Contribution ID: **90** Type: **Poster Presentation**

Title: Facile sensing characteristics of V2O5 nanostructured electrode from experimental and first principle approach.

Thursday, 11 July 2019 15:00 (2 hours)

To build an efficient and reliable nano-gas sensing device, critical study and analysis of the sensing material in terms of the parameters such as sensitivity and selectivity is a key requirement. In this study, experimental sensing performance of dopantless V2O5 to NH3 gas and its density functional facile properties are presented. The V2O5 sample material was synthesized from NH3VO4 via CVD at 400 ˚C under N2 flow for 12 h. Micro- and nano- structural and morphological characterizations revealed the material's structure as polycrystalline V2O5 nanorods. The material was tested for gas sensing application under different levels of NH3 flow. A linear sensitivity % with respect to the levels of NH3 concentration was observed. Furthermore, we also observed optimal sensor response at the operating temperature of 400 ˚C. Atomistic density functional calculations of adsorption energies for different numbers of NH3 gas molecules were performed on (001) and (110) surfaces of the V2O5 structure. High adsorption was observed in the case of the perpendicular plane; (001) surface compared with the parallel coordinated (110). The results suggest that, although the orientation has almost equal probability in (001) and (110), the (001) is more selective to NH3 than (110). Absolute value of adsorption energy per molecule with respect to different numbers of molecule does not only simulate the experimental sensitivity profile but also establish the high selective ability of (001) surface to NH3.

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No

Level for award
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N/A

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