Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Internal Seminar

Periodic trends in the crystal structure stability of d^{10} AB_2X_2 ternary solids

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Chemical compound space of extended systems comprises millions of stoichiometries that can crystallize in the 230 possible space groups. For a given composition, finding the most stable crystal structure remains an open problem in materials science. Clearly, in similarity with the situation in structural bioinformatics, chemical descriptors based inductive modelling holds the key for making further progress in this direction. Such efforts have been made to identify stable structures of some highly symmetric elemental and binary compounds. Some progress have been made in the structural classification of ternary materials using Pettifor structure maps. The present study aims to establish periodic trends in the crystal structure stabilities of the AB_2X_2 ternary compounds exhibiting non-trivial space group symmetries. The complete space of AB_2X_2 ternary compounds includes 122 and 1144 pnictides and chalcogenides that have been shown to exhibit valence fluctuation, p - wave or heavy fermion superconductivity.

The talk will discuss comparisons of lattice parameters predicted using several commonly employed density functional theory (DFT) approximations and identify a scheme that offers good speed-accuracy trade-off. For selected d^{10} subsets of the AB_2X_2 compounds, we present trends in cohesive energies and phonon frequencies. Variations across the periodic table is explained using band structures and densities of states. Strategies to archive the computed datasets in the MolDis Big Data analytics platform (https://moldis.tifrh.res.in/) will also be discussed.

Monday, Jun 3rd 2019

2:30 PM (Tea/Coffee at 2:00 PM)

Seminar Hall, TIFR-H