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Computational Modelling of FeS₂ Nanoparticles

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Nanoparticles have been the area of active research in the recent years due to their unique material properties, which distinguish them from the bulk materials due to the high surface atom ratio. Pyrite (FeS₂) structures at a nanoscale are considered to be one of few materials for photovoltaics capable of bridging the cost and performance gap of solar batteries. It also holds promise for energy storage applications as the material for high-performance cathodes. Computational modelling technique, molecular dynamics (MD) was performed to provide atomic or molecular level insights of the structural and dynamics of iron sulphide (FeS₂) nanoparticles (NP's). NP's of different sizes ranging from approximately 1 nm to 4.5 nm were considered. The effect of temperature on different sizes of NP's was determined via radial distribution functions (RDF's), energy as a function of temperature and structural changes. At low temperatures the RDF's have many and sharp peaks (the structure is still compact), at higher temperature the peaks are few and smooth which is an indicative of phase transition. Density Functional based Tight-Binding (DFTB+) code was utilized to study the electronic properties of the different sizes of nanoparticles, whereby the effect of temperature on the electronic properties. Band structures have indicated at low temperature there is a low band gap but at high temperature the material become metallic. Our findings have demonstrated that nanotechnology is the future for energy storage especially utilizing pyrite materials.

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