Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Simultaneous tunablility of electronic and phononic gap in SnS_2 under normal compressive strain BABU RAM[1], AADITYA MANJANATH[2], Ph.D student , ABHISHEK KUMAR SINGH[3], Assistant Professor — Ever since the discovery of graphene, 2D materials have emerged as an attractive field of research. Here, using density functional theory based calculations, we show tunability in the electronic structure of mono to multilayered SnS_2 under biaxial tensile (BT), biaxial compressive (BC), and normal compressive (NC) strains. We obtain a reversible semiconductor to metal (S-M) transition in mono to multilayered SnS_2 without changing the nature of the band gap (i.e. indirect). For the stability analysis with applied strain, we use bilayer (2L-)SnS_2 as our prototype system. Surprisingly, under a high NC strain, 2L-SnS_2 does not exhibit unstable modes. The phonon spectra of 2L-SnS_2 shows a gap in the optical region, which, most interestingly, increases with applied NC strain. Such a simultaneous tunability of the electronic as well as phononic properties of SnS_2 under applied strain can be exploited in many applications such as pressure sensors, micromechanical resonators, frequency filters, and in many other multi-physics devices.

[1]Materials Research Centre , Indian Institute of Science , Bangalore, India
[2]Materials Research Centre and Centre for Nanosience and Engineering, Indian Institute of Science, Bangalore, India
[3]Materials Research Centre, Indian Institute of Science, Bangalore, India

Abhishek Kumar Singh
Assistant Professor, Materials Research Centre, Indian Institute of Science, Bangalore

Date submitted: 06 Nov 2015 Electronic form version 1.4