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Atomistic simulations of iron sulphide mineral (marcasite-FeS2) based on a modified interatomic potential

Iron sulphides minerals are used for metal extraction and present in various types of rock such as igneous, sedimentary, and metamorphic ones. Marcasite-FeS2, an iron sulphide mineral is ubiquitous in nature, its oxidation plays a vital role in acid mine drainage, mineral resource recov-ery, and photoelectric material applications. In this work, we employed atomistic simulations to investigate the structural, dynamic, elastic and thermodynamic properties of marcasite-FeS2. To ensure the sufficient performance of atomistic simulations in various applications, the available interatomic potentials of marcasite are modified for better performance. The interatomic potential is validated to exhibits sufficient accuracy and transferability to various properties of bulk marca-site and surfaces. Moreover, the potential model is used for molecular dynamic simulations to study marcasite at elevated temperatures. The model predicts the melting temperature of marcasite to be in good agreement with the experimental. Furthermore, the model was used for the surface calculations of marcasite and predicted the most stable surface, i.e. {101} to compare better with the DFT data than the calculated surface energy with the original potential model. The developed inter-atomic potential can be used directly in future studies to investigate atomic-scale phenomena in minerals.

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