

SEMINAR NOTICE

*Department of Physics and Engineering Physics
University of Saskatchewan*

SPEAKER: Arnab Majumdar, PhD Candidate
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TOPIC: *Structural Phase Transition and Superconductivity
at High Pressure*

DATE: October 10th, 2017

TIME: 3:30-4:30 p.m.

PLACE: Physics 103

ABSTRACT:

Crystals show very interesting properties at high pressure. They can undergo phase transitions on being compressed and take up completely different crystal symmetries with novel properties. First principles metadynamics method can be employed to study the reconstructive phase transition and study the path taken for the structural transformation. This method approaches the problem by scanning the free energy surface to determine the most energetically favourable pathway for structural phase transition. The theory behind metadynamics simulations and its application in the case of AlH_3 and H_2S will be addressed in this talk.

H_2S was recently found to have a very high critical temperature at a very high pressure. This is in agreement with a prediction that covalent hydrides have the potential to be high- T_c superconductors. Using first principles calculations within the framework of the Bardeen Cooper Schrieffer (BCS) theory, the phonon mediated superconductivity properties can be studied in detail which will be reported in this presentation for the case of H_2S obtained from the metadynamics calculations. To give a similar idea, I will also talk on the critical temperature and electron-phonon coupling of the newly reported structure of FeH_5 .

Coffee and Cookies will be served in Physics lounge at 3:00 p.m. for those attending the seminar.