

Adsorption of Atmospheric Gases Using Atomic Clusters

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Abstract : First principles simulation, meaning density functional theory (DFT) calculations with plane waves and pseudopotential, has become a prized technique in condensed matter theory. Nanoparticles (NP) have been known to possess good catalytic activities, especially for molecules such as CO, O₂, etc. Among the metal NPs, Aluminium based NPs are also widely known for their catalytic properties. Aluminium metal is a lightweight, excellent electrical, and thermal abundant chemical element in the earth's crust. Aluminium NPs, when added to solid rocket fuel, help improve the combustion speed and considerably increase combustion heat and combustion stability. Adding aluminium NPs into normal Al/Al₂O₃ powder improves the sintering processes of the ceramics, with high heat transfer performance, increased density, and enhanced thermal conductivity of the sinter. We used VASP and Gaussian 03 package to compute the geometries, electronic structure, and bonding properties of Al₁₂Ni as well as its interaction with O₂ and CO molecules. Several MD simulations were carried out using VASP at various temperatures from which hundreds of structures were optimized, leading to 24 unique structures. These structures were then further optimized through a Gaussian package. The lowest energy structure of Al₁₂Ni has been reported to be a singlet. However, through our extensive search, we found a triplet state to be lower in energy. In our structure, the Ni atom is found to be on the surface, which gives the non-zero magnetic moment. Incidentally, O₂ and CO molecules are also triplet in nature, due to which the Al₁₂-Ni cluster is likely to facilitate the oxidation process of the CO molecule. Our results show that the most favourable site for the CO molecule is the Ni atom and that for the O₂ molecule is the Al atom that is nearest to the Ni atom. Al₁₂Ni-O₂ and Al₁₂-Ni-CO structures we extracted using VMD. Al₁₂Ni nanocluster, due to its triplet electronic structure configuration, indicates it to be a potential candidate as a catalyst for oxidation of CO molecules.

Keywords : catalyst, gaussian, nanoparticles, oxidation

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