Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

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.

Ashwin Ramasubramaniam
University of Massachusetts Amherst

Date submitted: 09 Nov 2011 Electronic form version 1.4