714	0.238 846
Co	0.226 803	2.385 471	0.374 087
Co	−2.055 085	−0.921 538	−0.898 320
Co	−1.345 555	0.550 215	0.982 397
Co	1.360 828	0.160 916	−2.862 506

Co_{13}	$E_{tot} = -494\,936.19\,\mathrm{eV}$	$\Delta E_{tot} = 672.74\,\mathrm{meV}$	
Co	−0.652 735	−2.340 977	−1.321 978
Co	−2.577 894	0.239 870	0.976 480
Co	0.206 884	−0.768 178	−2.851 072
Co	0.763 486	1.716 694	2.418 050
Co	1.027 017	−0.395 264	1.812 278
Co	−1.040 531	0.226 502	2.761 177
Co	2.217 373	0.221 231	−2.099 458
Co	0.315 881	1.268 858	−1.668 511
Co	1.763 648	1.147 254	0.187 645
Co	0.869 685	−0.840 322	−0.592 355
Co	−0.506 838	1.075 834	0.632 121
Co	−0.944 399	−1.324 879	0.886 610
Co	−1.441 576	−0.226 623	−1.140 987

Co_{13}	$E_{tot} = -494\,935.83\,\mathrm{eV}$	$\Delta E_{tot} = 1026.47\,\mathrm{meV}$	
Co	−0.528 191	−1.995 017	1.093 524
Co	2.278 948	0.378 422	−0.344 448
Co	−1.471 333	0.706 699	−1.666 691
Co	−2.278 198	−0.374 893	0.348 649
Co	1.299 774	−1.876 242	−0.483 566
Co	0.998 204	1.670 845	1.288 870
Co	0.000 569	0.000 124	0.000 231
Co	0.717 864	−0.229 921	−2.209 751
Co	−1.003 250	−1.666 782	−1.287 865
Co	1.473 996	−0.711 264	1.663 956
Co	−1.304 064	1.873 976	0.478 953
Co	0.529 146	1.994 991	−1.093 059
Co	−0.713 464	0.229 061	2.211 198

S9.1.3 Ni_{13}

Ni_{13}	$E_{tot} = -540\,329.16\,\mathrm{eV}$	$\Delta E_{tot} = 0.00\,\mathrm{meV}$	
Ni	0.004 833	2.233 941	−1.447 734
Ni	−0.066 735	−0.082 254	−1.422 265
Ni	0.140 114	−2.264 149	−0.807 756
Ni	2.003 753	0.975 014	−1.419 876
Ni	1.757 210	−0.818 255	0.207 804
Ni	−1.569 474	1.154 851	−0.066 320
Ni	−2.035 364	−1.129 685	−0.617 612
Ni	0.727 743	1.302 687	0.546 781
Ni	−0.878 941	1.037 488	2.265 803
Ni	−2.711 016	−0.190 176	1.429 989
Ni	1.217 084	−0.044 913	2.366 770
Ni	−0.471 940	−0.881 219	1.017 579
Ni	1.882 732	−1.293 332	−2.053 162

Ni_{13}	$E_{tot} = -540\,328.99\,\text{eV}$	$\Delta E_{tot} = 168.11\,\text{meV}$	
Ni	−2.239 052	−1.527 670	1.398 453
Ni	−0.202 374	0.590 359	−1.173 418
Ni	−0.358 677	−0.713 794	2.499 825
Ni	1.936 804	1.427 829	−1.025 148
Ni	1.804 662	−0.895 761	−0.902 776
Ni	−0.073 311	−1.491 648	−2.147 409
Ni	−0.089 494	1.595 806	2.597 663
Ni	1.173 623	0.361 358	1.010 185
Ni	−0.148 875	−1.560 378	0.271 661
Ni	0.213 976	2.335 345	0.372 336
Ni	−2.015 105	−0.903 063	−0.871 917
Ni	−1.362 937	0.586 319	0.915 936
Ni	1.360 760	0.195 297	−2.945 394

Ni_{13}	$E_{tot} = -540\,328.85\,\mathrm{eV}$	$\Delta E_{tot} = 310.00\,\mathrm{meV}$	
Ni	−0.004 376	−0.001 509	−0.001 648
Ni	−0.006 716	1.213 722	1.972 233
Ni	0.023 783	−1.237 502	2.022 816
Ni	−0.015 433	1.215 782	−1.972 619
Ni	0.016 684	−1.246 132	−2.018 474
Ni	1.185 919	1.966 742	−0.001 959
Ni	1.210 862	−1.975 041	0.000 179
Ni	−1.229 877	2.027 578	0.001 012
Ni	−1.186 476	−1.956 105	0.006 160
Ni	1.946 297	−0.014 121	1.219 298
Ni	1.939 421	−0.012 883	−1.231 162
Ni	−1.938 285	0.012 386	1.217 414
Ni	−1.941 803	0.007 085	−1.213 252

Ni_{13}	$E_{tot} = -540\,328.48\,\mathrm{eV}$	$\Delta E_{tot} = 675.95\,\mathrm{meV}$	
Ni	−1.927 928	−1.465 415	1.347 001
Ni	−1.166 667	1.125 448	−1.807 595
Ni	−0.000 070	−0.546 625	2.280 640
Ni	1.166 701	1.125 403	−1.807 697
Ni	2.011 745	−0.952 556	−1.013 137
Ni	0.000 019	−0.840 680	−2.278 611
Ni	1.927 842	−1.465 289	1.347 131
Ni	0.000 079	1.779 231	2.124 080
Ni	1.245 456	0.617 765	0.507 662
Ni	0.000 048	−1.480 349	0.006 711
Ni	0.000 058	2.437 624	−0.200 931
Ni	−2.011 708	−0.952 478	−1.013 059
Ni	−1.245 574	0.617 921	0.507 806

Ni_{13}	$E_{tot} = -540\,327.68\,\mathrm{eV}$		$\Delta E_{tot} = 1483.38\,\mathrm{meV}$
Ni	−1.595 252	−1.125 697	−2.612 190
Ni	−1.289 544	−1.118 117	−0.348 714
Ni	−0.938 968	−1.131 693	1.917 181
Ni	0.540 280	−1.105 657	−1.788 023
Ni	0.934 896	−1.111 982	0.508 125
Ni	1.171 423	−1.119 833	2.779 076
Ni	−1.610 533	1.120 022	−2.611 628
Ni	−1.302 339	1.101 658	−0.349 221
Ni	−0.952 730	1.105 949	1.915 644
Ni	0.527 288	1.123 131	−1.791 482
Ni	0.919 640	1.128 969	0.505 508
Ni	1.159 032	1.114 206	2.776 740
Ni	2.436 807	0.019 045	−0.901 017

S9.1.4 Cu_{13}

Cu_{13}	$E_{tot} = -588\,184.46\,\mathrm{eV}$	$\Delta E_{tot} = 0.00\,\mathrm{meV}$	
Cu	−0.803 550	−2.431 063	−1.399 728
Cu	−2.730 687	0.131 613	1.022 722
Cu	0.238 099	−0.780 148	−2.891 321
Cu	0.865 853	1.868 982	2.413 134
Cu	1.048 104	−0.431 742	1.804 398
Cu	−1.044 672	0.257 334	2.804 780
Cu	2.395 512	0.251 949	−2.064 950
Cu	0.290 919	1.302 441	−1.661 010
Cu	1.908 615	1.240 441	0.203 928
Cu	0.887 309	−0.882 910	−0.583 578
Cu	−0.537 603	1.109 837	0.620 717
Cu	−0.961 258	−1.446 080	0.903 223
Cu	−1.556 639	−0.190 656	−1.172 316

Cu_{13}	$E_{tot} = -588\,183.95\,\text{eV}$	$\Delta E_{tot} = 504.75\,\text{meV}$	
Cu	0.085 250	2.311 213	−1.499 347
Cu	−0.018 894	−0.073 305	−1.446 627
Cu	0.083 577	−2.354 403	−0.938 896
Cu	2.182 110	0.994 171	−1.465 996
Cu	1.822 675	−0.808 845	0.157 943
Cu	−1.616 672	1.178 912	−0.000 716
Cu	−2.112 247	−1.276 509	−0.587 229
Cu	0.751 712	1.345 859	0.564 464
Cu	−0.981 939	1.152 964	2.367 835
Cu	−2.813 760	−0.272 232	1.505 982
Cu	1.212 772	0.012 227	2.474 519
Cu	−0.501 291	−0.854 277	1.055 114
Cu	1.906 705	−1.355 776	−2.187 047

Cu_{13}	$E_{tot} = -588\,183.92\,\mathrm{eV}$		$\Delta E_{tot} = 538.42\,\mathrm{meV}$
Cu	0.000 000	−0.000 001	−0.736 617
Cu	−0.000 001	2.370 237	−0.635 565
Cu	0.000 001	−2.370 238	−0.635 563
Cu	2.155 396	1.241 500	−1.040 288
Cu	2.155 397	−1.241 500	−1.040 288
Cu	−2.155 397	1.241 500	−1.040 289
Cu	−2.155 396	−1.241 500	−1.040 288
Cu	3.255 789	0.000 000	0.739 988
Cu	−3.255 789	0.000 000	0.739 988
Cu	1.227 122	1.222 474	1.172 230
Cu	1.227 124	−1.222 476	1.172 231
Cu	−1.227 124	1.222 477	1.172 230
Cu	−1.227 122	−1.222 474	1.172 231

Cu_{13}	$E_{tot} = -588\,183.45\,\text{eV}$	$\Delta E_{tot} = 1004.26\,\text{meV}$	
Cu	−0.569 907	−2.040 767	1.142 683
Cu	2.339 883	0.395 156	−0.394 701
Cu	−1.518 056	0.734 625	−1.716 186
Cu	−2.340 530	−0.400 008	0.385 391
Cu	1.351 336	−1.926 401	−0.498 992
Cu	1.039 715	1.719 214	1.323 043
Cu	0.000 030	−0.000 017	0.000 004
Cu	0.759 291	−0.214 058	−2.272 843
Cu	−1.030 197	−1.722 876	−1.325 640
Cu	1.512 343	−0.729 267	1.723 504
Cu	−1.344 925	1.928 793	0.506 846
Cu	0.570 135	2.040 716	−1.142 613
Cu	−0.769 119	0.214 888	2.269 504

Cu_{13}	$E_{tot} = -588\,182.98\,\mathrm{eV}$	$\Delta E_{tot} = 1473.06\,\mathrm{meV}$	
Cu	−2.386 607	2.342 872	−0.535 556
Cu	−0.023 916	2.554 019	−0.425 828
Cu	2.344 525	2.381 695	−0.437 430
Cu	−2.538 682	−0.025 286	−0.516 591
Cu	−0.010 366	0.040 527	−0.674 135
Cu	2.511 466	0.015 501	−0.460 053
Cu	−2.307 298	−2.386 098	−0.611 808
Cu	0.064 258	−2.475 454	−0.569 650
Cu	2.439 118	−2.361 273	−0.490 810
Cu	−1.194 039	−1.226 086	1.133 742
Cu	−1.250 637	1.175 794	1.186 212
Cu	1.151 539	1.179 845	1.224 200
Cu	1.200 640	−1.216 055	1.177 705

S9.2 Adsorption Mol on TM_{13}

S9.2.1 Mol/Fe_{13}

CH_4/Fe_{13}	$E_{tot} = -453\,052.94$ eV	$\Delta E_{tot} = 0.00$ meV	
H	2.480 370	1.676 050	2.172 010
C	1.392 592	1.558 880	2.202 862
H	0.964 835	2.042 277	3.086 976
H	0.969 239	2.067 287	1.306 213
H	1.169 617	0.469 354	2.277 324
Fe	−2.033 468	−2.867 707	−0.387 264
Fe	1.416 317	−0.871 204	−1.381 406
Fe	−2.163 476	0.599 596	−2.756 356
Fe	−3.417 361	−0.737 624	−0.916 198
Fe	0.082 520	−2.847 133	−1.900 260
Fe	0.161 254	0.354 995	0.483 890
Fe	−0.996 880	−0.802 454	−1.146 668
Fe	−0.000 476	−0.704 571	−3.363 357
Fe	−2.152 684	−1.959 651	−2.777 283
Fe	0.158 404	−2.214 868	0.451 450
Fe	−2.081 977	1.236 055	−0.404 153
Fe	0.028 193	1.256 571	−1.918 372
Fe	−1.996 839	−0.905 285	1.061 662

