



Fabrication of Graphene-hBN Transistors for Characterization of Mott Insulators

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Introduction

Exfoliated graphene has proven to be a versatile platform for studying novel quantum states of matter due to its extraordinary electronic properties. Simultaneously, graphene can also play an auxiliary role in exploring the exotic physics of other 2D materials due to its easy availability and convenient symmetry. By placing an exfoliated graphene monolayer in a field-effect-transistor device geometry and growing air-sensitive thin films on it via molecular beam epitaxy (MBE), we can systematically investigate how electronic phases of these materials respond to gating-induced changes in carrier density.

Conventional DFT calculations of 1T-TaSe₂ band structure predict that it exhibits metallic behavior. However, experiments by the Crommie group have shown 1T-TaSe₂ hosts a Mott insulating ground state (Figure 1)[1]. When Coulomb interactions are taken into account during the analysis, the theory matches the experiment for certain bias voltages (Figure 2). Discrepancies in the low energy conduction bands, (circled in Figure 1 and 2) calls for further experiments and motivates this research.

Scanning Tunneling Spectroscopy Shows Orbital Texture

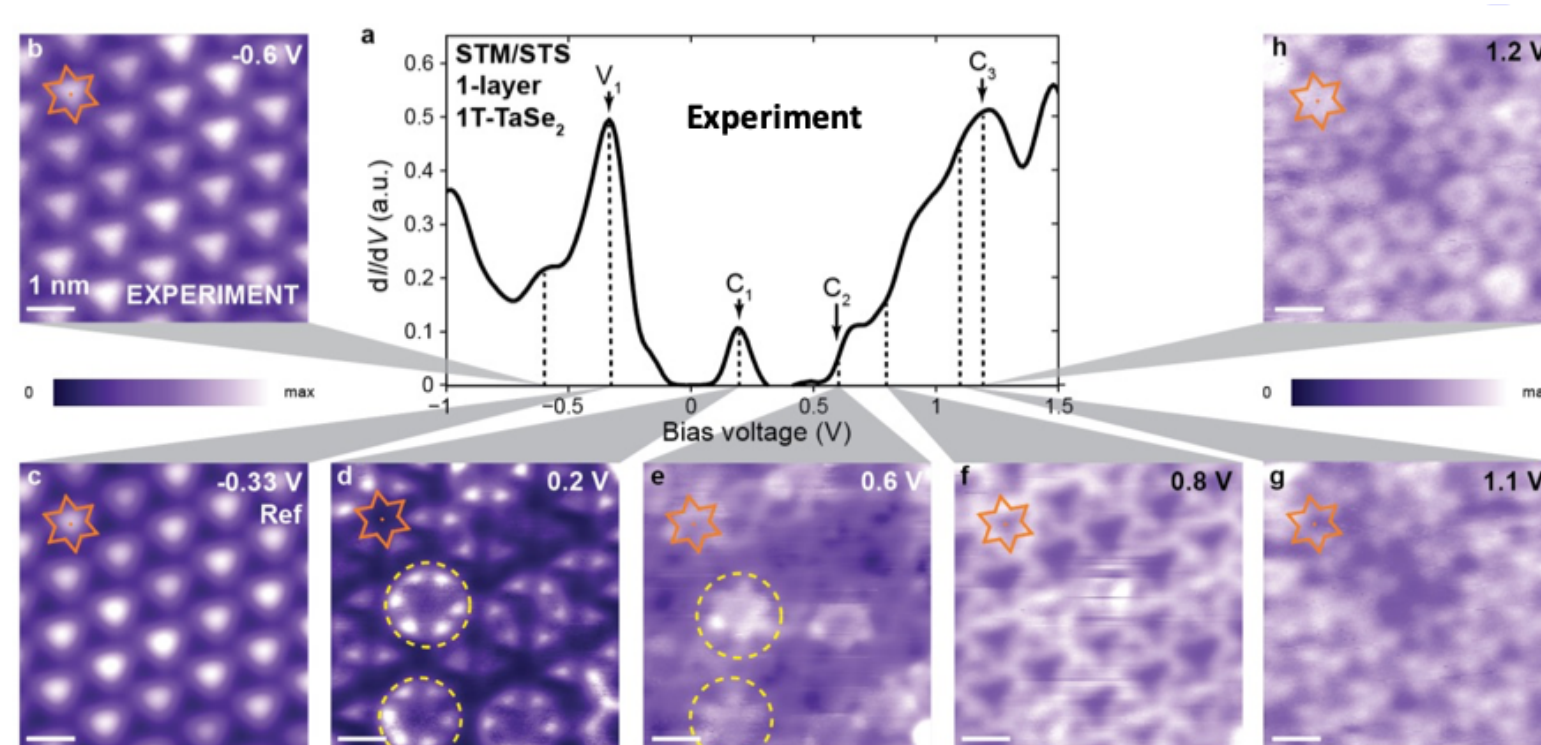


Figure 1: dI/dV maps are shown of the same patch of single-layer 1T-TaSe₂ for different energies, as indicated. Valence band states show state density smoothly distributed over each star-of-David cluster, but conduction band states show novel orbital texture. (STM imaging: Crommie group; growth: Mo, Shen groups)

