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The computational study of adsorption of cyanide ion on the surface of Pristine and Al doped boron phosphide nanotube: AIM, NBO, RDG, TD-DFT

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Abstract

Controlling and monitoring the HCN and CN ions concentration under the threshold limit value in both industrial and residential environments are of special interest. For detecting HCN gas and CN ion in the atmosphere, gas sensors have been considered promising alternatives for environmental measurements due to their low cost, high sensitivity, fast response and direct electronic interface [1–4]. In this project, we investigate the CN ion adsorption on the surface of pristine and Al&S doped (4,4) armchair and (8,0) zigzag models of boron phosphide nanotubes (BPNTs) by using Gaussian 16 software, at the wb97xd/ 6-31G(d, p) level of theory. The results showed that adsorption energy in the all adsorption models are negative, and all adsorption models are favorable in view of thermodynamic approach. The positive value of NBO analysis indicate that the charge transfer is occurred from the cyanide ion toward the nanotube, for this means the electrical properties of nanotube change significantly from original state. The quantum results show that with doping Al&S doped the activity of nanotube for adsorbing CN ion increase. The reduced density gradient and atom in molecule theory results confirm that the bonding nature of nanotube with CN ion is electrostatic and partial covalence. The computational results demonstrate that the pristine and Al&S doped BPNTs can be a suitable adsorbent for cyanide ion in the environmental system.

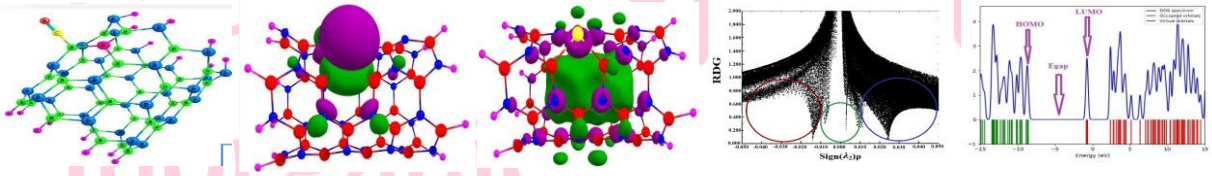


Figure 1: The RDG, DOS, HOMO-LUMO, and optimized sturctures of CN ion with BP nanotube

Keywords: *BPNTs, Al&S doped,* Cyanide ion, Static Electric Field, DFT

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