CH_4/Fe_{13}	$E_{tot} = -453\,052.94\,\mathrm{eV}$		$\Delta E_{tot} = 0.07\,\mathrm{meV}$
H	0.481 631	−0.642 457	2.454 674
C	−0.487 172	−0.443 731	2.968 865
H	−0.882 414	−1.400 079	3.325 308
H	−0.280 203	0.236 870	3.801 015
H	−1.268 352	0.035 843	2.335 186
Fe	0.126 394	−1.876 971	−1.115 500
Fe	2.443 482	1.364 264	−2.114 370
Fe	−1.702 327	1.388 372	−2.807 263
Fe	−1.989 653	−0.373 375	−1.145 434
Fe	1.720 092	−1.048 277	−2.765 143
Fe	1.290 489	2.015 790	−0.063 820
Fe	0.225 509	0.493 035	−1.623 523
Fe	0.601 385	0.983 658	−3.848 709
Fe	−0.839 447	−1.029 299	−3.192 315
Fe	2.158 280	−0.397 841	−0.458 383
Fe	−1.270 501	2.037 037	−0.500 499
Fe	0.328 595	2.868 302	−2.139 188
Fe	−0.146 837	0.004 342	0.603 299

CH_4/Fe_{13}	$E_{tot} = -453\,052.94\,\mathrm{eV}$		$\Delta E_{tot} = 2.55\,\mathrm{meV}$
H	−2.414 335	−0.227 503	1.155 859
C	−3.146 932	−0.252 675	0.316 102
H	−3.790 507	−1.125 567	0.463 955
H	−3.722 702	0.677 687	0.351 063
H	−2.697 278	−0.333 014	−0.700 178
Fe	0.549 033	−2.496 648	0.516 424
Fe	3.837 707	−0.556 650	−0.618 753
Fe	0.381 009	0.857 656	−2.003 211
Fe	−0.740 918	−0.355 385	−0.036 987
Fe	2.382 395	−2.611 197	−1.088 119
Fe	2.835 480	0.828 284	1.287 309
Fe	1.548 861	−0.455 190	−0.330 481
Fe	2.278 783	−0.533 488	−2.648 792
Fe	0.279 199	−1.735 772	−1.953 215
Fe	2.730 035	−1.769 903	1.341 684
Fe	0.724 742	1.696 577	0.429 023
Fe	2.556 604	1.588 789	−1.179 135
Fe	0.840 213	−0.378 114	1.988 340

CH_4/Fe_{13}	$E_{tot} = -453\,052.94\,\mathrm{eV}$		$\Delta E_{tot} = 2.83\,\mathrm{meV}$
H	−2.794 513	−2.903 208	−0.986 300
C	−1.933 393	−2.421 983	−1.460 608
H	−1.760 814	−2.816 736	−2.466 812
H	−2.166 736	−1.336 503	−1.556 421
H	−1.035 729	−2.659 688	−0.844 148
Fe	0.055 117	−0.859 871	2.047 322
Fe	3.086 494	0.902 638	−0.086 621
Fe	−0.789 691	1.769 755	−1.123 679
Fe	−1.593 930	0.966 833	1.210 213
Fe	1.877 749	−1.188 037	0.226 957
Fe	2.038 190	2.556 946	1.562 796
Fe	0.742 853	0.929 993	0.560 132
Fe	1.348 162	0.428 627	−1.734 859
Fe	−0.554 206	−0.697 276	−0.442 301
Fe	2.283 177	0.104 058	2.253 241
Fe	−0.381 404	3.060 327	0.901 876
Fe	1.440 850	2.727 593	−0.922 160
Fe	0.137 822	1.436 535	2.861 371

CH_4/Fe_{13}	$E_{tot} = -453\,052.93\,\mathrm{eV}$		$\Delta E_{tot} = 14.84\,\mathrm{meV}$
H	−2.024 329	1.842 751	−0.160 639
C	−1.381 039	2.718 596	0.098 387
H	−1.722 107	3.105 258	1.063 883
H	−0.288 092	2.503 805	0.188 960
H	−1.504 274	3.462 234	−0.695 271
Fe	−0.546 927	−3.340 344	0.533 551
Fe	2.795 410	−1.514 607	−1.182 121
Fe	−1.168 232	−0.837 787	−2.325 572
Fe	−2.004 548	−1.558 768	−0.123 765
Fe	1.460 282	−3.564 253	−1.106 831
Fe	1.850 179	0.065 100	0.435 894
Fe	0.386 351	−1.547 691	−0.688 592
Fe	0.972 792	−2.130 373	−2.990 432
Fe	−0.994 358	−3.189 587	−1.888 354
Fe	1.777 184	−2.254 682	1.088 792
Fe	−0.484 373	0.539 116	−0.224 110
Fe	1.265 255	0.121 320	−2.097 618
Fe	−0.263 846	−1.007 811	1.604 196

CO/Fe_{13}	$E_{tot} = -455\,037.14\,\mathrm{eV}$		$\Delta E_{tot} = 0.00\,\mathrm{meV}$
C	2.464 398	1.449 105	−1.068 309
O	3.029 259	2.119 769	−1.864 621
Fe	−0.991 713	−2.544 999	0.971 888
Fe	1.823 961	0.419 123	0.280 290
Fe	−1.451 365	0.648 704	−1.667 828
Fe	−2.645 151	−0.983 787	0.013 780
Fe	1.159 624	−2.078 336	−0.122 005
Fe	0.023 522	1.402 220	1.920 349
Fe	−0.411 272	−0.281 449	0.238 258
Fe	0.834 264	−0.172 049	−1.871 838
Fe	−0.807 056	−1.914 681	−1.505 269
Fe	0.596 404	−1.089 406	2.183 341
Fe	−2.036 325	1.444 078	0.699 160
Fe	0.152 695	2.017 830	−0.483 279
Fe	−1.741 245	−0.436 121	2.276 080

CO/Fe_{13}	$E_{tot} = -455\,037.12\,\mathrm{eV}$		$\Delta E_{tot} = 17.92\,\mathrm{meV}$
C	−1.615 620	−1.062 358	1.827 548
O	−2.366 428	−1.542 721	2.654 597
Fe	−0.145 019	−1.905 294	0.778 890
Fe	2.667 963	0.604 831	−0.742 999
Fe	−1.217 931	0.948 285	−2.086 751
Fe	−2.088 386	−0.218 422	0.078 688
Fe	1.709 212	−1.629 916	−0.872 264
Fe	1.411 369	1.880 641	0.904 336
Fe	0.297 503	0.197 072	−0.339 853
Fe	1.042 337	0.039 987	−2.624 822
Fe	−0.861 775	−1.447 635	−1.608 103
Fe	1.813 281	−0.567 099	1.432 135
Fe	−1.155 645	2.014 959	0.143 018
Fe	0.857 790	2.218 055	−1.523 121
Fe	−0.348 649	0.469 615	1.978 700

CO/Fe_{13}	$E_{tot} = -455\,037.12\,\mathrm{eV}$		$\Delta E_{tot} = 25.11\,\mathrm{meV}$
C	1.323 970	1.393 217	−2.516 297
O	1.942 280	2.276 234	−2.993 741
Fe	−0.482 981	−2.449 276	1.372 509
Fe	2.082 632	0.203 545	0.077 160
Fe	−1.975 986	0.530 945	−1.131 328
Fe	−2.541 616	−0.876 191	0.925 792
Fe	1.197 060	−1.963 043	−0.513 010
Fe	0.713 511	1.274 152	1.893 602
Fe	−0.249 384	−0.302 761	0.406 061
Fe	0.418 054	−0.029 570	−1.898 344
Fe	−1.309 230	−1.830 420	−1.002 873
Fe	1.467 044	−1.116 068	1.994 946
Fe	−1.763 725	1.416 472	1.176 580
Fe	0.052 507	1.879 797	−0.527 180
Fe	−0.874 136	−0.407 035	2.736 122

CO/Fe_{13}	$E_{tot} = -455\,037.01\,\text{eV}$		$\Delta E_{tot} = 137.28\,\text{meV}$
C	−0.741 790	−2.871 371	0.008 378
O	−1.215 783	−3.388 714	−0.981 298
Fe	−0.033 220	−1.672 835	1.124 863
Fe	2.466 981	1.222 779	−0.282 163
Fe	−1.518 883	1.082 566	−1.644 204
Fe	−2.189 826	−0.116 788	0.602 157
Fe	1.886 728	−1.251 856	−0.284 802
Fe	0.911 365	2.302 635	1.272 645
Fe	0.128 650	0.417 505	0.053 683
Fe	1.063 886	0.289 793	−2.059 745
Fe	−0.844 748	−1.214 390	−1.231 960
Fe	1.871 102	0.031 758	1.739 923
Fe	−1.550 405	2.168 285	0.519 442
Fe	0.357 237	2.484 228	−1.117 200
Fe	−0.591 293	0.516 406	2.280 279

CO/Fe_{13}	$E_{tot} = -455\,036.95\,\text{eV}$		$\Delta E_{tot} = 196.78\,\text{meV}$
C	2.147 018	−0.630 796	−1.545 400
O	2.736 582	−1.728 649	−1.607 834
Fe	−0.832 879	−1.947 097	1.330 739
Fe	2.006 957	0.782 509	−0.142 570
Fe	−1.999 426	0.986 274	−1.415 759
Fe	−2.721 100	−0.471 666	0.636 417
Fe	1.046 898	−1.661 179	−0.252 247
Fe	0.580 682	1.887 961	1.519 984
Fe	−0.377 629	0.154 535	0.232 030
Fe	0.474 214	0.200 776	−1.944 100
Fe	−1.438 052	−1.358 339	−1.190 097
Fe	1.333 124	−0.508 526	1.856 191
Fe	−1.925 383	1.816 582	0.853 482
Fe	−0.017 469	2.333 723	−0.830 904
Fe	−1.013 536	0.143 892	2.500 066

H_2/Fe_{13}	$E_{tot} = -451\,982.92\,\mathrm{eV}$		$\Delta E_{tot} = 0.00\,\mathrm{meV}$
H	−1.675 467	1.605 117	−2.586 402
H	−1.107 246	2.040 905	−2.096 230
Fe	−0.541 532	−2.343 873	1.382 127
Fe	2.504 486	0.033 465	0.026 763
Fe	−1.048 523	0.471 954	−1.455 218
Fe	−2.103 193	−0.391 097	0.724 073
Fe	1.441 810	−2.279 774	−0.274 836
Fe	1.183 336	1.325 421	1.863 879
Fe	0.189 743	−0.278 246	0.339 219
Fe	1.129 578	−0.485 083	−1.927 143
Fe	−0.818 503	−1.987 400	−1.001 186
Fe	1.515 387	−1.194 069	2.053 363
Fe	−0.961 099	1.799 619	0.934 207
Fe	0.956 967	1.808 248	−0.623 550
Fe	−0.665 743	−0.125 188	2.640 935

H_2/Fe_{13}	$E_{tot} = -451\,982.92\,\text{eV}$		$\Delta E_{tot} = 1.40\,\text{meV}$
H	−2.050 884	−0.220 099	2.016 626
H	−1.760 904	0.180 365	2.740 314
Fe	−0.028 127	−2.034 749	0.441 298
Fe	2.879 239	0.480 387	−0.655 094
Fe	−0.923 961	0.856 780	−2.234 213
Fe	−1.886 930	−0.428 216	−0.421 485
Fe	1.960 205	−1.836 321	−0.926 448
Fe	1.358 804	1.887 860	0.887 443
Fe	0.489 101	0.076 386	−0.501 200
Fe	1.323 574	−0.251 486	−2.665 020
Fe	−0.465 199	−1.709 627	−1.922 229
Fe	1.903 609	−0.541 515	1.285 695
Fe	−0.942 324	2.040 429	−0.107 250
Fe	1.217 492	2.112 125	−1.491 500
Fe	−0.520 127	0.346 598	1.570 970

H_2/Fe_{13}	$E_{tot} = -451\,982.92\,\mathrm{eV}$		$\Delta E_{tot} = 2.41\,\mathrm{meV}$
H	−0.419 977	0.217 694	3.455 785
H	0.196 505	0.710 247	3.047 608
Fe	−0.308 374	−2.164 225	0.572 104
Fe	2.330 329	0.336 498	−1.081 442
Fe	−1.737 081	0.785 469	−2.015 325
Fe	−2.313 505	−0.476 779	−0.009 003
Fe	1.384 364	−1.925 519	−1.280 521
Fe	1.188 409	1.449 104	0.850 644
Fe	0.009 177	−0.063 366	−0.477 671
Fe	0.644 038	0.013 246	−2.787 595
Fe	−1.047 952	−1.597 554	−1.906 101
Fe	1.780 358	−0.996 469	0.971 044
Fe	−1.393 277	1.740 691	0.356 111
Fe	0.267 331	2.053 379	−1.494 126
Fe	−0.580 345	−0.082 416	1.798 488

