Contribution ID: **20** Type: **Poster Presentation**

Computational Modelling of Minerals Sulfides

Thursday, 11 July 2019 15:00 (2 hours)

There are several computational techniques and experimental studied minerals sulfides. Group of sulfides in nature and significant importance because they serve as a source of economic for many applications. We used parameterization technique to study chalcopyrite, pyrite, marcasite and sulfides minerals structures using a Density Functional based Tight-Binding (DFTB+). We developed sets of parameters for FeCuS₂, MnS₂, FeS₂, CoS₂, NiS₂, CuS₂ and ZnS₂ mineral compounds. However, S-S interaction pairs produced some good bond lengths, lattice parameters, bulk modulus and elastic constant of minerals sulfides and gave a good agreement of computational-based calculations and experimental results. Density of states (DOS) and band structures chalcopyrite (FeCuS₂) DFTB+ calculations compare with other results showed that there is no bang gap. Cluster Expansion showed alloyed pyrite with Oxygen are stable phases increased band gap and Monte Carlo indicates that the is no phase transition at all different temperature but for photovoltaic applications of fabricating pyrite absorber because there is promise with optimum band gap.

Apply to be
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   award (Yes / No)?

No

Level for award
 (Hons, MSc,
   PhD, N/A)?

N/A

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