

Kinetics and Thermodynamics of CO Oxidation by $(\text{TiO}_2)_6$

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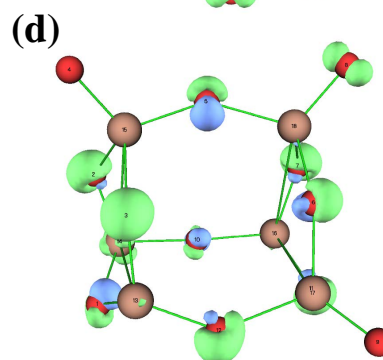
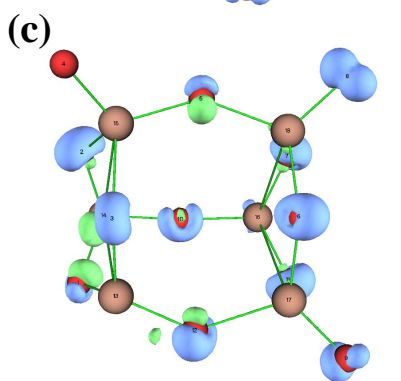
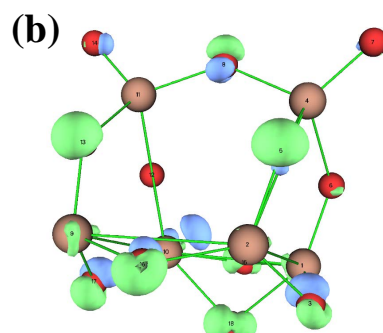
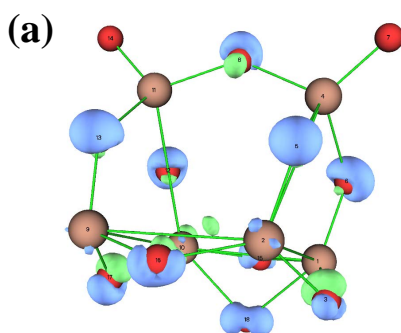
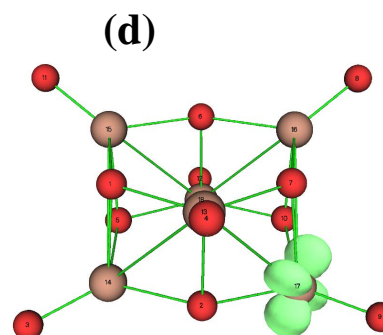
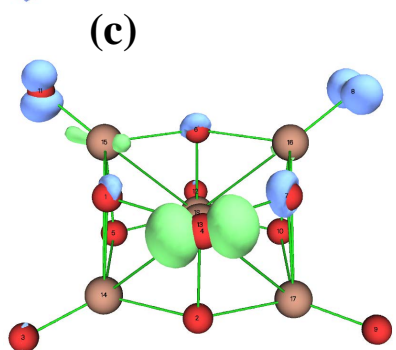
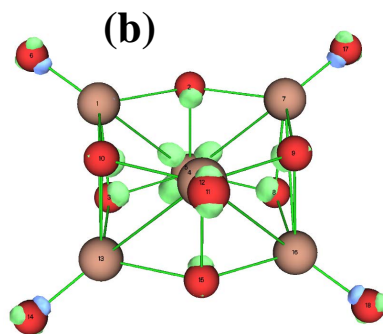
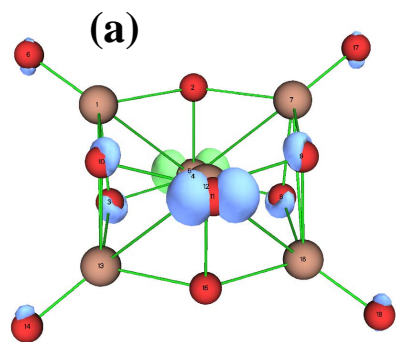
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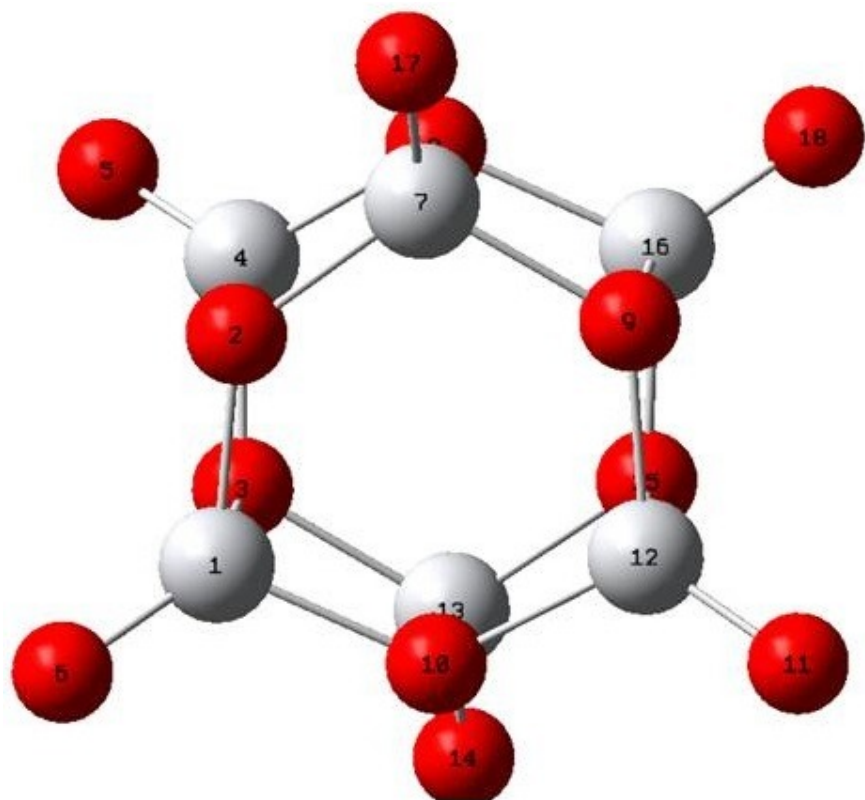
Abstract

