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Adsorption of Atmospheric Gases Using Atomic Clusters

Authors : Vidula Shevade, B. J. Nagare, Sajeev Chacko

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, O_2, 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/Al_2O_3 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 0_3 package to compute the geometries, electronic structure, and bonding properties of $Al_{12}Ni$ as well as its interaction with O_2 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 $Al_{12}Ni$ 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 Al_{12}-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 O_2 molecule is the Al atom that is nearest to the Ni atom. $Al_{12}Ni$-O_2 and Al_{12}-Ni-CO structures we extracted using VMD. $Al_{12}Ni$ nanocluster, due to in triplet electronic structure configuration, indicates it to be a potential candidate as a catalyst for oxidation of CO molecules.

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