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Tailoring vanadium pentoxide (V2O5) nanostructure properties to selective detection of nitrogen dioxide (NO2).

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Abstract

The density functional theory (DFT) method was used to critically investigate the absorption energy of pristine and doped α-V2O5 towards the detection of NO2 gas molecules. The different transition metals, including tungsten (W), copper (Cu), manganese (Mn), tin (Sn), and silver (Ag), were intercalated into α-V2O5 (110) surface using the substitution method to enhance the adsorption energy within the Cambridge Serial Total Energy Package (CASTEP) code. The results show that pristine α-V2O5 lack structural stability and show less negative adsorption energy when the concentration of NO2 molecules increases. α-V2O5 doped with Ag possesses the most negative adsorption energy compared to the pristine and the other dopant. Furthermore, the dopants such as Cu, Ag, and Mn have also enhanced the structural stability of V2O5 at higher concentrations of NO2 molecules. This study paves the way for the experimental fabrication of the most stable and highly selective α-V2O5 doped Ag sensor for selective detection of nitrogen dioxide.

Keywords: V2O5, Adsorption energy, transition metals, gas sensors

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