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Molecular dynamics simulation of TiO₂ nanoparticles using DFTB+ code

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Abstract content
   (Max 300 words)
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Special chars

Titanium nanoparticles, which are anticipated to a wide range of batteries industries, have been shown to exhibit enhanced properties compared to their bulk counterparts. This enhancement has mostly been attributed to their large surface area-to-volume ratio and has attracted enormous research interest in recent years. In this work, molecular dynamics simulations have been performed on anatase TiO₂ nanoparticles at different temperatures using DFTB+ code. Thermodynamic and structural properties such as total system energies and radial distribution functions are reported for the different nanoparticle sizes. At high temperatures, the structures are seen to transform from a highly crystalline to liquid form. Studies conducted on the change of final structure (after simulation) with respect to the initial structure (before simulation) revealed that after simulation, structural disordering (i.e., change in atom position) is more visible at the surface layer compared to the bulk of the final structure.

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD)?

MSc

Main supervisor (name and email)
and his / her institution

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Yes

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