Tunable band gaps in transition metal dichalcogenides
ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst, DORON NAVEH, ELIAS TOWE, Carnegie Mellon University — We investigate band-gap tuning in transition-metal dichalcogenide bilayers by external electric fields applied perpendicular to the layers. Using density functional theory, we show that the fundamental band gap of MoS$_2$, MoSe$_2$, MoTe$_2$, and WS$_2$ bilayer structures continuously decreases with increasing applied electric fields, eventually rendering them metallic. We interpret our results in the light of the Giant Stark Effect and obtain a robust relationship, which is essentially characterized by the interlayer spacing, for the rate of change of band gap with applied external field. Our study expands the known space of layered materials with widely tunable band gaps beyond the classic example of bilayer graphene and suggests potential directions for fabrication of novel electronic and photonic devices.