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Atomistic modeling of effects of irradiation on 2D materials

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Ion irradiation has successfully been used for introducing impurities and creating defects in two-dimensional (2D) materials in a controllable manner. Moreover, focused ion beams, especially when combined with in-situ or post-irradiation chemical treatments, can be employed for patterning and even cutting 2D systems with a high spatial resolution. The optimization of this process requires the complete microscopic understanding of the interaction of energetic ions with the low-dimensional targets. At the same time, lots of attention has recently been paid to the mechanisms of defect creation in 2D systems under electron irradiation in a transmission electron microscope, further motivating the research in this area.

In my presentation, I will dwell upon the multi-scale atomistic computer simulations of the impacts of electrons and ions onto free-standing (e.g., suspended on a TEM grid) and supported (deposited on various substrate) 2D materials, including graphene and transition metal dichalcogenides (TMDs), such as MoS2 and WS2. The theoretical results will be augmented by the experimental data obtained by the coworkers.

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