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Gas sensing mechanism of Ethylene on pure Co3O4 (311) surface: Density Functional Theory Study

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Advanced sensing technology is required for the detection of gases and volatile organic compounds (VOCs) for application in environmental monitoring, disease diagnosis, and smart agriculture. Among the many materials used as sensing layers, nanostructured semiconductor metal oxide-based sensing materials have recently gained preference owing to their outstanding sensitivity and high surface area. The flexibility to tune their morphology and surface characteristics also add upon to their most use in this field of gas sensors. Considerable experimental research has shown the behaviour of the semiconductor metal oxide-based gas sensors towards different gases; however, they do not provide a detailed understanding of the sensing mechanism. This work focuses on density functional theory (DFT) calculations to explore the electronic properties of the bulk Co3O4 and its (311) surface using the BIOVA Material Studio. The general sensing mechanism describing the performance of Co3O4 when exposed to ethylene molecules is also discussed.

Key words: Gas sensor, nanostructured, Co3O4, DFT calculations, ethylene, sensing mechanism

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

Yes

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

MSc

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