Mott Insulation: 1T-TaSe₂

A pressing question in the field of quantum materials is the behavior of states formed in a doped Mott insulator. Bulk 1T-TaSe₂ and the surface of bulk 1T-TaSe₂ are materials made up of layered transition metal dichalcogenides (TMDs). These materials are known to have unique insulating phases in the star-of-David charge density wave (CDW) state. However, the insulating nature of these materials is complicated by the stacking of layers, which has led to differing opinions on the effects of this stacking on the insulating phase. To better understand the respective contributions of electron correlation and interlayer coupling in quasi-2D materials, my colleagues are studying atomically thin 1T-TMDs as they offer an ideal platform to investigate these effects. Single-layer systems can be fully characterized in the absence of interlayer coupling, allowing for differentiation between contributions from electron correlation and interlayer coupling.

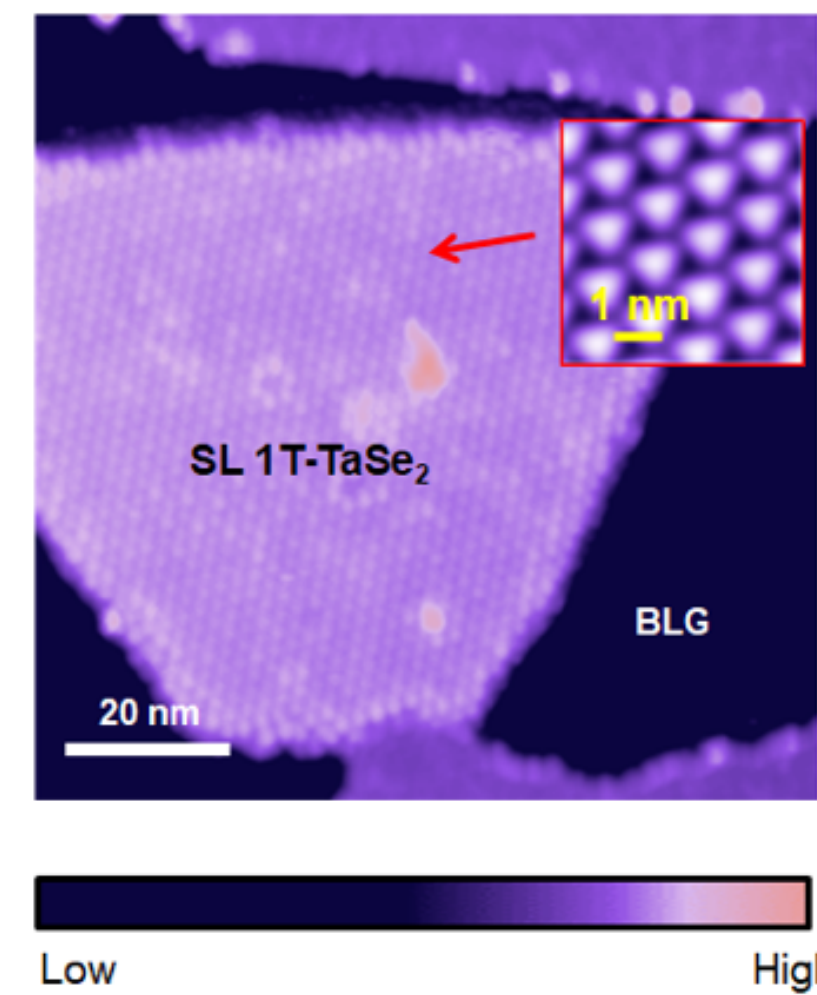


Figure 3: STM image of single-layer 1T-TaSe₂ exhibits the star-of-David phase. Each maximum in the wavefunction corresponds to a 13-atom cluster of Ta atoms. (STM imaging: Crommie group; growth: Mo, Shen groups).

