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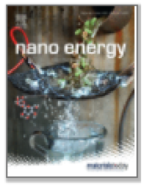

Tailoring the selectivity of ultralow-power heterojunction gas sensors by noble metal nanoparticle functionalization

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Abstract

Heterojunctions are used in solar cells and optoelectronics applications owing to their excellent electrical and structural properties. Recently, these energy-efficient systems have also been employed as sensors to distinguish between individual gases within mixtures. Through a simple and versatile functionalization approach using noble metal nanoparticles, the sensing properties of heterojunctions can be controlled at the nanoscopic scale. This work reports the nanoparticle surface functionalization of $TiO_2/CuO/Cu_2O$ mixed oxide heterostructures, where the gas sensing selectivity of the material is tuned to achieve versatile sensors with ultra-low power consumption. Functionalization with Ag or AgPt-nanoclusters (5–15 nm diameter), changed the selectivity from ethanol to butanol vapour, whereas Pd-nanocluster functionalization shifts the selectivity from the alcohols to hydrogen. The fabricated sensors show excellent low power consumption below 1 nW. To gain insight into the selectivity mechanism, density functional theory (DFT) calculations have been carried out to simulate the adsorption of H_2, C_2H_5OH and n-C_4H_9OH at the noble metal nanoparticle decorated ternary heterostructure interface. These calculations also show a decrease in the work function by ~2.6 eV with respect to the pristine ternary heterojunctions. This work lays the foundation for the production of a highly versatile array of sensors of ultra-low power consumption with applications for the detection of individual gases in a mixture.