2D Materials and van der Waals Heterostructures for Opto-electronics and Quantum Science

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The objective of this research is to fabricate single- to few-layer samples of materials which exhibit a layered character in the bulk or are theoretically predicted to be stable as single layers, and determine their fundamental properties. Just as graphene exhibits dramatically different properties than graphite, theory and initial experiment indicate that the properties of other single monolayer materials will be strikingly different from their bulk counterpart. For example, single layer MoS_2 is a direct gap semiconductor with strong room temperature luminescence, while two-layer and bulk MoS_2 are indirect gap semiconductors. Single monolayer WSe_2 hosts states which exhibit strong single photon emission behavior (quantum emitters), a property of keen interest in a variety of quantum science applications. Theory has predicted similar dramatic property evolution in many other single layer transition metal dichalcogenide materials (e.g., WS_2, $MoSe_2$, VTe_2) that include metals, insulators, semiconductors, ferromagnets, and even potential superconductors, but the basic science is not well understood.

A second objective is to develop a new paradigm for heterostructures unconstrained by lattice match by systematically stacking single monolayers of these two dimensional materials in a sequence of our choosing to form a **van der Waals heterostructure**. We will determine and understand the new electronic and optical properties these heterostructures exhibit, and develop a predictive capability to fabricate them with a property set of our design. The weak interlayer bonding enables a new approach for materials by design through van der Waals epitaxy of non-lattice matched 2D materials, an avenue not possible with traditional epitaxial approaches dominated by out-of-plane bonding. This represents a bottom up approach towards design and fabrication of new materials that do not exist in nature, and a new class of atomic-scale heterostructures that are expected to exhibit properties and functionality beyond the limits of their bulk counterparts. In addition, recent work has demonstrated that the twist angle between two layers can be used to strongly modify the overall properties, producing a moire superpotential and demonstrating that such structures provide a highly tunable quantum materials platform.

In this research, single layer and van der Waals heterostructure samples will be fabricated either by exfoliation from bulk material or by direct synthesis using techniques such as chemical vapor deposition or molecular beam epitaxy, and a wide spectrum of experimental techniques employed to determine the fundamental properties. Extensive instrumentation exists for structural, transport (charge and spin), and optical characterization. Because each constituent atom participates in electron transport while also being a surface atom, these monolayer materials are particularly sensitive to their environment and are obvious candidates for gas/chemical sensors or surface functionalization for biological applications.

Through combined fabrication and theory efforts, this program will enable discovery of materials with new properties and provide avenues to tune the fundamental excitations. The scientific goals have relevance to quantum science, low-power electronics, information processing, chemical/biological sensors, photo-detection, and energy harvesting. Topics of particular interest include

- quantum effects (e.g. single photon emitters)
- moire superlattices in twisted bilayers
- phase transitions as a function of gate voltage, surface doping or other external stimulus (e.g. 2H to 1T)
- ferromagnetic or antiferromagnetic 2D layers
- chemical vapor sensing
- integration of 2D materials with ferroic substrates (e.g. ferroelectric, ferromagnetic)
- prototype device heterostructures utilizing any of the above
- valleytronics / spintronics
- defects and defect passivation
- lateral heterostructures and alloys

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