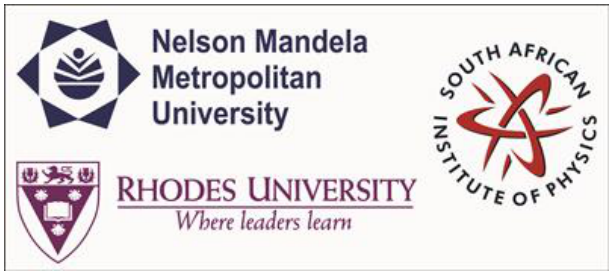

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The modified interatomic potentials of FeS₂ in atomistic simulations

Tuesday, 30 June 2015 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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The modified interatomic potentials were used for both energy minimization and molecular dynamics to study the surfaces and the bulk structure of pyrite. With energy minimization we calculated the surface energies of the surfaces {100}, {110}, {111} and {210}. They revealed that {100} surface is the most stable surface. When we compared the surface energies calculated from the original potentials and the adjusted potentials, it is clear that the adjusted potentials improve the stability of the surfaces. It was also revealed that water stabilizes the surfaces, since the surface energies decreases when hydrated. Molecular dynamics (MD) was used to see the effect of temperature on the surfaces.

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