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Computational Modelling of Minerals Sulfides

There are several computational techniques and experimental studied minerals sulfides [1-2]. Group of sulfides in nature and significant importance because they serve as a source of economic for many applications. It is also in a main various precious metals such as iron, cobalt, nickel and lead. We used parameterization technique to study iron sulfides, pyrite nanoparticles (NP's) and pentlandites structures using a density functional based tight-binding (DFTB+) [3] method. We developed sets of parameters for FeS2, CuS2, FeCuS2, Co9S8, Fe9S8, Ni9S8, and Fe4Ni5S8 mineral compounds. However S-S interaction pairs produced a 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. Pyrite nanoparticles (NP's) of different sizes ranging from approximately 1 nm to 4.5 nm were considered. The effect of temperature on different sizes of NP's was determined via radial distribution functions (RDF's), energy as a function of temperature and structural changes. At low temperature the RDF's have many and sharp peaks (the structure is still compact), at higher temperature the peaks are few and smooth which is an indicative of phase transition. Cluster Expansion shows alloyed FeS2 with oxygen all stable phases and Monte Carlo indicates that there no phase transition at all different temperature. However alloyed pyrite with oxygen produced an increased band gap. Material Studio (DFTB+ and DMol3), MedeA (VASP), DL_POLY [4] and UNCLE codes calculations all ran using CHPC Lengau cluster. Our observations is that compared to our local cluster, CHPC provided quick time, accuracy both ab-initio and large supercell and gave us good results of the codes.

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