Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Normal Compressive Strain Induced Metallic Transition of Semiconducting Bilayer Transition Metal Dichalcogenides ABHISHEK SINGH, SWASTIBRATA BHATTACHARYYA, Materials Research Centre, Indian Institute of Science Bangalore 560012 INDIA — First principle density functional theory based calculation was carried out to investigate the effect of strain on the band gap of bilayer semiconducting transition metal dichalcogenides (TMDs). The band gap of these materials was observed to decrease smoothly with the application of normal compressive strain. Most importantly, the materials exhibit semiconductor to metal (S-M) transition after a critical pressure (inter-layer distance) is reached. This critical pressure varies with the type and stacking pattern of the material. The S-M transition is attributed to lifting of degeneracy of the bands at the fermi level caused by inter-layer interactions via charge transfer from metal to chalcogens. The GGA result was validated by incorporating the band gap corrections using hybrid functionals and GW method. The tuning of band gap of TMDs by applying normal compressive strain opens a possibility to use these materials in various applications of nanoelectronics such as electromechanical sensors, switches etc.

Abhishek Singh
Materials Research Centre, Indian Institute of Science Bangalore 560012

Date submitted: 09 Nov 2012 Electronic form version 1.4