Defects and new phases in graphene and related systems: insights from multi-scale atomistic simulations

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Following isolation of graphene, many other 2D systems, e.g., single sheets of transition metal dichalcogenides (TMDs) have been manufactured. All these materials contain defects and impurities, which may govern their electronic and optical properties. Moreover, defects can intentionally be introduced using beams of energetic particles – ions and electrons. Formation of defects may also give rise to phase transformations in these materials. All of these calls upon the studies on defects and mechanisms of their formation. In my talk, I will present the results [1] of our recent theoretical studies of defects (native and irradiation-induced) in 2D systems obtained in close collaboration with several experimental microscopy groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of 2D materials. Finally, I touch upon the intercalation of Li and other alkali metal atoms into bilayer graphene and MoS_2.

[1] https://users.aalto.fi/~ark/publist.html