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Computational study of anatase TiO_2 nanotube as an anode material for lithium ion batteries

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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 TiO_2 nanotube 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 anatase TiO_2 nanotube anode is a material that conducts electric current and they do not expand to more than three times their volume during charging and then 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 anatase TiO_2 analogues (bulk and nanotubes) 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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