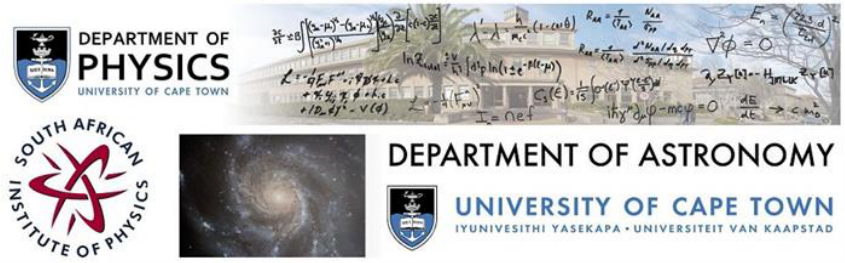

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Molecular dynamics simulations of the interactions between water molecules and sulphide nanoparticles

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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The interaction of water molecules with sulphide nanoparticles has a variety of important geological and technological processes. Nanoparticles have been the area of active research in the recent years due to their unique material properties, which distinguish them from the bulk material. Computational modelling method, molecular dynamics (MD) was performed to provide atomic or molecular level insights of the structural and dynamics of sulphides nanoparticles. MD provides an alternative to experimental approaches for analysis of the interaction between nanoparticles and water molecules. Radial distribution functions, density profiles, and phase changes were calculated to study the effect of water on the nanoparticles. We found that nanoparticles are stabilized in the presence of water, as compared to nanoparticles in vacuum, which undergoes structural changes.

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