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The structural, electronic and dynamical properties of pyrite-type minerals: DFT and Atomistic Simulations.

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Pyrite is the most common sulphide gangue mineral occurring in base metal sulphide ores around the world. FeS2 is one of the most commonly occurring metal sulphide minerals. Despite its low economic value, its properties have been explored extensively over the years. However, the study of properties of other pyrite-type minerals are still lacking. This work use computational modelling simulation methods to examine the properties of the pyrite-type minerals (MS2, where M = Co, Ni), that have a similar chemical composition. The work will be conducted through the derivation of interatomic potentials. Density Functional Theory (DFT) method was used to calculate the structure and elastic properties of pyrite-type minerals. Subsequently, the DFT data was used for the derivation of interatomic potentials for atomistic simulation. The constructed interatomic potentials were validated by subjecting the minerals to extreme conditions, i.e. temperatures and pressure through molecular dynamics simulations. The structure and elastic properties are in qualitative agreement with DFT data and those from literature. Furthermore, the potentials will be useful into the fundamental understanding of the collectors and surface interaction mechanisms involved in mineral processing.

Apply to be considered for a student ; award (Yes / No)?

No

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

N/A

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