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**Atomistic mechanisms of van der Waals epitaxy and property optimization of layered materials**

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Since the first isolation of graphene from graphite by mechanical exfoliation, atomically-thin or layered materials have been occupying the central stage of today's condensed matter physics and materials sciences because of their rich and exotic properties in two dimensions (2D). Many members of the ever-expanding 2D materials family share the distinct commonality of possessing relatively-weak van der Waals (vdW) interlayer coupling, whereas each member may invoke its own fabrication approaches, and is characterized by its unique properties. In this presentation, we first discuss the major atomistic processes and related morphological evolution in the epitaxial growth of graphene, such as nucleation, diffusion, feedstock dissociation, and grain boundaries, and further review the current status of the vdW epitaxy of newly discovered 2D materials. The review covers the vdW epitaxy of both monolayered 2D systems and their lateral or vdW-stacked heterostructures, emphasizing the vital importance of the vdW interactions in these systems. We also briefly highlight on some of the recent advances in the property optimization and functionalization of 2D materials, using examples from the fields of optics, electronics, spintronics, and catalysis. Work done in collaboration with Ping Cui, Wei Chen, Jun-Hyung Cho, and Zhenyu Zhang.