H_2/Fe_{13}	$E_{tot} = -451\,982.91\,\text{eV}$		$\Delta E_{tot} = 4.28\,\text{meV}$
H	−2.579 755	1.693 135	0.639 055
H	−2.315 921	2.357 240	1.110 721
Fe	0.033 981	−2.475 663	0.892 444
Fe	2.553 589	0.397 058	−0.666 373
Fe	−1.255 645	0.497 567	−1.743 778
Fe	−1.850 098	−0.994 501	0.239 258
Fe	1.679 802	−2.089 012	−0.868 899
Fe	1.473 952	1.322 587	1.322 555
Fe	0.363 888	−0.293 900	−0.123 491
Fe	0.887 622	−0.279 158	−2.490 578
Fe	−0.657 399	−1.991 980	−1.592 667
Fe	2.082 943	−1.014 772	1.433 921
Fe	−0.896 566	1.439 957	0.747 861
Fe	0.661 453	1.896 380	−1.124 131
Fe	−0.181 847	−0.464 940	2.224 101

H_2/Fe_{13}	$E_{tot} = -451\,982.85\,\mathrm{eV}$	$\Delta E_{tot} = 66.25\,\mathrm{meV}$	
H	1.820 426	−0.151 760	−3.024 919
H	2.085 224	0.396 676	−2.458 691
Fe	−1.043 632	−2.065 336	1.490 594
Fe	2.103 022	0.329 254	0.425 428
Fe	−1.636 990	0.714 510	−1.477 271
Fe	−2.700 758	−0.362 319	0.432 074
Fe	1.046 455	−2.039 297	0.232 894
Fe	0.668 238	1.760 817	1.769 451
Fe	−0.294 994	−0.023 197	0.405 458
Fe	0.703 435	−0.332 485	−1.657 301
Fe	−1.274 689	−1.799 146	−0.914 126
Fe	1.025 758	−0.755 351	2.318 993
Fe	−1.649 496	1.992 532	0.613 951
Fe	0.436 120	2.039 696	−0.636 575
Fe	−1.288 117	0.295 405	2.480 040

CH_3OH/Fe_{13}	$E_{tot} = -455\,101.40\,\text{eV}$	$\Delta E_{tot} = 0.00\,\text{meV}$	
H	−3.043 209	−1.433 862	−0.694 176
C	−3.263 836	−0.371 511	−0.549 470
H	−4.255 357	−0.135 467	−0.959 513
H	−3.212 638	−0.132 218	0.521 835
O	−2.245 782	0.357 898	−1.287 611
H	−2.376 940	1.313 311	−1.153 170
Fe	2.546 616	−2.024 438	1.166 877
Fe	3.549 907	1.294 617	−1.209 465
Fe	−0.236 750	0.086 891	−0.782 342
Fe	0.279 695	−1.164 784	1.401 815
Fe	3.499 120	−1.300 503	−1.140 119
Fe	2.629 721	2.178 300	1.056 554
Fe	1.913 450	0.062 759	0.094 713
Fe	1.810 741	0.001 273	−2.327 986
Fe	1.193 147	−2.044 105	−0.862 631
Fe	4.043 156	0.044 459	0.970 617
Fe	0.330 369	1.425 575	1.334 567
Fe	1.277 105	2.147 112	−0.973 360
Fe	2.016 154	0.125 484	2.525 486

CH_3OH/Fe_{13}	$E_{tot} = -455\,101.40\,\text{eV}$	$\Delta E_{tot} = 0.84\,\text{meV}$	
H	−3.457 295	−0.978 093	−0.714 790
C	−3.640 374	−0.083 639	−0.110 915
H	−4.647 014	0.307 050	−0.313 738
H	−3.520 987	−0.332 951	0.952 443
O	−2.646 902	0.893 666	−0.524 601
H	−2.732 947	1.692 554	0.024 244
Fe	−0.020 759	−1.599 650	1.095 549
Fe	3.788 786	−0.615 023	0.516 994
Fe	1.191 072	0.709 776	−2.194 861
Fe	−0.627 386	0.389 516	−0.414 583
Fe	2.072 707	−2.492 249	0.221 083
Fe	2.681 338	1.448 786	1.557 356
Fe	1.590 787	−0.115 551	0.051 289
Fe	2.826 355	−1.061 282	−1.814 350
Fe	0.494 824	−1.673 928	−1.446 902
Fe	1.989 435	−0.942 241	2.304 608
Fe	1.102 466	2.255 780	−0.116 165
Fe	3.203 308	1.371 224	−0.989 836
Fe	0.352 587	0.826 254	1.917 176

CH_3OH/Fe_{13}	$E_{tot} = -455\,101.40\,\mathrm{eV}$		$\Delta E_{tot} = 3.26\,\mathrm{meV}$
H	0.863 584	2.346 176	−2.400 583
C	−0.219 215	2.463 920	−2.291 764
H	−0.519 111	3.475 495	−2.598 075
H	−0.730 506	1.701 433	−2.895 482
O	−0.506 343	2.278 638	−0.879 073
H	−1.468 194	2.327 762	−0.737 406
Fe	0.559 191	−3.766 975	1.779 292
Fe	2.346 610	−0.626 505	0.111 801
Fe	−1.772 166	−1.307 040	−0.304 996
Fe	−1.755 395	−2.670 587	1.714 552
Fe	1.960 605	−3.010 451	−0.226 831
Fe	1.189 185	0.129 646	2.303 172
Fe	0.300 631	−1.649 449	0.914 065
Fe	0.516 858	−1.517 337	−1.499 302
Fe	−0.591 181	−3.433 560	−0.479 361
Fe	2.374 860	−1.995 666	2.129 983
Fe	−1.358 588	−0.288 554	2.047 304
Fe	0.034 163	0.484 880	0.039 768
Fe	0.081 392	−1.783 698	3.328 716

CH_3OH/Fe_{13}	$E_{tot} = -455\,101.40\,\mathrm{eV}$		$\Delta E_{tot} = 4.89\,\mathrm{meV}$
H	0.697 786	−3.184 450	−1.308 226
C	0.873 155	−3.304 757	−0.234 429
H	−0.092 078	−3.390 182	0.283 823
H	1.498 442	−4.189 692	−0.052 989
O	1.582 763	−2.111 115	0.196 027
H	1.720 174	−2.150 564	1.159 003
Fe	−1.083 668	0.179 796	1.724 853
Fe	1.750 716	1.974 007	−0.800 362
Fe	−2.220 908	1.872 571	−1.837 773
Fe	−2.858 414	1.458 943	0.648 622
Fe	0.682 940	−0.248 591	−0.087 819
Fe	0.703 138	3.692 446	0.573 182
Fe	−0.550 770	1.718 352	−0.078 373
Fe	−0.049 764	0.854 199	−2.287 261
Fe	−1.805 868	−0.253 919	−0.727 650
Fe	1.115 053	1.557 062	1.679 482
Fe	−1.778 614	3.665 203	−0.063 415
Fe	−0.022 746	3.257 074	−1.882 586
Fe	−1.050 618	2.580 085	2.139 541

CH_3OH/Fe_{13}	$E_{tot} = -455\,101.39\,\text{eV}$	$\Delta E_{tot} = 13.06\,\text{meV}$	
H	−3.105 034	−1.851 304	1.397 918
C	−2.414 120	−1.620 855	2.215 038
H	−2.952 802	−1.621 933	3.172 720
H	−1.597 355	−2.356 096	2.220 194
O	−1.902 001	−0.287 245	1.948 952
H	−1.230 569	−0.061 764	2.619 128
Fe	0.222 613	−2.079 252	−0.905 353
Fe	2.931 649	0.648 197	−0.935 084
Fe	−0.247 598	1.086 518	−3.592 818
Fe	−1.432 626	−0.534 738	−2.242 144
Fe	2.409 123	−1.608 992	−1.772 396
Fe	0.942 668	1.672 168	0.360 394
Fe	0.702 107	0.148 855	−1.535 559
Fe	2.096 160	0.402 150	−3.376 327
Fe	0.527 231	−1.431 696	−3.393 602
Fe	1.648 162	−0.717 761	0.562 084
Fe	−1.018 629	1.889 282	−1.399 046
Fe	1.270 657	2.400 001	−1.957 116
Fe	−0.824 795	0.033 454	0.207 912

S9.2.2 Mol/Co_{13}

CH_4/Co_{13}	$E_{tot} = -496\,039.71$ eV	$\Delta E_{tot} = 0.00$ meV	
H	−3.148 121	−2.555 812	0.069 044
C	−2.822 174	−1.563 143	−0.260 229
H	−3.648 930	−0.845 525	−0.244 646
H	−2.044 701	−1.212 197	0.459 486
H	−2.459 088	−1.654 332	−1.306 383
Co	1.000 638	2.840 521	0.046 112
Co	1.107 930	−1.947 858	0.340 360
Co	1.010 944	0.458 929	0.304 052
Co	2.730 721	−0.783 508	−0.777 160
Co	2.692 559	1.626 051	−0.929 520
Co	−0.573 437	−0.891 294	−0.883 631
Co	−0.609 673	1.583 682	−1.072 369
Co	2.771 854	−0.605 692	1.529 491
Co	2.735 005	1.726 768	1.382 516
Co	1.014 037	0.304 140	−2.070 843
Co	1.017 043	2.669 188	−2.207 264
Co	1.081 997	−2.037 341	−1.929 681
Co	4.339 895	0.515 692	0.354 827

CH_4/Co_{13}	$E_{tot} = -496\,039.71$ eV		$\Delta E_{tot} = 1.09$ meV
H	−0.687 393	4.185 397	0.640 891
C	−0.090 965	3.334 274	0.987 407
H	0.313 263	3.511 588	1.989 348
H	−0.771 112	2.450 782	1.039 247
H	0.760 657	3.207 348	0.284 979
Co	0.295 702	1.236 660	−0.166 759
Co	−1.338 164	−3.208 509	0.548 879
Co	−0.544 301	−0.962 484	0.284 741
Co	0.733 312	−2.855 096	−0.421 827
Co	1.556 032	−0.605 110	−0.776 721
Co	−2.363 844	−1.811 955	−1.020 034
Co	−1.507 388	0.444 863	−1.416 710
Co	0.596 051	−2.397 649	1.827 714
Co	1.410 017	−0.242 574	1.486 347
Co	−0.326 842	−1.413 500	−2.042 965
Co	0.526 119	0.772 425	−2.375 278
Co	−1.138 315	−3.594 660	−1.666 167
Co	2.577 172	−2.051 803	0.796 908

CH_4/Co_{13}	$E_{tot} = -496\,039.69\,\text{eV}$		$\Delta E_{tot} = 13.94\,\text{meV}$
H	1.114 422	2.549 120	−1.646 013
C	0.839 395	2.285 863	−2.692 694
H	0.086 467	1.467 535	−2.767 999
H	0.439 845	3.177 741	−3.186 175
H	1.750 733	1.930 176	−3.185 722
Co	−0.807 627	1.590 246	1.428 041
Co	−1.139 718	−3.176 897	1.701 358
Co	−1.025 562	−0.783 495	1.662 117
Co	0.796 186	−2.181 723	0.959 303
Co	0.962 857	0.225 981	0.835 706
Co	−2.412 791	−2.006 631	0.136 997
Co	−2.234 603	0.447 193	0.001 354
Co	0.368 262	−1.969 407	3.208 966
Co	0.534 675	0.353 384	3.082 115
Co	−0.530 665	−0.970 547	−0.656 233
Co	−0.314 773	1.377 778	−0.781 428
Co	−0.664 286	−3.319 688	−0.500 365
Co	2.237 183	−0.996 629	2.400 671

