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MOLECULAR DYNAMICS SIMULATION OF TiO2 NANOPARTICLES USING DFTB+ CODE

Titanium dioxide 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.

Summary

This present work is intended to give us a great appreciation for batteries by exploring basic parts, reactions and processes that make them work. Anatase TiO2 nanoparticles large surface area-to-volume ratio make this nano-structured material a potentially important candidate for use in efficient storage devices as an anode material. Finally, it is worth pointing out that anatase TiO2 nanotubes can work under extreme temperature without compromising its conductivity capability.

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