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Tailoring the properties of inorganic two-dimensional materials by post-synthesis introduction of impurities and defects

Arkady V. Krasheninnikov
Helmholtz Zentrum Dresden-Rossendorf,
Institute of Ion Beam Physics and Materials Research,
Dresden, Germany
a.krasheninnikov@hzdr.de

Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN, transition metal dichalcogenides (TMDs) or silica bilayers were manufactured. All these systems contain defects and impurities, which frequently govern the electronic and optical properties of these materials. Moreover, due to the very morphology of the 2D materials, which consist of essentially surface only, defects can easily be created by chemical treatment or irradiation, so that the properties of the materials can be tuned. For example, single impurities can be introduced by ion implantation or atom deposition, and when their concentration increases, a 2D alloy can be manufactured. Likewise, increasing vacancy concentration by sputtering atoms from a 2D TMD sheet can change the stoichiometry of the system and give rise to new features like inversion domains and grain boundaries or even new phases. In my talk, I will present the results [1-4] of our recent first-principles theoretical studies carried out with several experimental groups of how defects and impurities can be used to tailor properties of 2D materials or induce phase transformations in these systems.

References

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