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| Interfacial Interaction of Palladium with MoS2 and MoS2-rGO hybrids: **Labrini Sygellou** 1# 1 Foundation for Research and Technology, Institute of Chemical Engineering Sciences (FORTH/ICE-HT), Patras, GR-26504, Greece # \* sygellou@iceht.forth.gr |

abstract

Transition metal dichalcogenides, TMDs, are an exciting class of 2D materials, beyond graphene, with numerous potential applications such as catalysis, electronic devices, optoelectronics, energy storage and sensors. Among them, the MoS2 is the most studied. The drawbacks are the poor electrical conductivity, and the low number of active sites, which could be overcome by combining TMD nanoparticles with a conductive support such as graphite, carbon aerogels, reduced graphene oxide (rGO), carbon nanofibers, or carbon nanotubes (CNTs) and by phase transition from semiconducting 2H-MoS2 to metallic 1T-MoS2. For a few-layer MoS2 sample, the transition between the 2H and 1T phases requires the gliding of either sulfur (S) or Mo atom gliding. The transition has been achieved by alkali metal or hydrogen intercalation, substitutional doping, annealing accompanied by energetic electron-beam irradiation, plasmonic hot electrons and argon plasma. This opens the possibility of tuning the properties of MoS2 through phase engineering [[[1]](#endnote-1)]. A novel method for phase transition of the semiconducting 2H- to 1T-MoS2 is by metal substitution [[[2]](#endnote-2)]. The resulting 1T phase is reported to be thermodynamically unstable and relaxes to 1T′ or 2H over time or above a temperature range of 150 °C, which is in the range of standard sample processing temperatures for device applications.

In the present study, the interaction of Pd with MoSx and MoSx hybrids with reduced graphene oxide (MoSx-rGO), x≥2, has been extensively investigated by Synchrotron Radiation Photoelectron Spectroscopy (SRPES) and conventional X-ray photoelectron spectroscopy (XPS) [[[3]](#endnote-3)]. It was found that Pd interacts with S atoms with unsaturated electronic structures leading to the formation of PdSx surface compounds and to phase transition from the semiconducting 2H- MoS2 to the metallic 1T-MoS2 state. The stoichiometry of the substrate is a critical parameter since the phase transition does not occur on the stoichiometric MoS2, in contrast to non-stoichiometric surfaces MoSx, x>2 surfaces, where the phase transition occurs by Mo atoms substitution by Pd. In addition, the thermal stability depends on the surface chemistry. On stoichiometric MoS2-rGO htbrids, the 1T-phase is not stable whereas on sulfur-rich substrates, the 1T phase remains present up to about 4000C [[[4]](#endnote-4)]. Our conclusions highlight the need for sulfur excess to uphold the thermal stability of the 1 T phase up to 4000 C, irrespective of the presence of rGO. While rGO facilitates the formation of the 1T- phase in stoichiometric MoS2, it does not contribute to improving its thermal stability.

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