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A Multiscale computational approach to predict the elastic deformation fields in Moiré Patterns of 2D van der Waals interfaces and heterostructures HEMANT KUMAR, VIVEK SHENOY, University of Pennsylvania — Recent technological advancements in isolation and transfer of different 2-dimensional (2D) materials have led to renewed interest in Van der Waals (vdW) heterostructures. We report a multiscale computational method to predict the deformation of vdW heterostructures using density functional theory (DFT) informed continuum simulations. We validate our method by comparing its predictions with all atom atomistic simulations for the graphene-hBN bilayer system and computing the in-plane strains, local curvature for different misorientation angles between two lattices. We also present closed form solutions for the elastic field as a function of lattice mismatch, relative rotations and predict the deformation fields for MoS2-WS2, MoSe2-WSe2 systems that have been recently synthesized experimentally.

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