CH_4/Co_{13}	$E_{tot} = -496\,039.69\,\text{eV}$		$\Delta E_{tot} = 14.13\,\text{meV}$
H	0.719 721	−2.712 626	−1.342 253
C	0.403 444	−2.570 382	−2.401 023
H	−0.425 036	−1.836 402	−2.528 993
H	1.268 858	−2.176 099	−2.944 858
H	0.083 537	−3.536 188	−2.805 425
Co	−1.745 421	2.995 178	1.777 425
Co	−1.288 707	−1.767 444	1.671 228
Co	−1.568 586	0.605 927	1.821 789
Co	0.447 190	−0.378 923	1.033 216
Co	0.217 270	2.026 086	1.071 748
Co	−2.743 031	−0.712 927	0.204 133
Co	−2.984 663	1.738 236	0.253 777
Co	0.018 995	−0.439 378	3.282 057
Co	−0.208 362	1.881 171	3.327 197
Co	−1.074 907	0.724 582	−0.501 277
Co	−1.270 200	3.074 021	−0.427 436
Co	−0.797 719	−1.620 063	−0.543 274
Co	1.686 698	0.930 413	2.554 508

CH_4/Co_{13}	$E_{tot} = -496\,039.61\,\text{eV}$		$\Delta E_{tot} = 97.81\,\text{meV}$
H	−1.472 315	2.974 226	−2.343 139
C	−0.964 885	2.890 750	−1.376 303
H	−0.083 043	2.216 062	−1.515 195
H	−0.589 965	3.862 212	−1.037 683
H	−1.724 731	2.542 486	−0.627 315
Co	−1.029 663	0.423 016	2.023 779
Co	0.261 464	−4.004 766	0.936 693
Co	−0.427 699	−1.805 830	1.557 353
Co	1.677 560	−2.260 730	0.469 723
Co	1.008 338	0.008 814	1.026 552
Co	−1.490 449	−3.035 621	−0.247 244
Co	−2.154 260	−0.766 596	0.342 915
Co	1.438 125	−2.765 180	2.695 581
Co	0.832 367	−0.583 253	3.230 331
Co	−0.167 981	−1.233 197	−0.733 426
Co	−0.741 408	0.958 502	−0.184 776
Co	0.519 491	−3.395 991	−1.241 372
Co	2.777 236	−1.010 363	2.138 886

CO/Co_{13}	$E_{tot} = -498\,024.10\,\text{eV}$		$\Delta E_{tot} = 0.00\,\text{meV}$
C	−2.992 820	0.026 089	−1.006 656
O	−4.077 179	0.034 997	−1.483 179
Co	0.030 247	2.402 715	0.836 525
Co	−0.011 393	−2.402 266	0.838 373
Co	0.006 912	0.000 211	0.950 310
Co	1.682 375	−1.232 914	−0.181 902
Co	1.703 434	1.203 251	−0.182 852
Co	−1.619 269	−1.136 552	−0.404 635
Co	−1.599 394	1.163 836	−0.404 616
Co	1.687 967	−1.193 803	2.124 435
Co	1.708 390	1.166 094	2.123 524
Co	0.077 458	−0.001 282	−1.458 690
Co	0.076 588	2.405 877	−1.391 236
Co	0.034 965	−2.408 185	−1.389 426
Co	3.291 718	−0.028 070	1.030 027

CO/Co_{13}	$E_{tot} = -498\,023.96\,\mathrm{eV}$		$\Delta E_{tot} = 130.66\,\mathrm{meV}$
C	0.879 814	−0.132 684	−2.853 815
O	1.402 461	−0.170 302	−3.893 499
Co	−1.044 085	2.402 624	0.727 235
Co	−0.772 683	−2.393 465	1.031 979
Co	−1.024 242	0.002 252	0.945 713
Co	1.109 465	−1.087 330	0.768 177
Co	0.974 773	1.293 345	0.616 956
Co	−1.820 012	−1.373 500	−0.802 979
Co	−1.956 432	1.049 101	−0.957 078
Co	0.086 828	−0.971 057	2.823 379
Co	−0.043 487	1.323 085	2.677 590
Co	0.082 447	−0.076 893	−1.289 553
Co	−0.057 348	2.273 965	−1.277 564
Co	0.206 231	−2.408 196	−0.980 426
Co	1.976 273	0.269 057	2.463 886

CO/Co_{13}	$E_{tot} = -498\,023.86\,\text{eV}$		$\Delta E_{tot} = 236.71\,\text{meV}$
C	−2.176 236	−1.681 440	0.576 265
O	−3.118 070	−1.804 249	1.286 449
Co	−0.200 307	2.680 973	0.317 848
Co	−0.335 836	−2.129 013	0.460 163
Co	−0.303 355	0.307 715	0.491 907
Co	1.592 230	−0.943 132	−0.247 010
Co	1.657 313	1.444 180	−0.315 235
Co	−1.660 909	−0.948 285	−1.095 615
Co	−1.555 821	1.510 468	−1.190 758
Co	1.153 424	−0.904 087	1.993 081
Co	1.195 920	1.437 153	1.958 024
Co	0.242 510	0.259 625	−1.832 888
Co	0.317 686	2.615 633	−1.869 471
Co	0.221 773	−2.097 339	−1.779 943
Co	2.969 680	0.251 800	1.247 183

CO/Co_{13}	$E_{tot} = -498\,023.83\,\text{eV}$		$\Delta E_{tot} = 268.38\,\text{meV}$
C	0.752 338	2.455 826	−2.285 814
O	1.577 699	2.650 141	−3.083 013
Co	−1.093 253	1.854 419	1.217 319
Co	−0.610 479	−2.872 059	0.669 377
Co	−0.865 971	−0.535 941	1.041 160
Co	1.135 326	−1.462 448	0.126 854
Co	0.918 368	0.933 668	0.429 512
Co	−2.080 766	−1.657 861	−0.677 518
Co	−2.314 939	0.776 179	−0.364 001
Co	0.713 967	−1.702 514	2.383 731
Co	0.484 305	0.606 259	2.641 431
Co	−0.407 073	−0.236 508	−1.286 374
Co	−0.443 092	2.070 762	−1.064 087
Co	−0.156 549	−2.563 237	−1.521 710
Co	2.390 118	−0.316 686	1.773 133

CO/Co_{13}	$E_{tot} = -498\,023.28\,\mathrm{eV}$		$\Delta E_{tot} = 813.51\,\mathrm{meV}$
C	−1.794 867	−0.044 431	1.652 041
O	−2.660 222	−0.065 561	2.433 325
Co	−0.317 091	2.387 942	0.216 898
Co	−0.252 304	−2.400 025	0.159 637
Co	−0.528 529	−0.013 546	0.499 397
Co	1.566 745	−1.171 809	−0.484 488
Co	1.534 383	1.225 242	−0.455 735
Co	−1.618 815	−1.225 473	−1.315 742
Co	−1.651 547	1.212 919	−1.286 661
Co	1.141 526	−1.205 426	1.768 541
Co	1.108 841	1.193 500	1.797 019
Co	0.153 126	0.026 099	−2.003 340
Co	0.189 189	2.361 857	−1.995 578
Co	0.251 645	−2.307 443	−2.051 289
Co	2.877 916	0.026 152	1.065 975

H_2/Co_{13}	$E_{tot} = -494\,969.91\,\mathrm{eV}$		$\Delta E_{tot} = 0.00\,\mathrm{meV}$
H	0.090 442	2.421 812	2.340 231
H	0.804 155	2.011 724	2.821 075
Co	−0.912 900	1.990 789	−0.058 318
Co	−0.644 836	−2.746 962	0.197 900
Co	−0.864 315	−0.396 882	0.097 316
Co	1.214 964	−1.469 740	−0.291 958
Co	1.070 753	0.925 678	−0.460 992
Co	−1.830 466	−1.733 698	−1.559 917
Co	−1.988 281	0.710 545	−1.692 862
Co	0.472 100	−1.341 836	1.876 795
Co	0.318 928	0.994 923	1.721 653
Co	−0.033 376	−0.411 834	−2.123 009
Co	−0.161 038	1.927 821	−2.222 751
Co	0.182 060	−2.745 306	−1.923 642
Co	2.281 810	−0.137 034	1.278 479

H_2/Co_{13}	$E_{tot} = -494\,969.84\,\mathrm{eV}$		$\Delta E_{tot} = 67.03\,\mathrm{meV}$
H	1.884 969	−2.167 494	−0.402 564
H	2.352 734	−1.686 535	0.172 402
Co	−0.860 520	2.757 885	0.167 680
Co	−1.225 023	−1.948 796	0.756 326
Co	−1.099 777	0.410 444	0.552 995
Co	0.842 751	−1.047 314	0.187 349
Co	0.973 144	1.403 400	−0.125 107
Co	−2.273 718	−0.915 812	−1.067 551
Co	−2.082 412	1.504 753	−1.331 802
Co	0.066 153	−0.625 140	2.339 720
Co	0.268 803	1.691 846	2.052 558
Co	−0.296 789	0.100 799	−1.683 632
Co	−0.084 235	2.417 434	−1.952 092
Co	−0.489 422	−2.236 382	−1.374 512
Co	2.023 341	0.340 912	1.708 230

H_2/Co_{13}	$E_{tot} = -494\,969.81\,\text{eV}$		$\Delta E_{tot} = 97.02\,\text{meV}$
H	−2.868 423	1.348 284	−0.021 758
H	−3.228 906	0.785 694	−0.587 097
Co	−0.487 606	2.146 920	0.584 253
Co	0.116 406	−2.633 787	0.497 658
Co	−0.234 522	−0.290 996	0.664 306
Co	1.832 550	−1.220 633	−0.076 845
Co	1.498 600	1.182 675	−0.017 721
Co	−1.323 616	−1.595 128	−1.036 460
Co	−1.619 543	0.836 454	−0.956 682
Co	1.304 971	−1.266 769	2.191 083
Co	0.972 924	1.053 001	2.226 610
Co	0.362 174	−0.157 206	−1.654 310
Co	0.092 957	2.169 495	−1.645 717
Co	0.654 450	−2.498 085	−1.684 475
Co	2.927 584	0.140 083	1.517 151

H_2/Co_{13}	$E_{tot} = -494\,969.70\,\mathrm{eV}$		$\Delta E_{tot} = 208.49\,\mathrm{meV}$
H	1.312 584	2.010 871	−2.091 534
H	0.974 281	2.765 364	−2.315 213
Co	−0.843 304	2.018 268	0.957 598
Co	−0.952 500	−2.746 536	0.631 914
Co	−0.940 885	−0.372 009	0.873 179
Co	1.018 237	−1.615 220	0.253 794
Co	1.078 082	0.803 534	0.432 972
Co	−2.076 524	−1.454 103	−0.945 051
Co	−2.035 508	0.993 342	−0.760 141
Co	0.305 658	−1.665 627	2.444 078
Co	0.381 213	0.656 639	2.593 789
Co	−0.178 418	−0.275 991	−1.376 827
Co	−0.067 539	2.074 244	−1.191 815
Co	−0.194 033	−2.632 545	−1.490 601
Co	2.218 659	−0.560 230	1.983 860

H_2/Co_{13}	$E_{tot} = -494\,969.67$ eV		$\Delta E_{tot} = 237.91$ meV
H	0.543 698	2.175 412	−3.037 009
H	1.024 778	2.630 793	−2.462 020
Co	−0.661 824	2.079 305	0.628 270
Co	−0.983 643	−2.595 893	1.198 483
Co	−0.856 873	−0.227 306	0.975 051
Co	1.015 169	−1.661 427	0.524 019
Co	1.188 196	0.735 789	0.228 176
Co	−2.146 037	−1.587 875	−0.546 940
Co	−1.971 900	0.819 695	−0.802 275
Co	0.406 207	−1.255 562	2.711 658
Co	0.589 416	1.046 633	2.428 577
Co	−0.203 415	−0.601 541	−1.285 230
Co	0.063 213	1.671 872	−1.560 976
Co	−0.341 643	−2.903 042	−0.957 058
Co	2.334 657	−0.326 850	1.957 272

CH_3OH/Co_{13}	$E_{tot} = -498\,088.16\,\text{eV}$	$\Delta E_{tot} = 0.00\,\text{meV}$	
H	−0.939 280	−2.012 901	−2.899 481
C	−0.196 495	−2.616 031	−2.367 974
H	−0.054 079	−3.575 236	−2.884 194
H	0.747 887	−2.057 946	−2.303 416
O	−0.745 057	−2.855 372	−1.040 652
H	−0.101 839	−3.372 420	−0.524 986
Co	0.513 000	3.745 763	0.625 358
Co	−1.358 537	−0.362 156	2.222 983
Co	−0.459 042	1.745 558	1.522 575
Co	0.712 418	−0.298 723	1.198 085
Co	1.653 552	1.765 375	0.377 573
Co	−2.341 122	0.733 170	0.436 148
Co	−1.385 060	2.850 432	−0.394 871
Co	0.644 450	0.589 495	3.309 668
Co	1.550 029	2.589 906	2.520 279
Co	−0.314 805	0.846 376	−0.670 566
Co	0.633 456	2.857 369	−1.447 324
Co	−1.190 294	−1.205 316	0.120 959
Co	2.630 817	0.632 656	2.199 833

