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Density functional theory study of transitional metal doped ZnO nanostructures for gas sensing: Interaction of NH3 and NO2 with the doped ZnO surface

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The adsorption and interaction mechanisms of gaseous molecules on ZnO surfaces have received a substantial amount of attention recently as a direct result of the technical uses that they offer in gas sensing. The adsorption behaviour of molecules of NH3 and NO2 was examined using density functional theory on surfaces of undoped and M-doped ZnO (101) where (M = Ni, Co, and Cu). It was discovered that each of the adsorption energy values had a negative value, which suggests that both molecules absorb through the process of chemisorption rather than physisorption. According to the results of the adsorption energy calculations, the molecule of NH3 has an energetic profile that is more compatible with adsorption on the exposed ZnO surface than the NO2 molecule does. On the other hand, it was found that the surface of all the M-doped ZnO could support a robust adsorption arrangement for the NO2 molecule. The redistribution of charge density showed that the adsorbent and the adsorbate each had charge accumulation and depletion on their respective surfaces. The density of states and band structures were also studied in order to study the electronic behavior of molecules of NH3 and NO2 that had been adsorbed on surfaces of undoped and Sn-doped ZnO (101), respectively.

Apply to be considered for a student ; award (Yes / No)?

No

Level for award;(Hons, MSc, PhD, N/A)?

MSC

Primary authors: Mr MAKHUBELE, Matimu (University of Venda); DIMA, Ratshilumela Steve (University of venda); MAPHANGA, Rapela (CSIR); MALUTA, Nnditshedzeni Eric (University of Venda); KIRUI, Joseph (UNIVERSITY OF VENDA)

Presenter: DIMA, Ratshilumela Steve (University of venda)

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