Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

**Effect of pressure on electronic & optical properties of Cadmium Chalocogenides**[1] DHARMBIR SINGH, PIET, Samalkha, Panipat, Haryana, India, PAWAN KUMAR, J.C.D.M. College of Engineering, Sirsa, Haryana, India — We report effect of pressure on electronic & optical properties of Cadmium Chalcogenide. The theoretical computational studies of Cadmium Chalcogenide are carried out using the full-potential linear augmented plane wave (FP-LAPW) method. In this approach the Generalized-gradient-approximation (GGA) is used for the exchange–correlation (XC) potential. We have calculated the equilibrium lattice constant, electronic band structure dispersion, total & partial density of electron states, band gap, bulk modulus, and its pressure derivative. The calculated parameters are found in good agreement with experiment and other theoretical results. Furthermore, optical constants such as dielectric functions, refractive indices, reflectivity, absorption coefficient, optical conductivitity, loss functions of stable Cadmium chalcogende S were calculated for photon energies at ambient & high pressure.

[1]The authors would like to thank to their institute's Director for all the motivation and support

Dharmbir Singh
PIET, Samalkha, Panipat, Haryana, India

Date submitted: 29 Mar 2013 Electronic form version 1.4