CH_3OH/Co_{13}	$E_{tot} = -498\,088.12\,\text{eV}$		$\Delta E_{tot} = 31.34\,\text{meV}$
H	−1.554 207	−1.163 719	2.769 189
C	−2.308 441	−1.369 074	2.002 195
H	−3.165 967	−1.887 520	2.452 653
H	−2.614 296	−0.422 156	1.536 705
O	−1.669 290	−2.239 454	1.028 706
H	−2.320 926	−2.474 476	0.346 083
Co	0.720 087	3.243 051	−0.616 320
Co	−0.070 776	−1.444 683	−0.060 762
Co	0.286 684	0.913 925	−0.257 913
Co	2.046 732	−0.646 716	−0.616 903
Co	2.443 349	1.729 814	−0.896 856
Co	−0.975 442	−0.310 042	−1.899 508
Co	−0.604 758	2.088 709	−2.148 665
Co	1.401 943	−0.223 834	1.546 588
Co	1.743 665	2.057 560	1.268 582
Co	1.073 055	0.530 558	−2.476 327
Co	1.442 996	2.846 822	−2.724 285
Co	0.716 639	−1.798 107	−2.155 800
Co	3.408 952	0.569 340	0.902 637

CH_3OH/Co_{13}	$E_{tot} = -498\,088.10\,\text{eV}$	$\Delta E_{tot} = 58.72\,\text{meV}$	
H	0.266 705	2.282 604	2.917 315
C	−0.239 714	3.023 140	2.289 408
H	−0.772 707	3.747 319	2.920 562
H	0.501 553	3.528 203	1.654 977
O	−1.194 818	2.282 698	1.482 862
H	−1.655 891	2.898 901	0.887 727
Co	−0.465 393	0.793 598	0.226 792
Co	−0.322 910	−3.841 586	−0.999 427
Co	−0.427 298	−1.556 543	−0.301 137
Co	1.474 038	−2.452 709	−1.439 627
Co	1.391 146	−0.107 764	−0.807 401
Co	−1.783 913	−2.379 705	−2.092 509
Co	−1.828 862	−0.012 322	−1.482 332
Co	1.154 974	−3.002 499	0.772 955
Co	1.102 788	−0.758 188	1.374 753
Co	−0.032 473	−0.939 170	−2.564 758
Co	−0.062 653	1.339 863	−1.950 169
Co	0.025 348	−3.222 149	−3.145 165
Co	2.870 077	−1.623 690	0.255 179

CH_3OH/Co_{13} $E_{tot} = -498\,088.09\,\text{eV}$ $\Delta E_{tot} = 62.70\,\text{meV}$

H	−2.588 012	2.988 945	−1.557 311
C	−1.809 323	3.584 121	−1.069 380
H	−1.616 597	4.492 519	−1.655 695
H	−2.128 255	3.841 451	−0.049 864
O	−0.618 435	2.752 641	−1.050 294
H	0.116 509	3.243 405	−0.644 028
Co	−0.579 566	0.049 473	1.939 732
Co	0.988 943	−4.094 039	0.131 473
Co	0.180 054	−2.069 547	1.129 935
Co	2.123 315	−2.138 131	−0.282 472
Co	1.334 459	−0.049 546	0.643 564
Co	−1.006 110	−3.167 402	−0.640 309
Co	−1.802 722	−1.028 300	0.293 009
Co	2.288 064	−2.950 636	1.861 926
Co	1.532 760	−0.929 954	2.749 492
Co	0.049 440	−1.177 355	−1.072 123
Co	−0.674 095	0.890 556	−0.166 781
Co	0.857 145	−3.221 070	−1.946 017
Co	3.352 426	−1.017 131	1.385 144

CH_3OH/Co_{13}	$E_{tot} = -498\,088.00\,\text{eV}$		$\Delta E_{tot} = 152.60\,\text{meV}$
H	2.513 331	0.453 193	−1.751 754
C	2.125 303	−0.467 312	−2.201 667
H	2.628 732	−0.658 647	−3.159 888
H	2.288 350	−1.299 530	−1.501 263
O	0.713 115	−0.241 917	−2.425 483
H	0.313 502	−1.057 182	−2.777 887
Co	−1.206 817	2.753 259	1.269 451
Co	−1.961 233	−1.946 562	1.593 054
Co	−1.646 065	0.414 092	1.457 392
Co	0.176 869	−1.109 888	1.319 175
Co	0.557 068	1.263 216	1.161 739
Co	−2.627 506	−0.791 883	−0.339 680
Co	−2.257 062	1.610 911	−0.495 677
Co	−0.801 347	−0.764 368	3.376 820
Co	−0.439 400	1.512 695	3.222 801
Co	−0.519 275	0.090 546	−0.692 761
Co	−0.196 529	2.483 534	−0.714 002
Co	−0.949 196	−2.291 005	−0.376 286
Co	1.288 156	0.046 848	3.035 916

S9.2.3 Mol/Ni_{13}

CH_4/Ni_{13}	$E_{tot} = -541\,432.74\,\text{eV}$		$\Delta E_{tot} = 0.00\,\text{meV}$
H	−1.085 218	1.958 111	2.316 005
C	−0.960 184	2.896 598	1.713 155
H	−0.609 243	2.734 828	0.652 751
H	−1.933 324	3.395 476	1.662 406
H	−0.214 638	3.521 192	2.215 755
Ni	0.662 494	0.245 925	−2.903 406
Ni	0.365 820	−1.806 769	−1.894 574
Ni	0.330 244	−3.511 217	−0.378 729
Ni	2.538 606	−0.994 609	−2.165 321
Ni	2.019 645	−1.870 696	0.036 506
Ni	−1.073 587	−0.012 876	−1.341 558
Ni	−1.706 062	−2.300 888	−0.903 100
Ni	1.197 108	0.264 624	−0.670 797
Ni	−0.542 179	0.913 051	0.845 582
Ni	−2.424 288	−0.548 953	0.446 867
Ni	1.468 429	−0.207 510	1.560 637
Ni	−0.239 003	−1.388 630	0.580 547
Ni	2.205 378	−3.287 656	−1.772 725

CH_4/Ni_{13}	$E_{tot} = -541\,432.70\,\mathrm{eV}$		$\Delta E_{tot} = 44.83\,\mathrm{meV}$
H	−3.494 520	−1.494 721	−1.029 657
C	−2.436 466	−1.729 420	−1.185 522
H	−1.965 849	−0.863 680	−1.727 678
H	−1.977 990	−1.957 875	−0.188 293
H	−2.312 587	−2.616 153	−1.816 274
Ni	0.936 438	2.790 372	−1.890 311
Ni	1.100 262	0.549 122	−1.394 555
Ni	1.447 655	−1.444 059	−0.337 097
Ni	3.057 795	1.702 668	−1.744 132
Ni	3.007 166	0.269 654	0.202 314
Ni	−0.450 237	1.915 402	−0.226 576
Ni	−0.771 689	−0.497 333	−0.344 763
Ni	1.862 868	2.368 110	0.186 980
Ni	0.361 321	2.325 235	2.022 803
Ni	−1.404 229	0.887 584	1.595 559
Ni	2.555 165	1.432 027	2.180 464
Ni	0.814 339	0.271 370	1.141 567
Ni	3.073 240	−0.617 915	−1.927 622

CH_4/Ni_{13}	$E_{tot} = -541\,432.68\,\mathrm{eV}$		$\Delta E_{tot} = 60.92\,\mathrm{meV}$
H	−2.482 787	−0.540 471	1.803 433
C	−3.184 807	0.302 572	1.533 531
H	−2.780 980	1.069 461	0.808 002
H	−4.066 679	−0.150 333	1.067 134
H	−3.450 134	0.826 585	2.458 009
Ni	2.274 454	1.621 747	−2.021 915
Ni	1.599 401	−0.573 306	−1.862 379
Ni	1.152 333	−2.666 490	−1.045 657
Ni	3.845 143	−0.141 194	−1.764 577
Ni	3.057 059	−1.630 527	−0.067 009
Ni	0.395 407	1.084 456	−0.673 516
Ni	−0.603 745	−1.063 103	−1.202 997
Ni	2.630 602	0.725 077	0.069 955
Ni	0.909 120	1.047 865	1.677 373
Ni	−1.176 939	0.225 582	0.797 868
Ni	2.602 182	−0.575 718	1.974 162
Ni	0.824 993	−0.979 620	0.573 330
Ni	3.146 765	−2.315 762	−2.291 147

CH_4/Ni_{13}	$E_{tot} = -541\,432.63\,\mathrm{eV}$		$\Delta E_{tot} = 118.08\,\mathrm{meV}$
H	−2.836 517	0.563 024	0.936 933
C	−3.003 956	−0.175 642	1.786 434
H	−3.895 141	−0.765 923	1.547 913
H	−2.153 682	−0.887 954	2.003 320
H	−3.154 745	0.422 486	2.691 859
Ni	1.324 412	1.571 955	−2.889 419
Ni	1.127 585	−0.690 219	−2.493 493
Ni	1.223 140	−2.754 074	−1.515 062
Ni	3.240 815	0.212 061	−2.786 238
Ni	3.039 894	−1.288 599	−0.904 792
Ni	−0.216 509	0.806 719	−1.260 375
Ni	−0.817 661	−1.482 031	−1.466 379
Ni	2.141 221	0.934 306	−0.836 863
Ni	0.680 468	1.063 132	0.980 561
Ni	−1.303 970	−0.219 187	0.544 564
Ni	2.677 867	−0.171 584	1.114 568
Ni	0.850 063	−1.046 208	0.023 607
Ni	2.898 614	−2.108 373	−3.048 037

CH_4/Ni_{13}	$E_{tot} = -541\,432.61\,\text{eV}$		$\Delta E_{tot} = 137.85\,\text{meV}$
H	−1.864 395	0.388 877	−1.247 757
C	−2.250 276	1.387 888	−0.936 002
H	−2.124 589	2.078 392	−1.776 745
H	−3.305 056	1.272 198	−0.665 183
H	−1.713 315	1.804 990	−0.053 892
Ni	1.339 322	1.244 391	−1.146 138
Ni	1.460 582	−1.001 199	−0.659 907
Ni	1.776 562	−2.987 205	0.386 024
Ni	3.385 715	0.331 982	−0.539 761
Ni	3.036 356	−1.178 878	1.343 123
Ni	−0.445 444	0.245 502	0.144 443
Ni	−0.461 417	−2.183 832	0.001 503
Ni	1.721 925	0.805 990	1.075 835
Ni	−0.118 352	0.617 805	2.536 533
Ni	−1.585 965	−1.042 548	1.745 090
Ni	2.035 176	−0.110 797	3.175 793
Ni	0.722 189	−1.376 262	1.761 803
Ni	3.616 548	−1.997 756	−0.722 819

CO/Ni_{13}	$E_{tot} = -543\,417.24\,\mathrm{eV}$		$\Delta E_{tot} = 0.00\,\mathrm{meV}$
C	−2.492 171	0.923 381	2.144 921
O	−3.330 298	1.496 712	2.754 905
Ni	0.556 785	2.015 665	−1.854 070
Ni	0.489 815	−0.295 267	−1.816 608
Ni	0.663 186	−2.453 932	−1.075 376
Ni	2.541 408	0.752 112	−1.628 898
Ni	2.225 411	−0.952 299	−0.015 818
Ni	−1.085 760	0.913 071	−0.611 862
Ni	−1.490 952	−1.399 923	−1.179 104
Ni	1.113 051	1.173 114	0.228 723
Ni	−0.684 054	0.908 872	1.821 577
Ni	−2.358 053	−0.382 720	0.838 934
Ni	1.479 909	−0.163 263	2.044 169
Ni	−0.075 340	−1.019 555	0.600 568
Ni	2.447 063	−1.515 968	−2.252 061

