2D Materials

Room 205 ABCD W - Session 2D-TuA

2D Materials: Theory and Applications

Moderator: Kai Xiao, Oak Ridge National Laboratory

5:15pm **2D-TuA-13 Theoretical Study of van der Waals expitacy of Biayer Silicene on III-Sb substrates**, ***Kumar Vishal***, *Hong Huang, yan zhuang,* wright state university

Research development of integrated silicon photonics in the mid-infrared (MIR) range has gained considerable momentum over the past decades, driven by its vital applications in biochemical sensing, medicine, and even astronomy communications. However, progress has been hampered by the limitation by the energy bandgap and optical transparency in conventional material. Very recently, it has been reported that 2D bilayer silicon (BLSi) demonstrates unique optical properties across the MIR spectrum. By adjusting the strain, the optical absorptions can be tuned in a wide range of wavelength from 1.5 -11.5 mm. However, experimentally the maximum in-plane strain achieved is ∼7% in a lattice-matching expitaxial silicon. Remote- and Van der Waals expitaxy methods can break the lattice-mismatch constraint to obtain single crystal 2D materials, but with an insufficient in-plane strain preserved in the 2D films.

In this work, motivated by the recent achievement of dative expitaxy of single crystalline Cr5Te8 on WSe2 enduring a ∼16% lattice mismatch, we conducted a theoretical study based on density function theory (DFT). Our aim is to explore the feasibility of growing BLSi on two III-Sb substrates: GaSb and AlSb. These substrates were chosen due to their ability to provide sufficient in-plane strain (11.92% and 12.23% respectively) to assure energy bandgap opening in BLSi. The generalized gradient approximation (GGA) and the strongly constrained and appropriately normed (SCAN) meta - generalized gradient approximation (meta-GGA) have been employed in the computation to analyze the chemical bond formation and to optimize the energetically favorable atomic structures. Our findings suggest that Van der Waals epitaxy of BLSi on both of the III-Sb substrates is viable when the substrate's surfaces are terminated with the metallic atoms. By forming the dative bonds between the BLsi and the III-Sb substrates, substantial in-plane strain in BLSi can be preserved, leading to a low buckled BLSi with an opened energy bandgaps.

5:30pm **2D-TuA-14 Tuning Bandgap in Nanoporous Graphene through Molecular Design**, ***Mamun Sarker***, *Alexander Sinitskii,* University of Nebraska - Lincoln

Molecular design is a powerful tool for growing graphene nanostructures with atomic precision, enabling control over their electronic and physical properties. Precisely tuning these properties is essential for advancing the next generation of graphene-based 2D electronic devices. In this presentation, I will discuss the on-surface synthesis of novel nanoporous graphene (NPG) materials, whose electronic bandgaps can be tuned from semiconducting to nearly metallic through rational molecular design. These NPGs were synthesized using custom-designed polyaromatic precursors deposited on Au(111) and thermally activated under ultra-high vacuum via surface-assisted chemical reactions. Scanning tunneling microscopy (STM) reveals the structural integrity and periodicity of nanoporous networks. Scanning tunneling spectroscopy (STS), in combination with density functional theory (DFT), shows that strategic modifications in the pore size, topology, and connectivity can reduce the bandgap to as low as 0.05 eV, approaching metallic behavior. This work not only demonstrates the feasibility of tailoring graphene's electronic structure with sub-nanometer precision but also establishes a versatile platform for engineering low-bandgap 2D materials.

5:45pm **2D-TuA-15 How Transparent Is Graphene? An Analytical Model for Remote Epitaxy**, ***Jason Kawasaki***, University of Wisconsin Madison

We propose an analytical model for the remote bonding potential of the substrate ϕ_{remote} that permeates through graphene during remote epitaxy. Our model, based on a Morse interatomic potential, includes the attenuation due to (1) the increased separation between film and substrate and (2) free carrier screening from graphene. Compared with previous slab density functional theory calculations, which use the electrostatic potential as a proxy for bonding, our analytical model provides a more direct description of bonding, explicitly includes screening (which is often ignored), and is based on simple, interpretable, and well benchmarked parameters. We show that the magnitude of $\phi_{remote}(z)$ for typical semiconductor and oxide substrates is few meV or smaller, similar to the van der Waals potential of graphene. This suggests that the potential of graphene, plus the interference between the remote substrate and graphene potentials, must be considered when interpreting experiments on remote epitaxy. We use our model to interpret previous experiments from the remote epitaxy and related literature. True remote effects are often obscured by defect-seeded nucleation, e.g. pinhole epitaxy, that mimics the macroscopic behavior of idealized remote epitaxy. Our model also points to tests, based on tunable screening and spatial extent of the substrate potential, that may increase the strength of the remote potential towards the more idealized picture.

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