Electron Irradiation-Induced Defects and Phase Transformations in Two-Dimensional Transition Metal Dichalcogenides

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Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN, transition metal dichalcogenides (TMDs) and silica bilayers were manufactured. All these systems contain defects and impurities, which may govern the electronic and optical properties of these materials. Moreover, defects can appear during the characterization of the materials in transmission electron microscope. All of these calls upon the studies on defect properties and mechanisms of their formation under electron beam. In my talk, I will present the results [1-4] of our recent first-principles theoretical studies of defects (native and irradiation-induced) in inorganic 2D systems obtained in close collaboration with several experimental TEM groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of inorganic 2D materials. I will also present the results of our theoretical studies of electron-beam induced phase transformations in 2D TMDs when electric charge, mechanical strain and vacancies are present. Based on the results of our calculations, we propose an explanation for this phenomenon which is likely promoted by charge redistribution in the monolayer combined with vacancy formation due to electron beam and associated mechanical strain in the sample.

References

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Figures

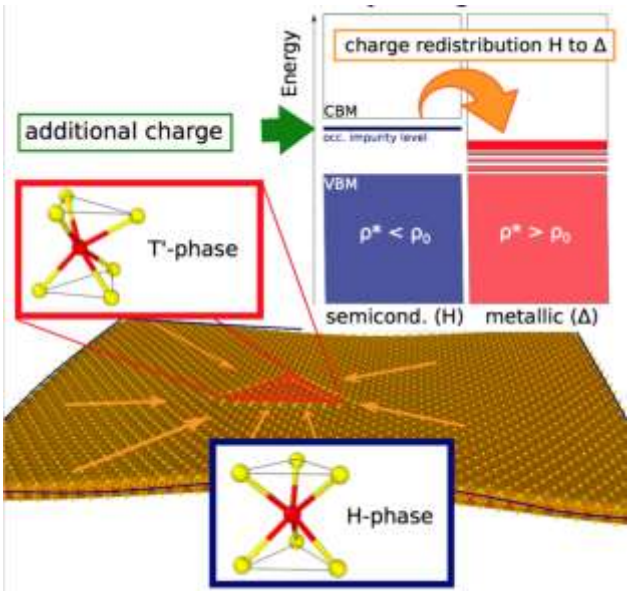

Figure 1: Schematic representation of charge-transfer mediated mechanism of the transition from the H to T' phase in 2D MoS_2.