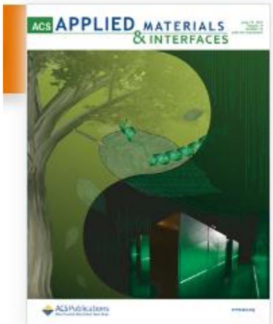

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ACS Applied Materials & Interfaces 2022, Vol.14, Iss. 25, pag. 29331–229344

Al_2O_3/ZnO Heterostructure-Based Sensors for Volatile Organic Compounds in Safety Applications

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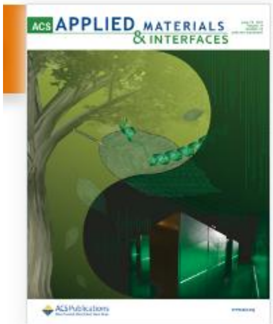
Abstract

Monitoring volatile organic compounds (VOCs) in harsh environments, especially for safety applications, is a growing field that requires specialized sensor structures. In this work, we demonstrate the sensing properties toward the most common VOCs of columnar Al_2O_3/ZnO heterolayer-based sensors. We have also developed an approach to tune the sensor selectivity by changing the thickness of the exposed amorphous Al_2O_3 layer from 5 to 18 nm. Columnar ZnO films are prepared by a chemical solution method, where the exposed surface is decorated with an Al_2O_3 nanolayer via thermal atomic layer deposition at 75 °C. We have investigated the structure and morphology as well as the vibrational, chemical, electronic, and sensor properties of the Al_2O_3/ZnO heterostructures. Transmission electron microscopy (TEM) studies show that the upper layers consist of amorphous Al_2O_3 films. The heterostructures showed selectivity to 2-propanol vapors only within the range of 12–15 nm thicknesses of Al_2O_3, with the highest response value of ~2000% reported for a thickness of 15 nm at the optimal working temperature of 350 °C. Density functional theory (DFT) calculations of the Al_2O_3/ZnO(1010) interface and its interaction with 2-propanol (2-C_3H_7OH), n-butanol (n-C_4H_9OH), ethanol (C_2H_5OH), acetone (CH_3COCH_3), hydrogen (H_2), and ammonia (NH_3) show that the molecular affinity for the Al_2O_3/ZnO(1010) interface decreases from 2-propanol (2-C_3H_7OH) ≈ n-butanol (n-



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C_4H_9OH) > ethanol (C_2H_5OH) > acetone (CH_3COCH_3) > hydrogen (H_2), which is consistent with our gas response experiments for the VOCs. Charge transfers between the surface and the adsorbates, and local densities of states of the interacting atoms, support the calculated strength of the molecular preferences. Our findings are highly important for the development of 2-propanol sensors and to our understanding of the effect of the heterojunction and the thickness of the top nanolayer on the gas response, which thus far have not been reported in the literature.

Keywords: zinc oxide, aluminium oxide, heterojunctions, volatile organic compounds, semiconducting metal oxides, gas sensors, gas response

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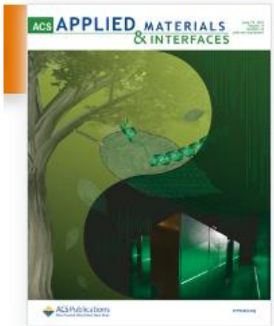

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