CO/Ni_{13}	$E_{tot} = -543\,417.13\,\mathrm{eV}$		$\Delta E_{tot} = 111.07\,\mathrm{meV}$
C	2.596 548	1.857 424	−1.869 664
O	3.482 139	2.545 899	−2.169 005
Ni	−0.957 255	1.782 228	−1.161 888
Ni	−0.659 285	−0.484 759	−1.069 979
Ni	−0.171 126	−2.609 644	−0.423 820
Ni	1.281 558	0.838 681	−1.409 849
Ni	1.364 422	−0.907 996	0.293 754
Ni	−2.182 446	0.589 867	0.405 862
Ni	−2.406 258	−1.747 764	0.014 783
Ni	0.152 810	1.109 890	0.712 786
Ni	−1.210 748	0.702 414	2.608 149
Ni	−2.897 079	−0.831 662	2.106 638
Ni	1.032 498	−0.076 725	2.468 695
Ni	−0.679 218	−1.223 106	1.411 846
Ni	1.253 439	−1.544 745	−1.918 309

CO/Ni_{13}	$E_{tot} = -543\,417.05\,\mathrm{eV}$		$\Delta E_{tot} = 191.68\,\mathrm{meV}$
C	0.191 836	2.075 130	1.847 844
O	0.549 904	3.112 274	2.287 230
Ni	−0.000 666	1.884 666	−1.631 587
Ni	−0.104 175	−0.409 687	−1.743 554
Ni	0.065 513	−2.614 485	−1.255 419
Ni	1.971 435	0.586 482	−1.613 989
Ni	1.674 906	−1.254 393	−0.154 761
Ni	−1.626 913	0.701 968	−0.349 771
Ni	−2.081 586	−1.511 147	−1.039 302
Ni	0.705 352	0.977 521	0.386 657
Ni	−0.961 322	0.663 780	1.970 852
Ni	−2.760 860	−0.653 063	1.129 540
Ni	1.147 636	−0.661 364	1.997 599
Ni	−0.578 048	−1.301 831	0.633 811
Ni	1.806 989	−1.595 853	−2.465 149

CO/Ni_{13}	$E_{tot} = -543\,416.81\,\text{eV}$		$\Delta E_{tot} = 423.56\,\text{meV}$
C	−0.465 164	2.787 712	−2.316 134
O	−0.711 131	3.877 302	−2.626 754
Ni	−0.107 740	1.189 906	−1.728 725
Ni	0.084 177	−1.011 071	−0.940 776
Ni	0.410 449	−2.909 875	0.363 687
Ni	2.060 029	0.113 149	−1.295 894
Ni	1.896 643	−1.064 421	0.813 824
Ni	−1.596 107	0.358 948	−0.012 642
Ni	−1.775 954	−1.989 111	0.130 412
Ni	0.704 661	0.951 595	0.470 623
Ni	−0.930 234	1.124 208	2.190 351
Ni	−2.585 748	−0.476 717	1.890 179
Ni	1.256 385	0.300 190	2.610 589
Ni	−0.333 432	−1.044 404	1.623 284
Ni	2.093 164	−2.207 411	−1.172 022

CO/Ni_{13}	$E_{tot} = -543\,416.71\,\mathrm{eV}$		$\Delta E_{tot} = 528.17\,\mathrm{meV}$
C	−0.754 869	0.031 771	−2.751 014
O	−1.287 591	0.008 037	−3.781 721
Ni	0.308 538	2.361 286	−0.644 059
Ni	0.064 825	0.103 262	−1.229 769
Ni	0.207 400	−2.141 801	−0.509 909
Ni	2.228 953	0.995 349	−0.723 623
Ni	1.853 779	−0.916 260	0.689 417
Ni	−1.337 146	1.216 014	0.542 985
Ni	−1.891 408	−0.901 702	−0.264 191
Ni	0.951 596	1.175 582	1.216 964
Ni	−0.754 641	0.816 637	2.823 351
Ni	−2.586 882	−0.267 198	1.867 285
Ni	1.294 877	−0.352 972	2.919 252
Ni	−0.362 063	−0.954 124	1.421 295
Ni	2.064 630	−1.173 879	−1.576 262

H_2/Ni_{13}	$E_{tot} = -540\,362.96\,\text{eV}$		$\Delta E_{tot} = 0.00\,\text{meV}$
H	−1.480 589	1.832 345	2.797 172
H	−0.629 421	1.840 870	3.027 367
Ni	0.171 678	1.951 111	−1.862 600
Ni	0.095 931	−0.362 540	−1.867 031
Ni	0.318 040	−2.551 222	−1.261 496
Ni	2.175 340	0.681 346	−1.843 865
Ni	1.915 874	−1.106 222	−0.236 850
Ni	−1.397 800	0.847 388	−0.502 907
Ni	−1.838 875	−1.448 409	−1.090 186
Ni	0.894 323	1.044 415	0.118 093
Ni	−0.759 111	0.802 156	1.854 912
Ni	−2.565 418	−0.534 102	0.922 022
Ni	1.387 786	−0.321 457	1.884 377
Ni	−0.317 985	−1.117 646	0.569 861
Ni	2.030 228	−1.558 034	−2.508 868

H_2/Ni_{13}	$E_{tot} = -540\,362.89\,\mathrm{eV}$		$\Delta E_{tot} = 68.15\,\mathrm{meV}$
H	2.763 107	−1.110 982	0.690 279
H	2.884 708	−1.275 347	−0.177 748
Ni	−0.637 285	2.457 221	−1.395 648
Ni	−0.606 117	0.145 456	−1.413 376
Ni	−0.354 896	−2.051 883	−0.927 264
Ni	1.379 836	1.273 050	−1.592 332
Ni	1.455 558	−0.628 864	−0.042 434
Ni	−2.044 694	1.290 698	0.077 804
Ni	−2.476 573	−0.990 458	−0.511 486
Ni	0.299 653	1.479 931	0.489 216
Ni	−1.106 728	1.120 078	2.351 415
Ni	−2.977 908	−0.103 966	1.635 630
Ni	0.979 920	0.098 146	2.196 070
Ni	−0.775 215	−0.732 515	0.961 420
Ni	1.216 634	−0.970 562	−2.341 544

H_2/Ni_{13}	$E_{tot} = -540\,362.88\,\text{eV}$		$\Delta E_{tot} = 79.80\,\text{meV}$
H	−2.324 693	−2.289 897	−0.617 482
H	−2.846 982	−1.789 930	−0.102 691
Ni	0.215 493	2.464 026	−1.659 391
Ni	0.290 609	0.188 323	−1.404 938
Ni	0.715 636	−1.909 043	−0.639 052
Ni	2.322 185	1.384 442	−1.741 788
Ni	2.310 605	−0.290 591	0.032 468
Ni	−1.138 942	1.431 326	−0.023 971
Ni	−1.532 568	−0.953 644	−0.356 984
Ni	1.209 038	1.797 010	0.306 178
Ni	−0.196 337	1.598 560	2.205 703
Ni	−1.974 944	0.216 004	1.744 688
Ni	1.966 789	0.650 528	2.158 831
Ni	0.190 864	−0.395 155	1.092 624
Ni	2.230 514	−0.894 949	−2.187 577

H_2/Ni_{13}	$E_{tot} = -540\,362.84\,\text{eV}$		$\Delta E_{tot} = 119.05\,\text{meV}$
H	−3.112 182	−0.651 439	2.461 771
H	−3.272 845	−1.188 207	1.781 047
Ni	0.235 485	2.351 374	−1.776 368
Ni	0.315 505	0.058 460	−1.729 748
Ni	0.706 356	−2.105 777	−1.064 610
Ni	2.295 139	1.182 013	−1.913 985
Ni	2.326 821	−0.548 321	−0.276 450
Ni	−1.136 676	1.169 821	−0.219 184
Ni	−1.486 746	−1.140 166	−0.841 731
Ni	1.186 440	1.528 169	0.153 652
Ni	−0.262 178	1.205 780	2.001 324
Ni	−2.063 164	−0.272 027	1.345 529
Ni	1.894 871	0.198 792	1.896 363
Ni	0.146 848	−0.700 377	0.727 939
Ni	2.226 327	−1.088 096	−2.545 548

H_2/Ni_{13}	$E_{tot} = -540\,362.60\,\mathrm{eV}$		$\Delta E_{tot} = 357.57\,\mathrm{meV}$
H	−0.763 161	−1.705 266	1.905 284
H	−0.321 966	−2.146 202	1.272 450
Ni	−0.125 792	2.581 591	−2.033 877
Ni	−0.118 227	0.276 080	−1.870 119
Ni	0.239 460	−1.857 700	−1.173 416
Ni	1.900 068	1.357 954	−2.017 544
Ni	1.796 581	−0.332 955	−0.320 672
Ni	−1.581 323	1.499 516	−0.525 824
Ni	−1.970 165	−0.808 686	−0.945 342
Ni	0.695 503	1.767 622	−0.028 941
Ni	−0.784 223	1.510 670	1.753 935
Ni	−2.621 232	0.225 679	1.062 340
Ni	1.365 024	0.542 528	1.793 679
Ni	−0.401 617	−0.636 609	0.793 794
Ni	1.809 062	−0.900 963	−2.599 097

CH_3OH/Ni_{13} $E_{tot} = -543\,481.10\,\text{eV}$ $\Delta E_{tot} = 0.00\,\text{meV}$

H	−3.279 957	1.938 933	2.385 466
C	−2.746 769	1.255 812	1.709 279
H	−3.388 269	0.407 691	1.449 493
H	−2.435 497	1.770 454	0.789 286
O	−1.594 437	0.694 816	2.397 953
H	−0.961 458	1.414 000	2.570 565
Ni	0.047 947	1.554 943	−2.036 602
Ni	1.276 842	−0.384 732	−2.285 134
Ni	2.514 959	−2.263 877	−1.841 706
Ni	2.419 619	1.524 724	−1.743 894
Ni	2.978 267	−0.409 784	−0.426 019
Ni	−0.791 960	−0.441 620	−1.135 443
Ni	0.161 669	−2.459 199	−2.010 060
Ni	0.949 599	0.805 305	−0.056 470
Ni	−0.461 423	−0.561 427	1.290 168
Ni	−1.210 971	−2.400 827	−0.019 679
Ni	1.908 441	−0.429 694	1.647 421
Ni	1.018 170	−1.724 456	−0.037 265
Ni	3.595 223	−0.291 062	−2.647 354

CH_3OH/Ni_{13}	$E_{tot} = -543\,481.10\,\text{eV}$		$\Delta E_{tot} = 3.09\,\text{meV}$
H	3.509 014	−0.901 902	−1.314 607
C	3.430 433	−0.050 174	−0.631 678
H	3.068 639	−0.400 207	0.345 275
H	4.405 170	0.449 053	−0.536 494
O	2.474 905	0.865 478	−1.235 034
H	2.313 251	1.595 771	−0.611 831
Ni	−1.212 594	1.698 051	−1.368 883
Ni	−1.581 396	−0.571 089	−1.511 152
Ni	−1.887 878	−2.771 211	−1.027 649
Ni	0.606 227	0.133 859	−1.474 104
Ni	−0.003 713	−1.719 422	0.008 708
Ni	−2.909 339	0.785 099	−0.055 542
Ni	−3.742 509	−1.325 941	−0.770 185
Ni	−0.600 823	0.541 673	0.537 747
Ni	−2.234 108	0.437 018	2.226 597
Ni	−4.243 974	−0.426 713	1.386 462
Ni	−0.327 125	−1.003 853	2.220 243
Ni	−2.177 488	−1.429 956	0.904 326
Ni	0.064 338	−2.043 144	−2.262 230

CH_3OH/Ni_{13}	$E_{tot} = -543\,481.10\,\text{eV}$		$\Delta E_{tot} = 3.30\,\text{meV}$
H	2.318 730	2.528 976	0.049 183
C	2.951 403	1.636 528	0.009 378
H	4.005 820	1.926 992	−0.100 426
H	2.795 578	1.043 182	0.921 261
O	2.528 142	0.894 110	−1.167 399
H	3.021 856	0.055 766	−1.199 571
Ni	−1.333 882	1.523 656	−0.706 133
Ni	−1.459 838	−0.742 690	−1.069 325
Ni	−1.456 655	−3.003 197	−0.812 054
Ni	0.626 497	0.207 886	−1.183 077
Ni	0.402 179	−1.842 613	0.132 135
Ni	−2.757 102	0.282 802	0.657 819
Ni	−3.420 343	−1.836 212	−0.206 571
Ni	−0.381 618	0.259 686	0.974 979
Ni	−1.781 545	−0.217 191	2.803 791
Ni	−3.765 694	−1.224 941	2.083 511
Ni	0.260 696	−1.399 758	2.434 303
Ni	−1.674 404	−1.917 285	1.279 952
Ni	0.243 810	−1.916 056	−2.162 184

