Predictive theory of tunneling spectroscopy for point defect identification in two-dimensional semiconductors

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Project Summary: This project will develop a predictive first-principles framework for understanding how individual point defects control charge flow in two-dimensional semiconductor heterostructures, by directly comparing to tunneling spectra measured by our collaborator, Prof. Michael Crommie (2023 Vannevar Bush Faculty Fellow). Recent scanning tunneling spectroscopy (STS) studies have revealed sub-band-gap features associated with defect levels, yet their interpretation remains incomplete because previous theoretical models have not fully incorporated the combined effects of tunneling dynamics, vibronic coupling, dielectric confinement, and band alignments that govern the measured spectra. Establishing a predictive framework is therefore essential, as STS provides a unique capability to directly probe the electrical properties of defects in low-dimensional semiconductors. The resulting computational approach may also enable the identification of defects and host materials for future applications in low-power memory, advanced sensing, and neuromorphic computing.