catalysts

Supplementary Material: Conversion of Carbon Monoxide into Methanol on Alumina-Supported Cobalt Catalyst: Role of the Support and Reaction Mechanism—A Theoretical Study

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Tables:

Table S1. The calculated energy ($E_{cluster}$) of Co_4 clusters with different number of unpaired electrons

Number of unpaired electrons	$E_{cluster}$, eV
10	-2871.125081
12	-2873.933653
14	-2872.605828

Table S2. The calculated interaction energy (E_{int}) between Co_4 cluster and Al_2O_3.

The interaction energy E_{int} is calculated by formula: $E_{int} = E(Co_4\text{-}Al_2O_3) - E(Co_4) - E(Al_2O_3)$.

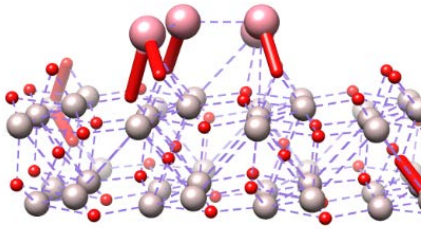
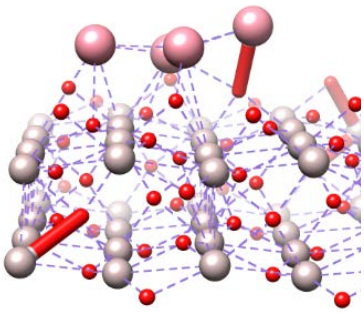
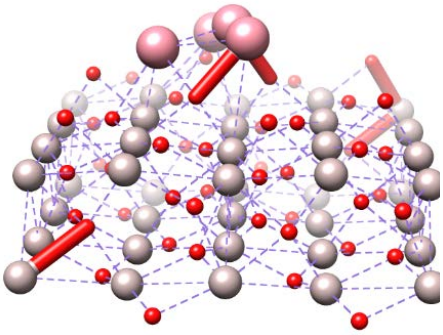
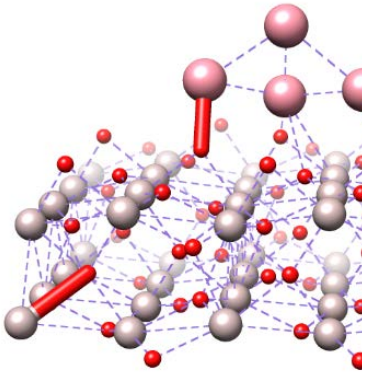
Structure	E_{int}, kJ.mol^{-1}	Structure	E_{int}, kJ.mol^{-1}
	-1027.3		-1023.3
	-1023.5		-1050.4

Table S3. The calculated adsorption energies (E_{ads}) for the adsorption of CO on Co_4 and Co_4/Al_2O_3 systems.

E_{ads} = E(CO-Adsorbent) - E(CO) - E(Adsorbent), where adsorbent: Co_4 or Co_4/Al_2O_3.

