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Sorption of NO, CO and CH4 on indium phosphide nanowires supported with molecular modelling

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Temperature Programmed Desorption (TPD) is crucial spectroscopic method used to determine thermodynmic and kinetic parameters of desorption processes. Sorption of gases from Group III-V semiconductor nanowires is a fascinating area of nanoscience, because they reveal potential of gas sensing. These nanowires have a potential to be used in various applications such as photonics, electronics including micro and nanoelectromechanical systems (MEMS and NEMS). They have relatively tuneable small direct bandgaps (Indium Phosphide (InP) = 1.34 eV) which makes them suitable for use in optoelectronic devices as well. InP surface in particular, has an interesting electron reach/deficiant active sites that could form part of the gas binding sites. The sorption of gases such as Methane (CH_4), Carbon Monoxide (CO) and Nitric Oxide (NO) were studied using TPD. In this study, it was discovered that InP nanowires binds through chermisoption to both CO and NO and binds very weakly through physisorption to CH_4. The heat of desorption enthalpies were found to be 140 kJ/mol, 80 kJ/mol and 48 kJ/mol for CO, NO and CH_4 respectively. The experimental enthalpies were compared to the theoretical values (binding energies) obtained through molecular modelling. The binding modes of the gases to the surface of InP nanowires were studied by Diffuse Reflectance Infrared Fourie Transorm Spectroscopy (DRIFTS) together with adsorption modelling. This study reveals the nature and strength of interaction between NO, CO, CH_4 gas molecules on the surface of InP nanowires and the sorption temperature range.

Biography

Sanele Nyembe has completed his Msc from University of Witwatersrand, Johannesburg and currently doing his PhD with the same university. He works as a Scientist at Mintek-Nanotechnology Innovation Centre, Research and Development. He has published 2 papers in reputed journals from his PhD work and 1 publication from other projects.

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