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Computational modelling of sulfides minerals

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Abstract content
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Sulfides minerals are an important group of minerals. They are many found in nature and of industrial significant because they serve as a source of various metal pyrites. We used Dmol, Vienna Ab-initio Simulation Package (VASP) and Density Functional Tight-Binding (DFTB+) modules to study electronic and structural properties of pyrite, marcasite, as well as phases and surface of cobalt binary sulfides structures. We parameterized cobalt sulfide (CoS) using DFTB+ and calculated different structures of cobalt sulfides and showed good structural properties with other calculations. We used DFTB+ method to calculate both ab-initio and molecular dynamic simulations for large structures of FeS₂ at high temperatures of 1500 K. The structural properties such as lattice parameters, bulk modulus and elastic constants in FeS₂ were in good agreement with previous other calculations and experimental results. The DFTB+ molecular dynamics calculation of FeS₂ showed the Radial Distribution Function (RDF), Density of States (DOS) and decreased the band gap at high temperature. Using DFTB+ we alloyed iron sulfide with oxygen and showed the band gap increased.

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