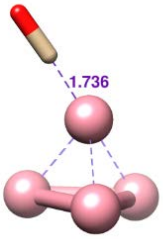
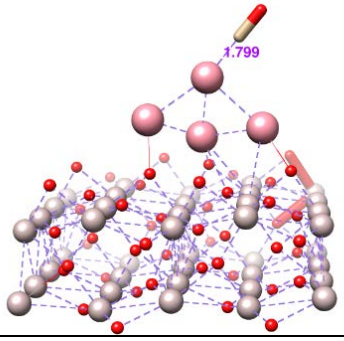
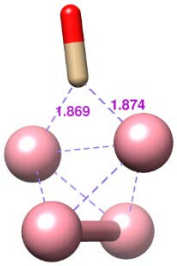
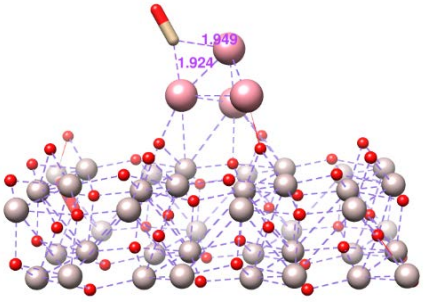
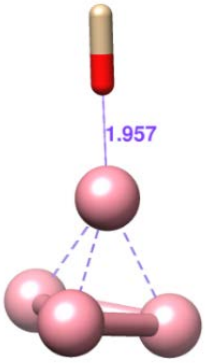
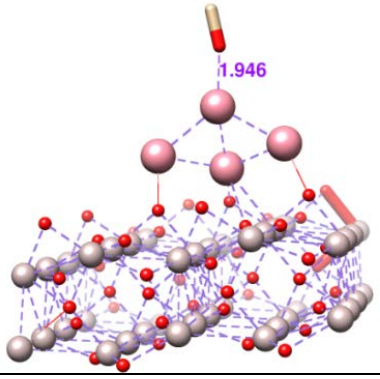
Adsoprtion of CO on Co_4			
C–Co Configurations			
Structure	**E_{ads}, kJ.mol^{-1}**	**Structure**	**E_{ads}, kJ.mol^{-1}**
d-1 configurations			
	-186.9		-231.9
d-2 configurations			
	-201.4		-237.3
O–Co Configurations			
Structure	**E_{ads}, kJ.mol^{-1}**	**Structure**	**E_{ads}, kJ.mol^{-1}**
	+21.8		-58.8

Table S4. The calculated adsorption energies (E_{ads}) for the adsorption of H_2 on Co_4 and Co_4/Al_2O_3 system.

E_{ads} = E(H_2-adsorbent) - E(CO) - E(adsorbent), where adsorbent: Co_4 or Co_4/Al_2O_3.

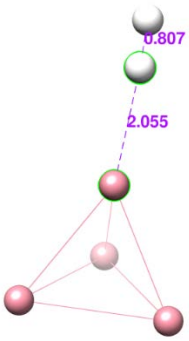
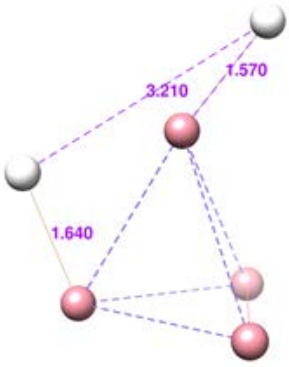
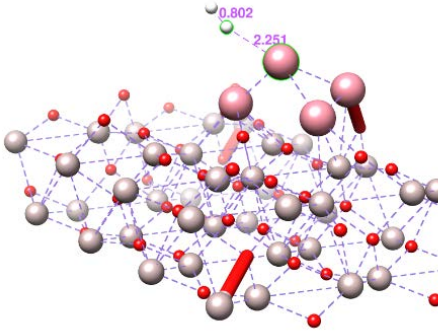
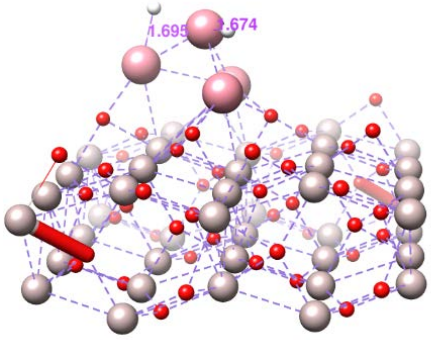
Structure	E_{ads}, kJ.mol^{-1}	Structure	E_{ads}, kJ.mol^{-1}
Molecular adsorption		**Dissociative chemisorption**	
	+32.0		-99.9
	-110.4		-280.7

Table S5. The calculated adsorption energies (E_{ads}) for the adsorption of CO and H_2 on Al_2O_3 system.

