Use of Chemical Vapor Induced 2H-to-1T Phase Transition in MoX_2 (X=Se, S) Transition Metal Dichalcogenide Films for Enhanced Chemical Sensing

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Abstract:
Chemical vapors that are strong electron-donors can impart charge to the surface of transition metal dichalcogenide (TMD) films while interacting with the film only via a weak physisorption bond. This interaction makes TMDs ideal candidates for conductance-based vapor and gas sensors [1]. We examine the exposure of monolayer MoS_2 and $MoSe_2$ films to various strong electron donor chemical vapor analytes. These TMDs can exist in both the 2H (semiconducting) and 1T (metallic) phases, and the adsorption of strong electron donors may induce a phase transition from 2H to 1T. The properties of the various phases of these TMD films can be utilized to enhance their sensing properties. We show that this can be accomplished with phase engineering of the contacts, which creates more sensitive, selective, and versatile sensors. We also show that optical interrogation of the phase state of the chemically exposed films may offer a possible new paradigm for a novel class of passive chemical vapor sensors. These TMD materials, being sensitive to strong electron donors, are particularly sensitive to the vapors emitted by chemical nerve agents and certain types of explosives, in particular those of the type used in the recent Brussels terror attack and in the ongoing Syrian civil war.

[1] Friedman, AL, Perkins FK, Hanbicki AF, Culbertson JC, and Campbell PM, Nanoscale **8** (2016) 11445.

Figures

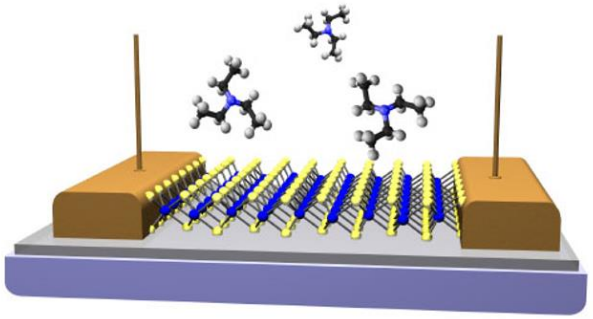

Figure 1: TMD device with physisorbing chemical vapor analyte ions.

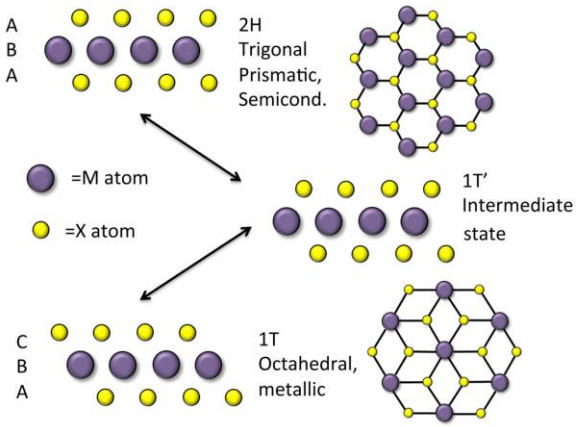

Figure 2: Model of the 2H-1T phase transition in MoX_2 films. The 2H phase is trigonal prismatic and the material is a semiconductor. The 1T phase is octahedral and the material is metallic. The 1T' phase is an intermediate state.