Integrating atomistic simulations with microscopy to probe defect dynamics in 2D materials

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In this talk, I will present some of our recent work on the use of machine learning (ML) to seamlessly bridge the electronic, atomistic and mesoscopic scales for materials modeling. Our automated ML framework aims to bridge the significant gulf that exists between the handful of research groups that develop new interatomic potential models (often requiring several years of effort) and the increasingly large user community from academia and industry that applies these models. Our ML approach showed marked success in developing force fields for a wide range of materials from metals, oxides, nitrides, hetero-interfaces to two-dimensional (2-D) material. This talk will also briefly discuss our ongoing efforts to integrate such cheap yet accurate atomistic models with AI techniques to perform inverse design and deep learning to improve spatiotemporal resolutions of microscopy and ultrafast X-ray imaging.