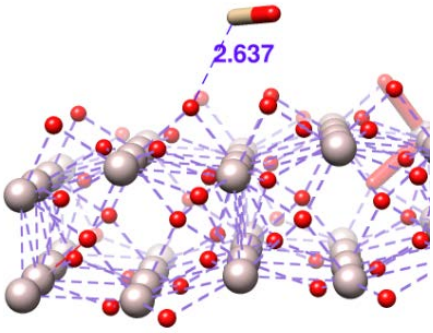
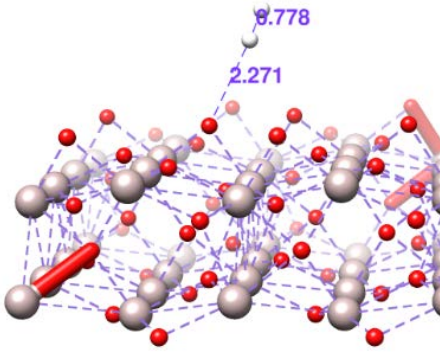
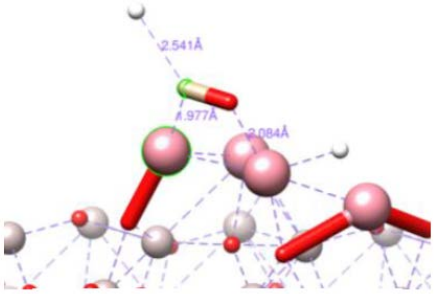
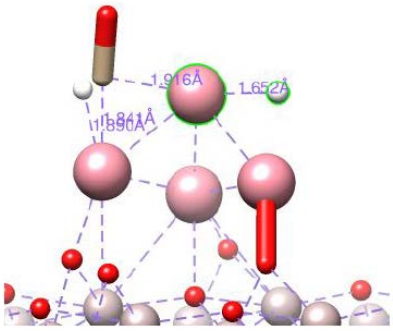
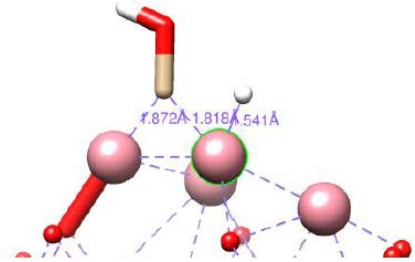
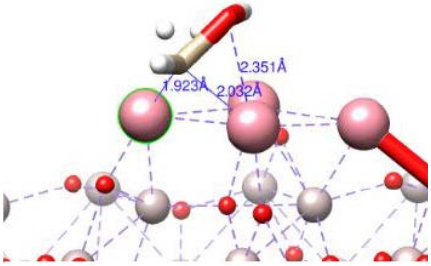
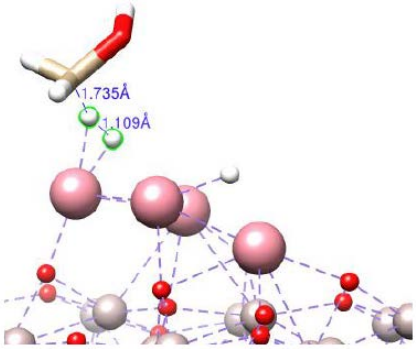
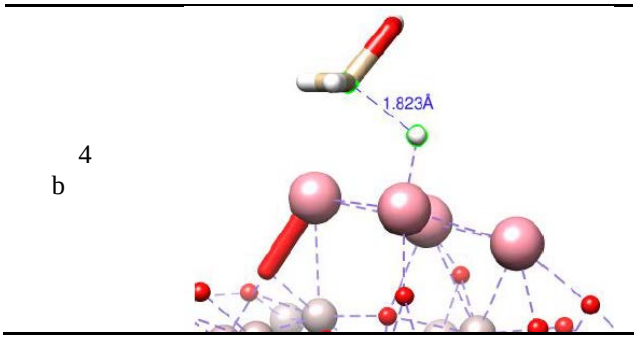
Structure	$E_{ads\ (CO)}$, kJ.mol^{-1}	Structure	$E_{ads}(H_2)$, kJ.mol^{-1}
	-59.8		-32.7

Table S6. Transition state structures of CO hydrogenation on Co_4/Al_2O_3

Step	Transition State Structure
1a	
1 b	
2	
3a	
4a	



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b