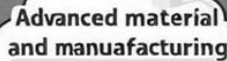




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## ICAMM-0P-24

### A comprehensive study on Pristine and Pt-doped ZnO nanotubes towards detection of CO<sub>2</sub> gas: a comparison

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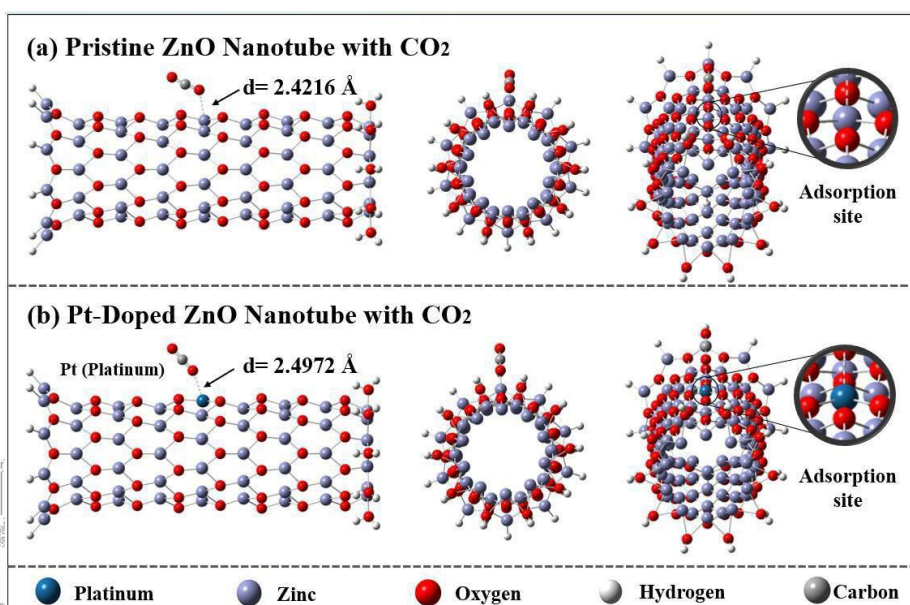
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#### Abstract:

The study compares the performance of pristine ZnO nanotube and platinum (Pt)-decorated ZnO nanotube for detecting CO<sub>2</sub> using the first-principle computational method in Gaussian 09W and Gauss View 6.0 software. Carbon dioxide (CO<sub>2</sub>), a greenhouse gas and a major contributor to global warming was chosen as the adsorbed gas molecule for both types of nanotubes, resulting in two systems viz. CO<sub>2</sub> adsorbed pristine ZnO nanotubes (Type-A) and CO<sub>2</sub> adsorbed Pt-doped ZnO nanotubes (Type-B). The interaction between the gas molecule and the sensing material was analyzed using various electronic parameters such as molecular electrostatic potential (MEP), Mulliken charge analysis, density of states (DOS), highest occupied molecular orbital (HOMO), and lowest unoccupied molecular orbital (LUMO). It was observed that Pt-decorated ZnO nanotube showed better interaction, resulting in strong adsorption with an adsorption energy of (-0.344 eV), compared to pristine ZnO nanotube with an adsorption energy of (-0.092 eV). However, the binding distance between the adsorbed gas molecule and the sensing material was found to be reduced in the case of the Type-A system (2.4217 Å) compared to the Type-B system (2.4972 Å). This study highlighted the importance of CO<sub>2</sub> detection in maintaining air quality and reducing environmental degradation. The introduction of a Pt atom onto the ZnO nanotube structure increased the surface interaction ability by creating additional active sites and altering charge distribution, thereby enhancing stronger interaction with the CO<sub>2</sub> molecule compared to pristine ZnO nanotube.



**Figure 1.** Optimized structure of (a) CO<sub>2</sub> adsorbed pristine ZnO nanotube (b) CO<sub>2</sub> adsorbed platinum (Pt)-doped ZnO nanotube

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