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Computational study of TiO₂ polymorphs as an anode material for energy storage devices

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Abstract content
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Energy production and storage plays an important role concerning our daily life, e.g. electronic devices. The increasing demand for powering systems of portable electronic devices and zero-emission vehicles stimulates research towards high energy and high voltage systems is a challenge. In lithium-ion battery, graphite is a widely used anode material, but it has some disadvantages as compare to anatase TiO₂ nanotube anode such as electrical disconnection, structural deformation, and initial loss of capacity. Given these exciting properties, it becomes necessary not only to synthesize such solid-state and molecular systems but also to model their properties at an appropriate size and time scale. In this work we have predicted the structural parameters for TiO₂ polymorphs and these parameters were found to be in agreement with an experimental data. We also calculated the band gap energies, predicted band structures and density of states for these polymorphs in an effort to validate the DFTB+ potentials. The geometry optimizations were performed using DFTB+ potentials that we derived. Moreover, these properties will determine which TiO₂ polymorph can be used as an anode material in future storage devices.

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