CH_3OH/Ni_{13} $E_{tot} = -543\,481.07\,\text{eV}$ $\Delta E_{tot} = 36.02\,\text{meV}$

H	2.218 804	−2.082 950	−2.017 513
C	1.620 268	−2.641 411	−1.290 733
H	1.781 425	−3.720 729	−1.422 104
H	1.893 067	−2.322 005	−0.274 727
O	0.231 470	−2.318 753	−1.575 443
H	−0.327 124	−2.746 421	−0.901 839
Ni	−1.350 706	3.752 789	0.490 391
Ni	−0.938 355	1.749 162	−0.664 861
Ni	−0.290 802	−0.372 555	−1.249 300
Ni	0.764 319	3.250 943	−0.445 003
Ni	1.275 975	0.940 660	0.077 133
Ni	−2.273 817	1.776 354	1.317 760
Ni	−2.451 509	0.000 653	−0.264 570
Ni	0.042 467	2.296 001	1.612 140
Ni	−1.006 015	0.835 214	3.138 882
Ni	−2.721 784	−0.355 275	2.101 901
Ni	1.226 336	0.450 231	2.361 668
Ni	−0.607 792	−0.102 177	1.093 485
Ni	0.913 771	1.610 267	−2.087 271

CH_3OH/Ni_{13}	$E_{tot} = -543\,480.70\,\text{eV}$	$\Delta E_{tot} = 402.21\,\text{meV}$	
H	−2.505 666	−1.341 619	1.879 734
C	−1.757 001	−1.994 016	1.416 278
H	−1.716 134	−2.950 432	1.957 674
H	−2.027 143	−2.157 805	0.362 174
O	−0.493 664	−1.303 543	1.532 710
H	0.200 022	−1.829 599	1.092 241
Ni	0.890 894	3.633 759	−2.095 005
Ni	0.517 779	1.366 870	−2.145 879
Ni	0.319 902	−0.833 052	−1.631 689
Ni	2.704 461	2.103 439	−2.037 972
Ni	2.104 328	0.290 048	−0.509 837
Ni	−0.850 125	2.717 395	−0.786 811
Ni	−1.589 214	0.555 517	−1.431 499
Ni	1.408 495	2.531 574	−0.130 902
Ni	−0.241 629	2.502 543	1.545 386
Ni	−2.221 031	1.601 164	0.647 914
Ni	1.718 005	1.138 431	1.648 550
Ni	−0.144 992	0.495 661	0.380 762
Ni	2.238 770	−0.088 904	−2.777 659

S9.2.4 Mol/Cu_{13}

CH_4/Cu_{13}	$E_{tot} = -589\,287.47$ eV	$\Delta E_{tot} = 0.00$ meV	
H	3.301 721	−1.123 348	1.612 911
C	2.779 947	−0.380 261	2.224 497
H	3.389 381	−0.062 634	3.077 045
H	2.577 965	0.507 125	1.592 046
H	1.853 925	−0.847 524	2.619 385
Cu	−1.437 539	−1.172 001	−1.670 668
Cu	−3.410 668	−0.319 625	1.692 569
Cu	−1.450 627	1.092 736	−2.619 179
Cu	−0.319 064	2.180 378	3.091 247
Cu	0.484 920	0.400 636	1.710 076
Cu	−1.431 431	−0.085 299	3.151 461
Cu	0.391 357	2.604 739	−1.796 709
Cu	−1.760 657	2.604 955	−0.756 971
Cu	0.241 492	2.664 180	0.699 402
Cu	−0.214 223	0.621 987	−0.621 127
Cu	−1.794 450	1.448 394	1.366 152
Cu	−1.312 924	−1.005 025	0.808 745
Cu	−2.822 925	0.432 397	−0.593 800

CH_4/Cu_{13}	$E_{tot} = -589\,287.41$ eV		$\Delta E_{tot} = 59.39$ meV
H	−3.384 237	0.052 738	0.493 906
C	−3.559 292	1.149 510	0.451 639
H	−4.201 151	1.425 033	1.295 136
H	−2.624 892	1.744 735	0.518 256
H	−4.038 771	1.376 040	−0.506 576
Cu	0.306 700	−2.846 533	−1.411 585
Cu	−1.362 197	0.140 278	0.680 305
Cu	1.610 266	−1.449 873	−2.973 085
Cu	2.378 386	1.451 820	2.130 686
Cu	2.301 773	−0.897 508	1.693 133
Cu	0.267 327	0.120 188	2.540 183
Cu	3.841 823	−0.613 907	−2.124 692
Cu	1.881 015	0.706 069	−1.891 422
Cu	3.414 797	0.558 899	0.036 067
Cu	2.162 316	−1.479 517	−0.646 285
Cu	0.962 429	0.753 037	0.346 302
Cu	0.180 954	−1.667 900	0.776 829
Cu	−0.137 244	−0.523 108	−1.408 795

CH_4/Cu_{13}	$E_{tot} = -589\,287.40$ eV		$\Delta E_{tot} = 73.15$ meV
H	−2.276 376	0.541 849	−1.594 787
C	−2.895 330	−0.353 763	−1.761 548
H	−2.430 512	−1.242 139	−1.301 582
H	−3.879 754	−0.196 615	−1.307 002
H	−2.986 571	−0.525 245	−2.839 709
Cu	0.641 081	−2.476 577	−0.489 102
Cu	−1.512 218	−0.074 094	1.914 012
Cu	1.265 453	−0.790 642	−2.160 006
Cu	1.817 407	2.272 249	2.872 983
Cu	2.360 989	−0.011 113	2.404 374
Cu	0.262 843	0.410 178	3.524 604
Cu	3.275 860	0.610 631	−1.565 443
Cu	1.060 197	1.357 889	−1.067 822
Cu	2.795 842	1.669 973	0.650 274
Cu	2.080 717	−0.628 144	0.083 763
Cu	0.440 831	1.188 400	1.260 836
Cu	0.465 135	−1.372 281	1.736 474
Cu	−0.485 595	−0.380 557	−0.360 317

CH_4/Cu_{13}	$E_{tot} = -589\,287.36\,\text{eV}$		$\Delta E_{tot} = 113.43\,\text{meV}$
H	−2.026 018	0.384 529	−3.794 985
C	−1.383 482	0.052 196	−4.625 838
H	−0.398 911	−0.282 457	−4.253 053
H	−1.867 947	−0.787 113	−5.136 791
H	−1.226 377	0.890 861	−5.312 780
Cu	−1.032 357	−1.849 550	−0.492 902
Cu	−3.493 140	0.127 795	1.974 935
Cu	−0.545 781	0.009 863	−2.018 684
Cu	−0.464 251	2.747 776	3.246 531
Cu	0.325 368	0.581 591	2.619 554
Cu	−1.843 035	0.707 772	3.701 643
Cu	1.283 288	1.572 940	−1.263 920
Cu	−1.005 899	2.044 732	−0.781 390
Cu	0.642 807	2.412 868	1.013 792
Cu	0.194 101	0.091 684	0.251 871
Cu	−1.668 619	1.646 224	1.507 959
Cu	−1.376 723	−0.932 321	1.809 304
Cu	−2.357 243	0.103 440	−0.240 755

CH_4/Cu_{13}	$E_{tot} = -589\,287.35\,\text{eV}$		$\Delta E_{tot} = 119.18\,\text{meV}$
H	1.030 050	4.145 128	2.727 318
C	0.586 296	3.186 154	3.015 316
H	0.077 687	3.256 418	3.982 832
H	−0.160 626	2.902 792	2.248 611
H	1.401 099	2.440 161	3.104 340
Cu	1.119 044	−3.917 076	−1.634 547
Cu	−1.808 314	−2.040 551	0.333 743
Cu	1.583 441	−2.159 805	−3.271 660
Cu	0.733 950	1.071 288	1.658 279
Cu	1.811 497	−1.047 956	1.353 586
Cu	−0.456 543	−1.118 686	2.165 128
Cu	3.133 847	−0.319 427	−2.483 705
Cu	0.764 358	−0.094 384	−2.318 026
Cu	2.132 943	0.636 147	−0.404 189
Cu	2.044 679	−1.784 253	−0.946 152
Cu	−0.110 363	−0.356 087	−0.070 352
Cu	0.416 429	−2.849 027	0.514 030
Cu	−0.422 406	−2.117 132	−1.729 689

CO/Cu_{13}	$E_{tot} = -591\,271.22\,\mathrm{eV}$	$\Delta E_{tot} = 0.00\,\mathrm{meV}$	
C	2.265 718	−0.659 845	2.358 313
O	3.122 791	−1.193 628	2.907 517
Cu	−0.851 758	−2.494 804	−1.483 619
Cu	−3.090 606	−0.015 074	0.691 027
Cu	−0.222 601	−0.861 925	−3.202 421
Cu	0.247 975	2.337 531	1.745 968
Cu	0.877 715	0.049 152	1.433 062
Cu	−1.353 212	0.485 086	2.403 576
Cu	1.771 777	0.550 935	−2.623 758
Cu	−0.457 133	1.322 264	−2.192 456
Cu	1.278 657	1.672 967	−0.440 526
Cu	0.556 553	−0.623 785	−0.948 303
Cu	−1.049 179	1.149 823	0.143 331
Cu	−1.092 007	−1.317 321	0.687 513
Cu	−2.004 689	−0.401 377	−1.479 224

CO/Cu_{13}	$E_{tot} = -591\,271.06\,\mathrm{eV}$		$\Delta E_{tot} = 153.88\,\mathrm{meV}$
C	−0.917 807	−2.666 576	1.666 213
O	−1.054 965	−3.697 794	2.158 108
Cu	−0.397 994	−2.162 749	−1.403 598
Cu	−2.475 195	0.489 053	0.893 046
Cu	0.269 132	−0.540 255	−3.083 650
Cu	0.945 049	2.725 929	1.784 377
Cu	1.369 874	0.371 584	1.442 486
Cu	−0.700 092	0.959 832	2.536 925
Cu	2.319 099	0.755 950	−2.527 065
Cu	0.137 249	1.674 922	−2.107 350
Cu	1.887 176	1.946 215	−0.381 323
Cu	1.080 007	−0.350 546	−0.826 699
Cu	−0.444 733	1.558 581	0.240 960
Cu	−0.592 054	−1.043 272	0.902 884
Cu	−1.424 747	−0.020 876	−1.295 319

CO/Cu_{13}	$E_{tot} = -591\,271.02\,\mathrm{eV}$		$\Delta E_{tot} = 197.09\,\mathrm{meV}$
C	−2.889 956	−0.714 600	−0.765 609
O	−4.022 663	−0.732 067	−1.041 778
Cu	0.332 863	−2.528 527	−0.989 289
Cu	−2.118 917	−0.293 902	1.159 045
Cu	0.800 377	−0.800 718	−2.679 378
Cu	1.030 383	2.280 588	2.398 477
Cu	1.758 314	0.064 807	1.953 845
Cu	−0.490 222	0.330 943	2.914 787
Cu	2.719 096	0.696 685	−2.052 105
Cu	0.434 489	1.328 372	−1.597 726
Cu	2.108 166	1.749 189	0.172 602
Cu	1.547 345	−0.554 161	−0.401 991
Cu	−0.186 146	1.140 960	0.704 908
Cu	0.011 519	−1.438 322	1.226 325
Cu	−1.034 649	−0.529 246	−1.002 113

CO/Cu_{13}	$E_{tot} = -591\,271.00\,\mathrm{eV}$		$\Delta E_{tot} = 211.00\,\mathrm{meV}$
C	2.273 526	2.627 178	−0.096 146
O	2.959 894	3.550 241	−0.140 189
Cu	−0.784 627	−3.017 159	−1.253 302
Cu	−3.082 444	−0.677 938	1.124 719
Cu	−0.172 442	−1.290 676	−2.844 890
Cu	0.190 686	1.501 048	2.421 896
Cu	0.808 580	−0.684 804	1.747 965
Cu	−1.346 124	−0.407 481	2.852 895
Cu	1.799 693	0.026 596	−2.196 200
Cu	−0.430 452	0.853 727	−1.711 838
Cu	1.294 857	1.106 659	0.073 789
Cu	0.591 359	−1.174 871	−0.567 655
Cu	−1.073 678	0.548 221	0.632 982
Cu	−1.080 517	−2.025 246	1.021 167
Cu	−1.948 312	−0.935 495	−1.065 195

