HETEROGENEITY IN BEYOND GRAPHENE 2D MATERIALS

Introduction

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Atomically thin 2D layered materials have shown remarkable physical and chemical properties, which are promising electronic and quantum materials for future devices, quantum information science, and energy applications. However, 2D materials also display remarkable heterogeneities. At atomic scales, 2D sheets contain point defects including vacancies, intentional dopants, and impurities. At the mesoscopic level, these imperfections include misoriented grains and layers, mixed phases, strain and charge transfer induced by the substrate, adsorbates, and the dielectric environment. Actually, 2D materials are a model system to explore the fundamentals of heterogeneities. Such materials allow direct correlation of nanoscale structure-property relationships enabled by the ultrathin thickness of 2D materials which confine all the electrons in the thin layer and make their properties highly sensitive to their heterogeneities. In addition, 2D materials have the well-defined single crystalline structures, which is perfect for both direct atomic structure characterization of their heterogeneity by electron microscopy and theoretical modeling and simulation. While these heterogeneities are of manufacturing concern for controllable, uniform, and large area synthesis of these materials, they also present opportunities to localize defects, dopants, isotopes, and edge to realize new optoelectronic functionality and quantum states in 2D layered materials. For instance, the defects in 2D materials could be used not only to tune their optical and electronic properties, but also to enable spin splitting to induce layer-modulated magnetism in non-magnetic 2D materials. Localized defect and strain in 2D materials also could spatially confine excitons for quantum emitters. Disorder, confinement, and symmetry breaking

often contribute to the emerging quantum states in layered 2D materials for future applications in quantum information science. To fully reveal these opportunities, a synergistic strategy to fundamentally understand and control heterogeneity of 2D materials and the emerging functionality must be developed.

This Focus Section highlights several representative and noteworthy research accomplishments in the area of heterogeneity of 2D materials. These include a comprehensive review of the role of strain in 2D materials on their properties and phase transition and how to control the deformation of 2D materials for engineering functionalities; the development of paths to control the formation of 2D alloys such as $\text{SnS}_x\text{Se}_{2-x}$ through van der Waals (vdWs) epitaxial growth; an overview of various manufacturing strategies for wafer-scale 2D transition metal dichalcogenide (TMD) heterostructures; advanced characterization of the charge transfer in WS_2 - ReSe_2 vdWs heterostructures by time-resolved laser spectroscopy; and the strain-induced interlayer stacking shift in 2D TMD bilayers at atomic scale by in-situ scanning transmission electron microscopy; and the theoretical prediction of a new 2D Janus structure of TaS_2 with distinct optical and electronic properties through fluorination and hydrogenation. These contributions highlight the transformational opportunity that heterogeneity can play in 2D materials and heterostructure for future electronics, quantum information science, and energy applications.

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