Theoretical DOS and Orbital Texture for Single Layer 1T-TaSe₂

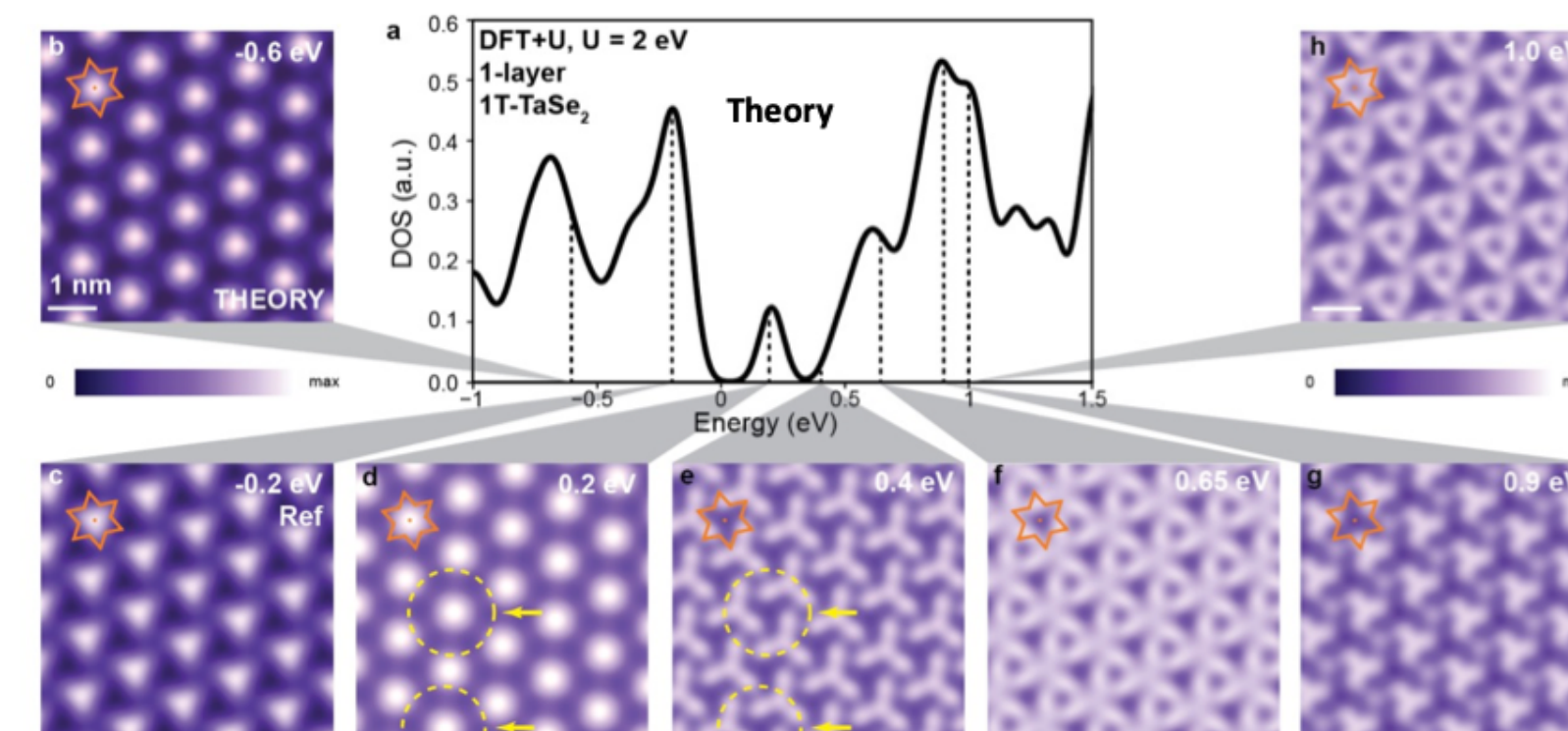


Figure 2: Theoretical density of states and wavefunction distributions (local density of states) for single-layer 1T-TaSe₂ at different energies calculated via DFT+U. (STM imaging: Crommie group; growth: Mo, Shen groups)

Fabrication: Graphene FET

We aim to fabricate a gate-tunable device for investigating Mott insulator phase transitions under electrostatic doping using scanning tunneling microscopy (STM). To achieve this, graphene is mechanically exfoliated from graphite, then transferred onto hexagonal boron nitride (hBN) via a polymer-assisted transfer technique, before annealing the sample in a forming gas to further eliminate possible surface contamination. Such a FET device will be suitable for MBE growth of novel 2D materials, notably 1T-TaSe₂. There are stringent constraints on the conditions of exfoliated graphene flakes: they must be in monolayer form to reduce screening and achieve effective gating, and they must be atomically clean (free from adsorbates) to facilitate MBE growth. We use digital contrast in the images of flakes to distinguish between atomic heights (Figure 4). Due to their microscopic size, the production of effective flakes is stochastic. Part of this research includes the optimization of exfoliation through scientific methods.

