

Gas sensing properties of ultrathin 2D materials and passivation strategies to prevent their degradation: the case of Layered Amorphous metal oxide structures

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2D Transition Metal Dichalcogenides (TMDs) and Metal Chalcogenides (MCs) with atomic scale thickness, being all reacting surfaces, have been extensively proposed as alternative materials of traditional nano-crystalline Metal Oxides (MO) for gas sensing applications. However, these layered interfaces, with the general chemical formula MX_2 where M is a transition metal (i.e. Mo, W) and X is a chalcogen, generally S, Se or Te, suffer from spontaneous oxidation under dry/wet air ambient conditions, adversely effecting both base line resistance (BLR) and sensor's signal (i.e. R_a/R_g or R_g/R_a) reproducibility over the long run [1]. Aim of this presentation is to discuss some oxidation mechanisms of TMDs and MCs addressing possible passivation strategies to prevent further degradation and improve their electrical stability for gas sensing applications [2]. Specifically this contribution reports: (i) an outline of a liquid phase exfoliation method to synthesize few layers of WSe_2 and $SnSe_2$ from commercial crystals [3]; (ii) a possible strategy, by suitable thermal treatment, to induce controlled oxidation in air of few layers WSe_2 and $SnSe_2$ leading to the formation of template self-assembled amorphous α - WO_3 and α - SnO_2 over 2D- WSe_2 [4] and 2D- $SnSe_2$ [5]; (iii) a description of how XPS, HRTEM and grazing Incidence GI-XRD microstructural characterization techniques can be utilized to assess the formation of amorphous phases over exfoliated WSe_2 and $SnSe_2$. Specifically, for the case of α - SnO_2 , by annealing as exfoliated 2D- $SnSe_2$ at temperatures below the crystallization temperature of SnO_2 (200°C) an amorphous oxidized skin-layer, homogeneously passivating the 2D- $SnSe_2$ is formed. The duration of the oxidation process has been optimized by "in operando" monitoring the base line resistance (BLR) while changing the annealing conditions, with the aim to yield base lines resistances and sensor's signal reproducible responses to oxidizing and reducing gases in dry/wet conditions. The amorphous α - SnO_2 skin, homogeneously covering the underlying 2D $SnSe_2$ flakes, represents the reacting surface to oxidizing/reducing gases of the α - SnO_2 / $SnSe_2$ heterostructure, paving the way for new class of template self-assembled Layered Amorphous Metal Oxides Sensors interfaces (LAMOS).

- [1] Q. Li, et al. J. Mater. Chem. A. **7**, 4291 (2019).
- [2] V. Paolucci, et. al, Sensors Actuators, B Chem. **350C**, 130890 (2022)
- [3] V. Paolucci, et. al. ACS Sustain. Chem. Eng. **8**, 18830 (2020).
- [4] C. Cantalini et. al, Sensors Actuators, B Chem. **243**, 812 (2017).
- [5] V. Paolucci, et. Al, ACS Appl. Mater. Interfaces. **12**, 34362 (2020).

