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Computational modelling of sulphides mineral (FeS₂)

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Abstract content
   (Max 300 words)
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Sulphides minerals are important group of minerals. They are found in nature and are of significant industrial and economic importance. They are the main source of various precious metals such as iron, cobalt, nickel and lead. Density functional based Tight Binding (DFTB+) method was used to investigate the electronic and structural properties of pyrite. DFTB+ molecular dynamics simulation was used to study the large structures of FeS₂ at high temperatures. The density of states (DOS) showed a decreased band gap at high temperatures. However alloyed FeS₂ with oxygen produced an increased band gap. The electronic and structural properties such as lattice parameters, bulk modulus and elastic constants of FeS₂ are in good agreement with previously studied theoretical and experimental results.

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