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The optoelectronic properties of in-plane grain boundaries and out-of-plane interfaces in two-dimensional transition metal dichalcogenides

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Two-dimensional monolayer transition metal dichacogenides (TMDs) are a promising new class of nanomaterial for energy harvesting systems. Monolayer group 6 TMDs (MX2, M = Mo, W, X = S, Se) are direct bandgap semiconductors with strongly bound excitons giving potential for diverse physical phenomena such as multiple exciton generation, trion formation, spin valley coupling and hot electron extraction. In this talk, we will study the behavior of electrons and excitons along in- and out-of-plane interfaces of monolayer materials. Using chemical vapor deposition, we produce high-quality, large-area monolayer molybdenum disulfide. Using electron microscopy, optical spectroscopy and electrical transport, we show that these monolayers contain in-plane grain boundaries composed of 8-4-4 ring defects in the hexagonal lattice and that that these grain boundaries impact the local optical and electronic properties of the material. We examine the role of interlayer coupling by building heterostructures of similar and dissimilar monolayer materials using ultra-clean transfer techniques. First, we build bilayers of molybdenum disulfide with a well-defined interlayer twist. Using optical spectroscopy, we observe that the layers electronically hybridize to form an indirect optical transition and that we can continuously tune electronic and optical properties of the bilayer with the twist angle. Next, we study the properties of an atomically thin p-n junction formed by a MoS2-WSe2 heterostucture. From photoluminescence and scanned photocurrent measurements, we demonstrate a photovoltaic response in the junction, mediated by charge transfer across the van der Waals interface.