Inorganic two-dimensional materials under electron irradiation: stability, evolution of the atomic structure, and beam-mediated doping

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Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN sheets, transition metal dichalcogenides (TMD) with a common structural formula MeX₂, where Me stands for transition metals (Mo, W, Ti, etc.), X for chalcogens (S, Se, Te), and SiO₂ layers were manufactured. Among them, TMD sheets have received a particular attention, as these materials exhibit intriguing electronic, optical and mechanical properties which can be controlled by varying material composition. Moreover, the properties can further be tuned by introduction of defects and impurities. In my talk, I will present the results [1] of our first-principles theoretical studies of defects in inorganic 2D systems -- TMDs and silica layers obtained in collaboration with several experimental transmission electron microscopy groups. I will also touch upon defect production in 2D systems under impacts of energetic electrons. I will further discuss defect and impurity-mediated engineering of the electronic structure of 2D materials. Finally I will address defects in truly one-dimensional ionic crystals, chains of CsI and also discuss BN chains.

[1] http://www.acclab.helsinki.fi/~akrashen/publist.html