CO/Cu_{13}	$E_{tot} = -591\,270.67\,\text{eV}$		$\Delta E_{tot} = 548.12\,\text{meV}$
C	2.181 107	−1.248 371	−1.440 366
O	3.101 280	−1.921 651	−1.686 942
Cu	−1.510 449	−2.020 058	−1.247 182
Cu	−2.963 783	0.388 586	1.499 492
Cu	−0.572 180	−0.219 030	−2.655 629
Cu	0.756 008	1.869 175	2.698 469
Cu	0.835 488	−0.358 665	1.814 170
Cu	−1.092 975	0.187 499	3.106 235
Cu	1.683 796	0.618 797	−1.988 515
Cu	−0.275 493	1.763 709	−1.310 096
Cu	1.494 296	1.528 167	0.347 723
Cu	0.530 673	−0.911 754	−0.523 777
Cu	−0.844 983	1.373 918	1.016 237
Cu	−1.270 768	−1.275 344	1.103 718
Cu	−2.052 017	0.225 024	−0.733 535

H_2/Cu_{13}	$E_{tot} = -588\,217.47\,\mathrm{eV}$		$\Delta E_{tot} = 0.00\,\mathrm{meV}$
H	0.216 940	2.750 773	−1.600 349
H	0.886 024	2.574 807	−2.017 275
Cu	−1.055 475	−2.569 665	−1.392 368
Cu	−2.818 278	−0.048 091	1.141 808
Cu	0.228 589	−0.867 595	−2.656 470
Cu	0.820 724	1.022 758	2.927 246
Cu	0.791 347	−1.205 058	2.055 955
Cu	−1.267 135	−0.376 034	3.015 158
Cu	2.437 846	−0.206 392	−1.598 265
Cu	0.477 223	1.101 298	−1.214 994
Cu	1.938 490	0.556 040	0.737 454
Cu	0.697 556	−1.267 225	−0.357 788
Cu	−0.521 476	0.663 729	0.989 837
Cu	−1.270 870	−1.850 306	0.958 094
Cu	−1.561 505	−0.279 039	−0.988 043

H_2/Cu_{13}	$E_{tot} = -588\,217.36\,\mathrm{eV}$		$\Delta E_{tot} = 106.02\,\mathrm{meV}$
H	−1.460 640	−3.340 199	−1.699 479
H	−1.622 875	−3.393 868	−0.913 360
Cu	−1.042 078	−1.777 228	−1.098 637
Cu	−2.386 557	1.165 540	1.270 583
Cu	0.199 569	−0.297 555	−2.667 435
Cu	1.548 743	2.175 014	2.541 423
Cu	1.258 479	−0.102 970	1.960 920
Cu	−0.643 967	0.984 842	3.012 915
Cu	2.551 785	0.313 300	−1.921 998
Cu	0.701 272	1.764 165	−1.472 349
Cu	2.351 649	1.390 669	0.322 411
Cu	0.907 746	−0.495 342	−0.401 834
Cu	−0.065 431	1.730 288	0.816 412
Cu	−0.937 266	−0.698 769	1.169 476
Cu	−1.360 428	0.582 115	−0.919 049

H_2/Cu_{13}	$E_{tot} = -588\,217.36\,\mathrm{eV}$		$\Delta E_{tot} = 108.64\,\mathrm{meV}$
H	−1.894 615	−2.348 451	1.290 687
H	−1.948 007	−2.530 284	0.505 383
Cu	−0.674 375	−1.724 905	−1.928 477
Cu	−2.438 069	0.927 648	0.610 341
Cu	0.733 131	−0.079 212	−3.051 156
Cu	1.170 114	1.819 534	2.524 913
Cu	1.045 947	−0.433 878	1.681 993
Cu	−0.993 146	0.512 635	2.554 912
Cu	2.888 193	0.406 739	−1.886 151
Cu	0.970 054	1.825 117	−1.583 972
Cu	2.327 577	1.234 425	0.397 096
Cu	1.066 833	−0.583 277	−0.720 808
Cu	−0.109 364	1.461 868	0.549 849
Cu	−1.030 491	−1.048 768	0.511 608
Cu	−1.113 784	0.560 807	−1.456 220

H_2/Cu_{13}	$E_{tot} = -588\,217.28\,\mathrm{eV}$		$\Delta E_{tot} = 184.92\,\mathrm{meV}$
H	3.235 429	0.017 465	−2.758 886
H	3.575 133	0.341 438	−2.110 225
Cu	−1.527 252	−2.312 278	−0.968 308
Cu	−3.409 278	0.496 038	1.173 456
Cu	−0.296 956	−0.820 271	−2.491 145
Cu	0.205 797	2.049 014	2.676 212
Cu	0.269 903	−0.292 017	2.205 000
Cu	−1.830 818	0.572 329	3.032 369
Cu	1.921 292	0.098 006	−1.604 049
Cu	−0.158 768	1.302 324	−1.366 360
Cu	1.321 959	1.241 518	0.593 539
Cu	0.220 629	−0.827 729	−0.168 986
Cu	−1.144 003	1.306 500	0.852 000
Cu	−1.748 365	−1.201 456	1.238 971
Cu	−2.150 702	−0.020 721	−0.925 497

H_2/Cu_{13}	$E_{tot} = -588\,217.28\,\mathrm{eV}$	$\Delta E_{tot} = 191.94\,\mathrm{meV}$	
H	−0.518 383	−1.347 039	−3.835 271
H	0.105 245	−0.891 760	−4.029 272
Cu	−0.769 944	−2.391 719	−0.509 639
Cu	−2.644 389	0.401 133	1.706 384
Cu	0.146 497	−0.890 034	−2.262 005
Cu	0.939 511	2.263 236	2.805 608
Cu	1.157 447	−0.085 625	2.384 539
Cu	−0.900 879	0.722 937	3.411 573
Cu	2.336 873	0.219 437	−1.548 911
Cu	0.251 381	1.311 983	−1.171 665
Cu	1.935 620	1.427 780	0.633 303
Cu	0.880 525	−0.750 120	0.051 959
Cu	−0.493 551	1.341 488	1.134 591
Cu	−0.873 300	−1.181 158	1.697 619
Cu	−1.552 652	−0.150 539	−0.468 815

CH_3OH/Cu_{13}	$E_{tot} = -591\,335.84\,\text{eV}$	$\Delta E_{tot} = 0.00\,\text{meV}$	
H	2.326 188	−0.779 103	2.488 125
C	1.740 236	−1.539 306	1.961 450
H	2.011 712	−1.533 327	0.895 200
H	1.931 858	−2.526 936	2.404 218
O	0.347 725	−1.177 177	2.145 057
H	−0.202 731	−1.813 185	1.655 309
Cu	−2.788 957	−0.607 451	−1.900 524
Cu	−3.230 862	2.915 167	−0.063 323
Cu	−1.032 946	0.091 469	−3.477 192
Cu	0.678 208	2.770 021	1.527 493
Cu	−0.288 379	0.611 326	1.253 153
Cu	−1.804 770	2.407 356	1.892 006
Cu	1.308 577	−0.001 125	−2.525 040
Cu	0.027 010	2.023 167	−2.484 070
Cu	1.335 552	1.416 956	−0.470 881
Cu	−0.605 494	0.016 583	−1.118 253
Cu	−0.855 241	2.519 852	−0.284 603
Cu	−2.528 863	0.660 725	0.218 157
Cu	−2.340 102	1.727 774	−2.050 104

CH_3OH/Cu_{13}	$E_{tot} = -591\,335.80\,\text{eV}$	$\Delta E_{tot} = 38.87\,\text{meV}$	
H	−3.501 401	−0.430 978	0.897 441
C	−3.050 952	0.266 221	1.611 572
H	−2.592 256	1.100 612	1.062 206
H	−3.820 735	0.629 764	2.306 178
O	−2.048 080	−0.491 589	2.340 737
H	−1.643 406	0.092 204	3.004 747
Cu	0.317 919	−2.231 437	−2.575 394
Cu	−0.421 020	−1.196 406	1.241 273
Cu	0.032 751	0.008 619	−3.572 317
Cu	2.971 341	1.289 658	1.405 951
Cu	3.221 042	−0.547 646	−0.106 381
Cu	1.940 667	−0.957 068	1.909 862
Cu	2.028 684	1.545 941	−3.451 778
Cu	0.353 522	1.605 419	−1.769 000
Cu	2.718 014	1.676 925	−1.058 157
Cu	1.855 976	−0.419 918	−2.086 290
Cu	0.992 262	0.551 791	0.308 460
Cu	1.229 595	−1.954 663	−0.273 301
Cu	−0.583 922	−0.537 453	−1.195 808

CH_3OH/Cu_{13}	$E_{tot} = -591\,335.72\,\text{eV}$	$\Delta E_{tot} = 117.66\,\text{meV}$	
H	3.653 181	−0.286 471	−0.608 887
C	3.132 128	−1.085 802	−1.146 061
H	3.865 537	−1.782 647	−1.575 153
H	2.459 728	−1.606 337	−0.449 534
O	2.384 358	−0.439 326	−2.210 587
H	1.886 897	−1.121 742	−2.693 493
Cu	−2.646 434	−1.434 934	−1.075 474
Cu	−3.887 495	0.704 486	2.025 261
Cu	−1.520 605	0.362 992	−2.312 617
Cu	0.022 227	1.637 041	3.272 501
Cu	−0.178 879	−0.467 943	2.169 237
Cu	−2.043 038	0.196 180	3.553 284
Cu	0.859 724	0.882 195	−1.574 835
Cu	−0.984 671	2.081 317	−0.710 560
Cu	0.734 812	1.434 745	0.894 543
Cu	−0.676 707	−0.332 903	−0.185 806
Cu	−1.644 055	1.494 125	1.564 897
Cu	−2.402 872	−1.016 275	1.367 475
Cu	−3.013 832	0.781 292	−0.304 189

CH_3OH/Cu_{13}	$E_{tot} = -591\,335.70\,\text{eV}$		$\Delta E_{tot} = 145.39\,\text{meV}$
H	2.102 597	1.385 947	2.676 646
C	2.769 394	0.769 023	2.064 303
H	3.815 494	0.981 523	2.326 311
H	2.540 180	−0.292 217	2.238 690
O	2.515 436	1.141 930	0.688 409
H	3.060 775	0.586 462	0.101 201
Cu	−1.835 609	−2.845 023	−2.144 906
Cu	−4.135 524	0.012 446	−0.495 780
Cu	−0.464 689	−1.315 469	−3.481 679
Cu	−1.023 967	1.642 848	1.679 353
Cu	−0.743 838	−0.712 378	1.270 687
Cu	−2.978 051	0.107 483	1.648 763
Cu	1.513 844	−0.415 133	−2.276 897
Cu	−0.518 065	0.832 234	−2.371 665
Cu	0.591 542	0.840 486	−0.147 036
Cu	−0.328 500	−1.294 309	−1.056 002
Cu	−1.860 424	0.815 719	−0.376 469
Cu	−2.514 768	−1.686 390	−0.052 289
Cu	−2.505 828	−0.555 181	−2.291 638

CH_3OH/Cu_{13}	$E_{tot} = -591\,335.52\,\text{eV}$	$\Delta E_{tot} = 322.46\,\text{meV}$	
H	2.870 386	−1.438 245	−1.589 976
C	2.610 001	−1.602 275	−0.537 568
H	3.187 942	−2.456 702	−0.152 930
H	2.859 304	−0.693 534	0.033 503
O	1.198 948	−1.876 813	−0.506 750
H	0.915 440	−1.957 451	0.422 969
Cu	−2.139 428	−1.387 427	−1.357 534
Cu	−3.825 241	0.996 017	1.344 872
Cu	−1.186 027	0.367 996	−2.789 705
Cu	−0.160 125	2.626 315	2.586 343
Cu	−0.022 283	0.373 676	1.821 510
Cu	−2.025 307	0.969 877	3.009 800
Cu	1.010 831	1.396 452	−2.087 980
Cu	−1.041 627	2.350 326	−1.412 718
Cu	0.721 829	2.141 543	0.284 023
Cu	−0.296 782	0.029 289	−0.588 919
Cu	−1.687 685	2.003 297	0.874 435
Cu	−2.076 706	−0.585 313	1.004 265
Cu	−2.827 052	0.820 974	−0.913 621

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