

The interaction of Phosgene gas with the pristine and B-doped Si₁₂C₁₂ nanocluster: A DFT, TD-DFT, RDG and AIM

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Abstract

Fullerenes are also a well-known class of carbon-based and SiC nanostructures with a cage-shaped configuration, employed in diverse applications, including superconductors [1], gas storage [2], nano-electronic magnetic devices, biotechnology [3–4]. In this project, we investigated the effects of B doped, and phosgene adsorption on the structural and electrical properties of SiC nano cluster by using density functional theory method. At the first time, we examined different configurations for adsorbing phosgene on the outer surface of nano cluster, after optimizing all models; we selected 15 stable models for this study. From optimized models the quantum parameters, RDG, NMR, HOMO-LUMO orbitals and thermodynamic properties are calculated by using cam-B3LYP/6-31G (d,p) level of theory. The calculated results indicated that the bond angle and bond length of nanocluster around doping and adsorbing position increase significantly from original values. The result of NMR graphs reveal that the chemical shielding parameters with doping (B atoms) and adsorbing phosgene increase. The quantum parameters such as gap energy and global hardness of system decrease significantly from pristine models, and so the reactivity and conductivity of system increase. The reduced density gradient and atom in molecule theory results demonstrated that the nature of bonding between SiC nanocluster with phosgen is van der Waals type and the doped nano cluster is a good candidate for adsorbing phosgene molecule.

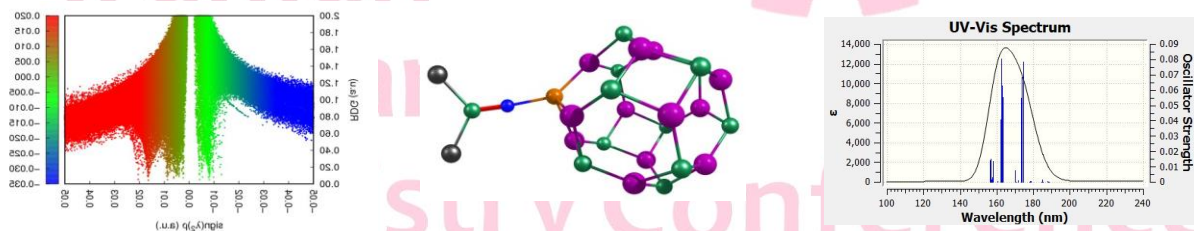


Figure : The optimized structure and RDG and UV-visible spectrum of SiC₁₂ nanocage @Ph complex

Keywords: Si₁₂C₁₂ nanocage, Phosgene, DFT, AIM

References

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