The Organic-2D Heterointerface

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Graphene, an atomically thin layer of carbon, is a semi-metal that can be used in applications such as transparent conducting electrodes in flexible electronics. The electronic and chemical properties of graphene can be engineered through a variety of methods such as by molecular adsorption [1,2], or fabricating graphene nanoribbons [3,4]. Unlike graphene, transition metal dichalcogenides (TMDs) such as MoS_2 and WSe_2, are semiconductors with tunable direct bandgaps dependent on the number of atomic layers, and have potential electronic and optoelectronic applications. We use high resolution scanning tunneling microscopy/spectroscopy (STM/STS) to study the atomic structure and intrinsic electronic properties of MoS_2 layers (mono-, bi-, tri-) directly deposited on HOPG substrates by chemical vapour deposition (CVD) [5]. We report an unexpected bandgap tunability with distance from the grain boundary in single-layer MoS_2, which also depends on the grain misorientation angle. We have similarly investigated the atomic scale grain boundary electronic properties of CVD-grown WSe2 monolayers, and report novel dislocation defects at low-angle grain boundaries [6].

The increasing availability of two-dimensional (2D) TMDs brings additional opportunities for them to be used as interlayers in "van der Waals (vdW) heterostructures" and organic/inorganic flexible devices. We studied perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) monolayers adsorbed on single-layer tungsten diselenide (WSe2), bare graphite and Au(111) surfaces, revealing a strong dependence of the PTCDA HOMO-LUMO gap on the electronic screening effects from the substrate [7]. The monolayer WSe_2 interlayer provides substantial – but not complete – screening at the organic/inorganic interface. Recent results of the $C_{60}F_{48}$-WSe_2 monolayer heterointerface will also be discussed [8]. Our results lay a foundation for the exploitation of the complex interfacial properties of hybrid heterostructures based on organics and TMD monolayers.

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