Molecular level insights into the mechanism and thermodynamics of CO oxidation by a $(\text{TiO}_2)_6$ cluster have been obtained through density functional calculations. Thereby, we have considered as an example, two different structural isomers of $(\text{TiO}_2)_6$ with the purpose of understanding the interplay between local structure and activity for the CO oxidation reaction. Active sites in the two isomeric forms were identified on the basis of global and local reactivity descriptors. For the oxidation of CO to CO₂ we considered both sequential and simultaneous adsorption of CO and O₂ on $(\text{TiO}_2)_6$ cluster through the ER and LH mechanisms, respectively. Three different pathways were obtained for CO oxidation by $(\text{TiO}_2)_6$ cluster, and the mechanistic route of each pathway were identified by locating the transition-state and intermediate structures. The effects of temperature on the rate of the reaction was investigated within the harmonic approximation. The structure-dependent activity of the cluster was rationalized through reactivity descriptors and analysis of the frontier orbitals. Finally, we also considered the effects of a support, i.e., graphene, on the oxidation mechanism.

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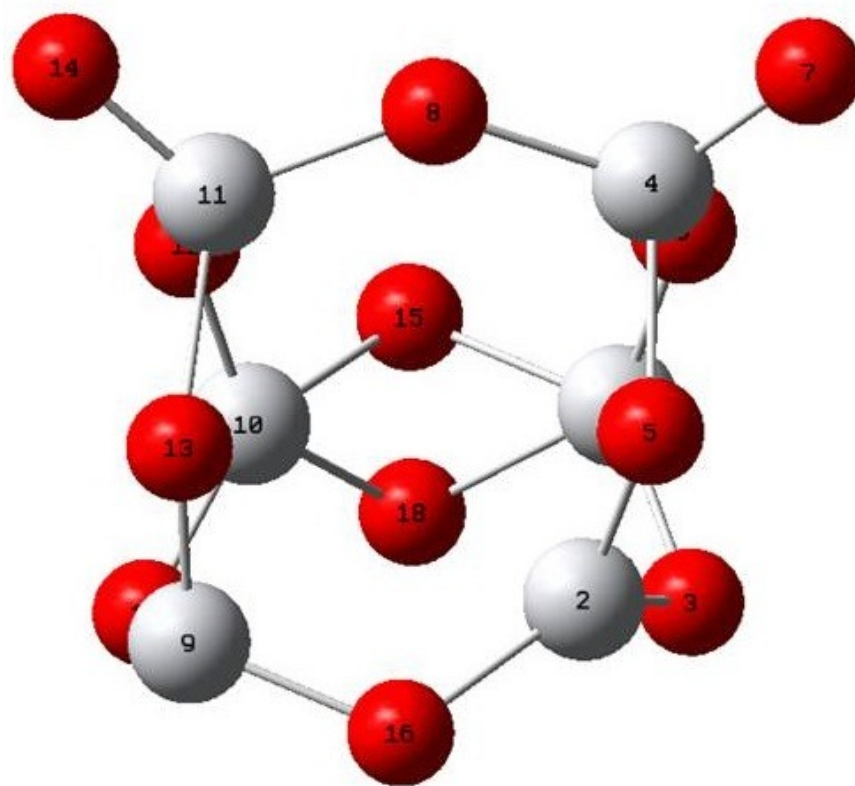
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S1(D_{3d})

E=0.00 eV



S2 (Cs)

E=4.21 eV

