Contribution ID: **344** Type: **Poster Presentation**

Computational modelling study of PtAs₂ and PtAsS structures

Wednesday, 13 July 2011 17:00 (2 hours)

<p>We have investigated the electronic, structural and optical properties of the PtAs< sub >< /sub>2 and PtAsS structures using the density functional theory in the framework of Vienna Ab initio Simulation Package (VASP) code within the generalized gradient approximations of Perdew, Burke and Erzenhof (GGA-PBE) . The total energy calculation of PtAs < sub >< /sub>2 and PtAsS have been computed and predict equilibrium lattice parameters that are in good agreement with the experiment. Elastic constants of these structures compare well with experimental measurements, both PtAs< sub >< /sub>2 and PtAsS gave positive independent elastic moduli, condition of mechanical stability. We found good correlation between heats of formation, elastic constants and phonon dispersion curves, all satisfying stability conditions. In particular the phonon dispersion display real frequencies along high symmetry direction of the Brillion zone.

Level (Hons, MSc,
   PhD, other)?

MSc

Consider for a student
   award (Yes / No)?

yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

yes

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