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Adsorption of H2S on La-ZnO Surface Using DFT+U Method

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Gas sensing is the detection of toxic gases in the environment/atmosphere for air quality and safety control. It iss based on the principle of transforming the gas adsorption effects on the surface of the active material into a detectable signal in terms of its changed electrical, optical, thermal, mechanical, magnetic (magnetization and spin), and piezoelectric properties. In this work, DFT+U method was used to investigate the properties of H2S adsorbed on to La doped ZnO (101) surface. The calculations are based on the adsorption of H2S on pure and doped with La-ZnO surface to see how doping affects the adsorption process in gas sensing. The calculated lattice parameters are consistent with the experimental results. Doping with La increase the absorption energy.

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

yes

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

Hons

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