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DFTB study of Li_xTiO₂ with trigonal bipyramid structures: an insight into lithium-ion battery anode materials

In lithium-ion battery, graphite is a widely used anode material, but it has some disadvantages as compare to TiO2 nanoparticles anode such as electrical disconnection, structural deformation, and initial loss of capacity. The choice of the anode material is very important for an effective development of a high energy density batteries and the use of high capacity electrode materials (anode & cathode) is an essential factor.
The computational simulation calculations have been performed at CHPC (Lengau) for our systems using 48 cores. The TiO2 trigonal bipyramid (TB) structures anode is a material that conducts electric current and they do not expand to more than 5% their original volume during charging and shrink again during discharge. 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 study TiO2 polymorphs (bulk and nanospheres) in an effort to understand how the DFTB+ potentials influence structural parameters and electronic properties. Our structural and electronics parameters are in good agreement with the experimental results.

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