First-principles studies of defects in 2D materials

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Recently, low dimensional materials such as graphene, hexagonal boron-nitride (hBN), and transition metal dichalcogenides have emerged among the hottest classes of materials owing to their unique properties and promising properties for future applications. In particular, combined density functional theory and real-space imaging studies have been known as a very powerful technique to directly investigate the structure, properties, chemistry and dynamics of defects in low dimensional materials [1-5]. In this talk, I will briefly introduce some of the recent defect studies in lateral graphene–hBN hybrid and SnSe materials. Novel observation in their electronic structures and related physical properties will be presented and discussed along with experimental results.

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