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Effect of temperature on the structure and dynamic properties of metal sulphide nanostructures via molecular dynamics simulation

Tuesday, 26 June 2018 15:00 (2 hours)

Metal sulphide nanostructures via molecular dynamics (MD) simulations at different temperatures are presented and discussed in order to understand their structure and dynamic properties. Nanostructured metal sulphides have attracted the attention of researchers in the fields of materials science, physics and chemistry. They have enhanced structure and dynamic properties due to their large surface-to-volume ratio; hence making them desirable to a wide range of industries. They are promising materials for catalysis, batteries and photovoltaic, however the understanding on the structure and dynamic conditions of large-scale nanostructures are still to be explored more. Computational modelling technique, MD was performed to provide atomic or molecular level insights of the structure and dynamic properties of nanostructured metal sulphides. The effect of temperature on different sizes of nanostructures are analysed in a form of structure and dynamic properties; namely radial distribution functions, potential energy and diffusion coefficient. The results showed that temperature associated with the melting transition and stability increased with an increase in the nanoparticle size. New insight into MD study of nanostructured metal sulphides is obtained and providing guidance to experiments.

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