Defects in two-dimensional transition-metal dichalcogenides and silica bilayers

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Isolation of a single sheet of graphene indicated that strictly two-dimensional (2D) materials can exist at finite temperatures. Indeed, inorganic 2D systems such as hexagonal BN sheets, transition metal dichalcogenides (TMD) with a common structural formula MeX_2, where Me stands for transition metals (Mo, W, Ti, etc.), X for chalcogens (S, Se, Te), and SiO_2 layers were later manufactured by various methods. All these materials have defects, which naturally affect their properties. Moreover, defects can deliberately be introduced by ion and electron irradiation to tailor the properties of the system [1].

In my talk, I will present the results of our first-principles theoretical studies of defects in inorganic 2D systems -- TMDs and silica obtained in collaboration with several experimental groups [2-4]. I will also touch upon defect production in 2D systems under impacts of energetic electrons [2,3]. I will further discuss defect and impurity-mediated engineering of the electronic structure of 2D materials such as TMDs [3-4] and BN [5,6].

Besides, I will discuss mixed TMDs, such as $MoS_{2x} Se_{2(1-x)}$, which can be referred to as 2D random alloys [7]. Our simulations indicate that 2D mixed ternary random alloy $MoS_2/MoSe_2/MoTe_2$ compounds are thermodynamically stable at room temperature, so that such materials can be manufactured by CVD or exfoliation techniques. Moreover, our simulations predicted that the direct gap in these materials can continuously be tuned depending on relative component concentration, as confirmed later on by several experimental groups.

I will finally touch upon defects in bilayer 2D silica [8] and show that defects are strikingly similar to those in graphene [9] with their morphology governed by the hexagonal symmetry of the lattice [10,11].

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