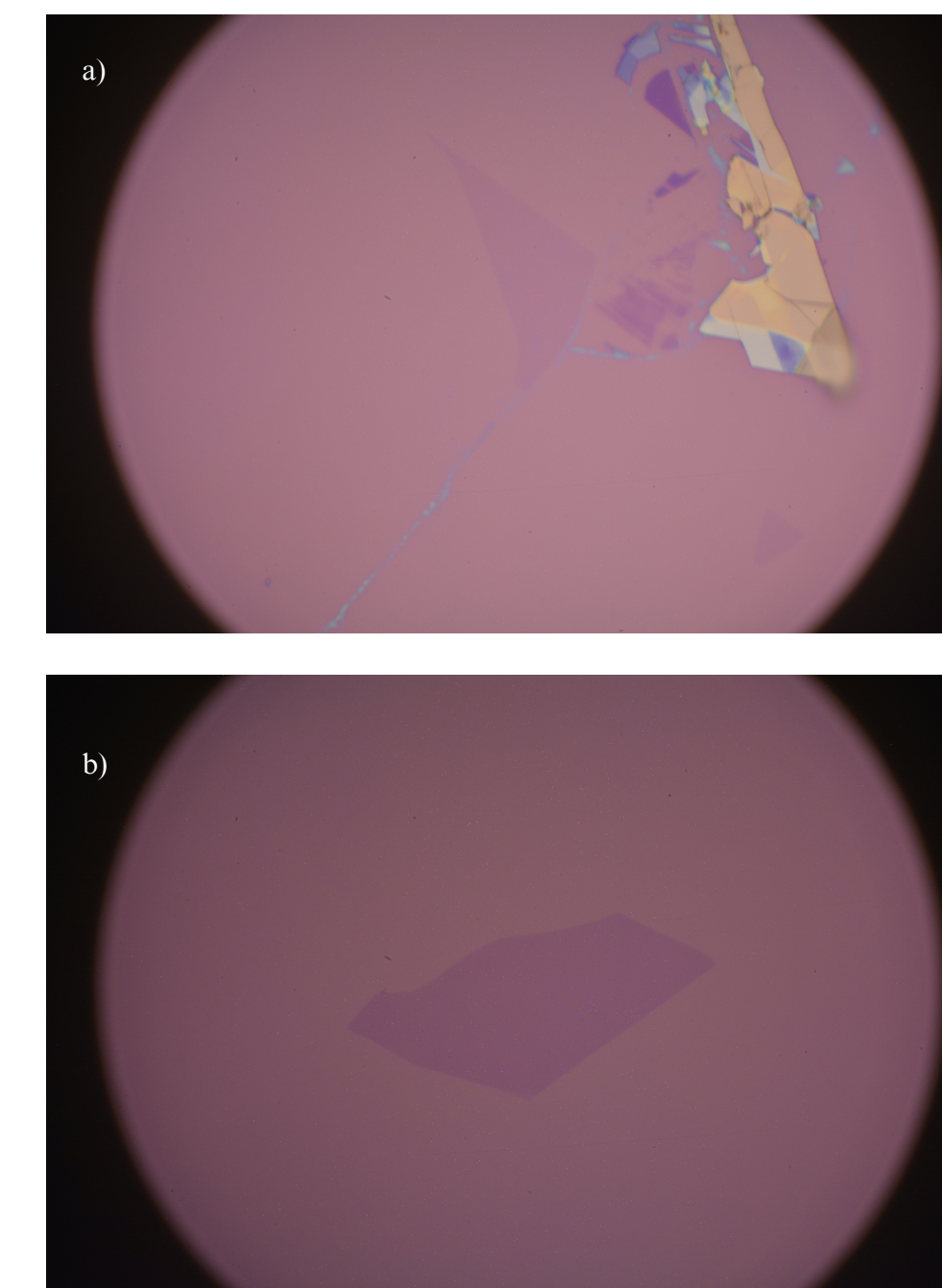


Figure 4: Graphite flakes under 100x magnification. a) and b) are monolayer (graphene) and bilayer graphite, respectively. Note the visual similarity requiring computational methods for distinguishing the two.

