The role of surface oxidation on the gas sensing properties of 2D layered chalcogenides: the evidence of 2D/2D *a*-SnO_2/$SnSe_2$ heterostructures

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Despite their widespread potential in gas sensing applications, 2D exfoliated metal dichalcogenides (MDs) show poor chemical stability under dry/wet conditions at operating temperatures (OTs) ranging from 25°C to 150°C, that limits their practical exploitation in sensing applications [1–3]. Aim of this work is to focus on new perspectives to passivate material surface preventing further degradation, with the practical case-study of gas sensing properties of 2D SnO_2/$SnSe_2$ heterostructures obtained by controlled oxidation of exfoliated $SnSe_2$ flakes. We report that, provided suitable thermal treatments, it is possible to synthesize a new class of 2D heterostructures comprising amorphous SnO_2 (*a*-SnO_2) metal oxide grown over pristine few layered $SnSe_2$ MDs.

We demonstrated by means of HRTEM, XPS and XRD techniques that annealing in static air at 200°C, i.e. below the crystallization temperature of SnO_2, and different times ranging from 2h to 170h induces surface oxidation of $SnSe_2$ leading to the formation of a self-assembled *a*-SnO_2 skin layer over the underling 2D-$SnSe_2$ flakes, with excellent gas sensing properties to oxidizing and reducing gases. Sensing tests were carried out on a-SnO_2/$SnSe_2$ at an OT of 100°C to NO_2 and H_2 gases and different relative humidities ranging from 40% to 80% RH, also investigating the long-term stability of the response over one year. The gas sensing responses of a-SnO_2/$SnSe_2$ heterostructure to increasing concentrations of NO_2 in the range 400 ppb-1.5 ppm and 40% RH show response to NO_2 with corresponding limits of detection of 400 ppb. Electrical tests in the presence of different amount of humidity highlight that water vapor improves sensor's response to NO_2. On the contrary, while the detection limit to H_2 is found to be 5 ppm, the effect of humidity is to hinder the response, suggesting a competitive mechanism.

These results explain that it is possible by suitable thermal treatment, to induce a self-terminating passivation process leading to an amorphous *a*-SnO_2 oxide over $SnSe_2$ which prevent the underlying 2D – $SnSe_2$ structure for further oxidation and achieve excellent gas sensing responses.

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