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Computational study of anatase TiO2 as an anode material energy storage devices

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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. 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.

HPC content

CHPC(Lengau) have been used in most of my PhD calculations. I used DFTB+ which is an implementation of the Density Functional based Tight Binding (DFTB) method within material studio(Biovia). DFTB+ offers an approximate density functional theory based quantum simulation tool with functionalities similar to ab initio quantum mechanical packages while being one or two orders of magnitude faster. When optimizing the structure of molecules and solids at CHPC, my calculation where faster as compare to the ones that I ran localy.

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