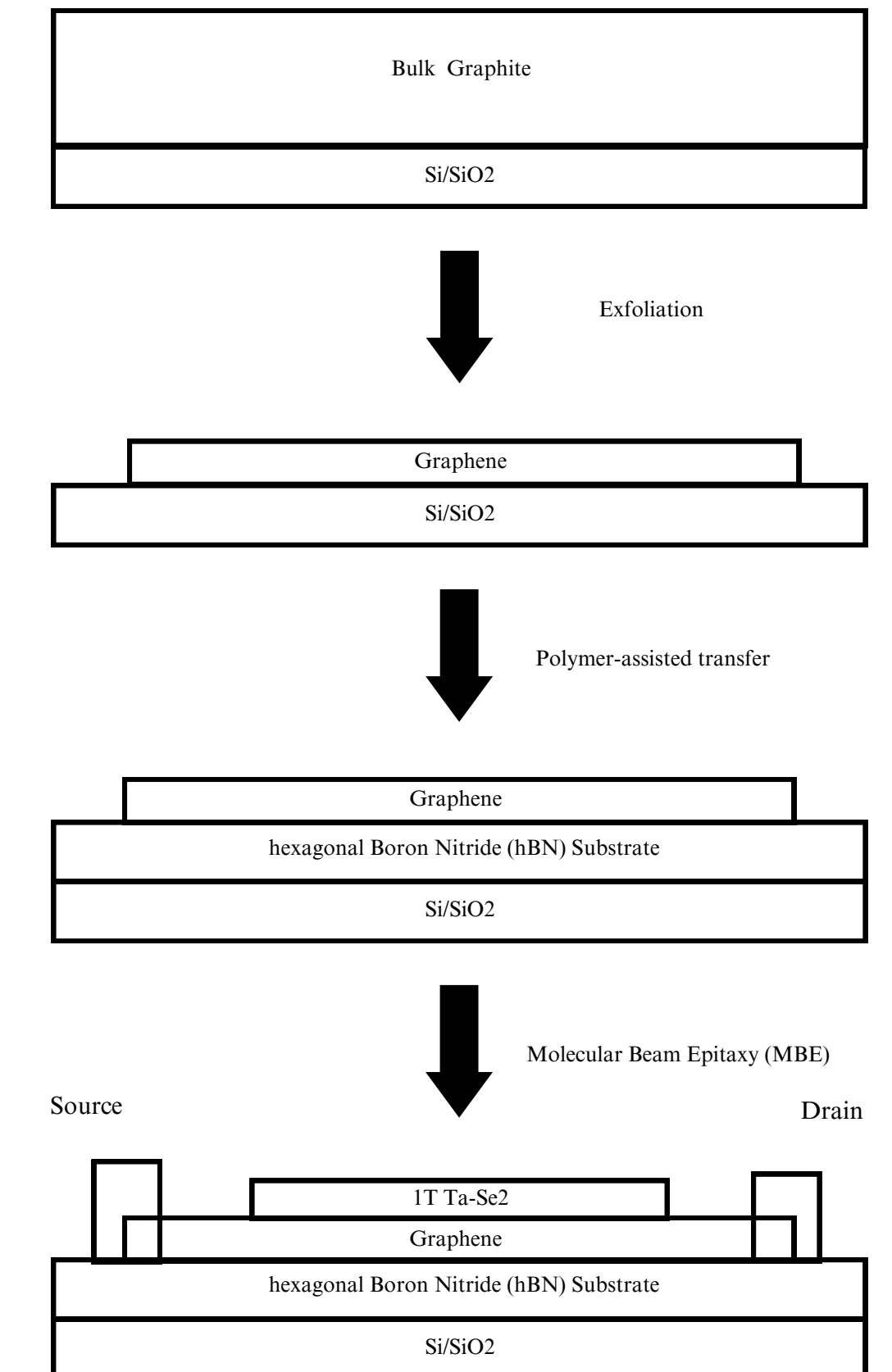


Figure 5: Graphene FET Schematic

Electrostatic doping is achieved by applying a gate voltage to the graphene FET, which allows for continuous control of the electron density in the 1T-TaSe₂ without inducing structural defects. My colleagues and collaborators will use STM to probe the electronic structure of 1T-TaSe₂ directly, providing the first local characterization of a doped 2D Mott insulator.

References:

1. Chen, Y., Ruan, W., Wu, M. et al. Strong correlations and orbital texture in single-layer 1T-TaSe₂. Nat. Phys. 16, 218–224 (2020).
2. S. Colonna, F. Ronci, A. Cricenti, L. Perfetti, H. Berger, and M. Grioni, Mott Phase at the Surface Of 1T-TaSe₂ Observed by Scanning Tunneling Microscopy, Phys. Rev. Lett. 94, (2005).