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Master Thesis Defense

Entitled

FUNCTIONALIZATION OF 2D-ZnO FOR SELECTIVE GAS-SENSING: FIRST-PRINCIPLES ANALYSIS

by

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Abstract

The scope of this MSc thesis is to theoretically search for suitable materials and relevant factors (e.g., dopants and catalysts) to induce gas-sensing (GS) selectivity towards harmful gases such as H2, H2S and CO2, under ambient conditions. We chose as material 2D-ZnO Honeycomb in the form of nano-ribbon (ZnO-NR), which is very promising in the gas-sensing applications. We employed a state-of-the-art computational method, based on a combination of the density-functional theory (DFT) and the Non-Equilibrium Green's Functions (NEGF) formalism, which both are incorporated in Atomistic Tool-Kit (ATK)* package. This package is famous by its reliability in estimating the IV-characteristics. The thesis consists of three phases: (1) Effect of dopants on gas-sensing: Three organic-atoms (e.g., N, C, F) were initially attempted. But selectivity towards the detection of H2 was achieved only in N-doped ZnO-NR. Special trend, discovered about the secrete of such selectivity, was the existence of negative-differential resistance (NDR) in the IV-characteristics of ZnO-NR:N. (2) Origins of NDR: the previous results led us to search for the origins of NDR in N-doped ZnO-NRs. We have investigated the effect of placing the doping atom N in three different positions across ZnO-NR, with respect to the edges (i.e.,(i) at the O-rich edge, (ii) at the center, and (iii) at the Zn-rich edge.) Results show a clear trend that NDR shifts to higher energies than Fermi level, as well as both NDR and the Top-to-Valley-Current Ratio (TVCR)get reduced, when N atom is moved from O-rich to Zn-rich edges. We concluded that the unpaired electron on N-atom, when it gets charged, causes the localization/curdling of wave-function at Fermi-level and consequently causes back-scattering and draw-back of current (so named NDR). (3) Effect of catalysts on gas-sensing: Five transition-metal atoms (Pt, Pd, Au, Ag, and Fe) were used as ad-atom decorating ZnO-NR aiming to induce selectivity towards gases of interest (H2, H2S, and CO2) in existence of other gases (e.g., O2, N2, H2O) at room temperature (RT). Results show that both Pt and Pd have poor selectivity at RT. Whereas, Fe is found to yield high selectivity toward detecting CO2, while both Au and Ag have selectivity towards H2S, at RT. All our findings are in excellent agreements with experimental data.

Keywords: Ab-initio calculations, Adsorbates on surfaces, Catalysis, Chemisorption, Gas-sensing, Physisorption, Surface structure, Transition metal oxides, ZnO.