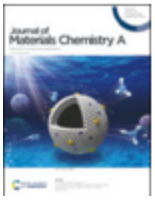
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Surface functionalization of ZnO:Ag columnar thin films with AgAu and AgPt bimetallic alloy nanoparticles as an efficient pathway for highly sensitive gas discrimination and early hazard detection in batteries

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Abstract

For a fast and reliable monitoring of hazardous environments, the discrimination and detection of volatile organic compounds (VOCs) in the low ppm range is critically important, which requires the development of new chemical sensors. We report herein, a novel approach to tailor the selectivity of nanocomposite thin film sensors by investigating systematically the effect of surface decoration of Ag-doped ZnO (ZnO:Ag) columnar thin films. We have used AgPt and AgAu noble bimetallic alloy nanoparticles (NPs) to decorate the surfaces of ZnO:Ag and we have measured their resulting gas sensing properties towards VOC vapors and hydrogen gas. The gas response of the nanocomposite containing AgAu NPs to 100 ppm of ethanol, acetone, n-butanol, 2-propanol and methanol vapors was increased on average by a factor of 4 compared to the pristine ZnO:Ag columnar films. However, decoration with AgPt NPs led to a considerable reduction of the gas response to all VOC vapors and an increase of the response to H2 gas by roughly one order of magnitude, indicating a possible

route to tailor the selectivity by surface decoration. As such, the reported NP-decorated ZnO:Ag thin film sensors should be suitable for the detection of H2 in Li-ion batteries, which is an early indication of the thermal runaway that leads to complete battery failure and possible explosion. To understand the impact of NP surface decoration on the gas sensing properties of ZnO:Ag thin films, we have employed density functional theory calculations with on-site Coulomb corrections and long-range dispersion interactions (DFT+U–D3-(BJ)) to investigate the adsorption of various VOC molecules and hydrogen onto the Ag-doped and NP-decorated (10[1 with combining macron]0) surface of zinc oxide ZnO. The calculated surface free energies indicate that Ag5Au5/ZnO(10[1 with combining macron]0):Ag is the most favourable system for the detection of VOCs, which based on its work function is also the most reactive towards these species. Our calculated adsorption energies show that Ag9Pt/ZnO(10[1 with combining macron]0):Ag has the largest preference for H2 gas and the lowest preference for the organic adsorbates, which is in line with the high selectivity of AgPt/ZnO:Ag sensors towards the hydrogen molecule observed in our experiments.