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Feasibility study of DFTB+ parameterization Li, Ti and O systems

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Abstract content
   (Max 300 words)

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. We use a Density-Functional-based Tight Binding (DFTB+) parameterization approach to calculate the Slater-Koster (SK) potentials. The accuracy of Density Functional Theory (DFT) and efficiency of Tight-Binding (TB) will be treated within parameterization procedure to generate a set of DFTB+ parameters that gives the best possible match of DFT energies for anataseTiO₂ with Li structure. Full geometry optimization was performed using LDA and GGA functional's potentials on both bulk and nanotubeTiO₂ structures. Our computational results predict that the lattice parameters of anatase are in good agreement with the available and theoretical data.

Apply to be
 consider 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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Would you like to
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No

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