INSTITUTE SEMINAR

Friday, 19 September 2014 4:00 pm Fermion

Speaker:

Abhishek K. Singh

Materials Research Centre, Indian Institute of Science, Bangalore 560012

Title:

Reversible Tuning of *"Electronic Structure"* of Semiconducting Transition Metal Dichalcogenides

Abstract:

Transition- metal dichalcogenides (TMDs) offer a wide range of 2D materials: metals, superconductors, charge-density-wave systems, Mott insulators, and semiconductors depending on the combination of metal and chalcogen atom. Semiconducting two-dimensional TMDs include MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 and have emerged as promising materials for a range of applications. Tuning the band gaps of 2D materials—for their potential application in electromechanical devices, tunable photodetectors, and lasers—has been a challenge in band gap engineering. We will present the effect of normal compressive strain (NCS) on the electronic properties of semiconducting bilayer TMDs. Using first principle density functional theory we have shown that the band gap of bilayer semiconducting TMDs can be reduced smoothly by applying normal compressive strain (NCS). The materials exhibit semiconductor to metal (S-M) transition after a critical pressure (inter-layer distance) is reached. 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 tuning of band gap of TMDs by applying normal compressive strain opens a new way to use these materials in various applications such as electromechanical sensors, tunable photo detectors and switches.

- Swastibrata Bhattacharyya and Abhishek K. Singh, Phys. Rev. B 86, 075454 (2012).
- A. P. Nayak*, S. Bhattacharyya*, J. Zhu, J. Liu, X. Wu, T. Pandey, C. Jin, A. K. Singh, D. Akinwande, and J-F. Lin, Pressure-Induced Semiconducting to Metallic Transition in Multilayered MoS_2, Nature Communications, **5**, 3731 (2014)