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SCC-DFTB parameterization of potentials for simulation of pure TiO₂ and lithiated TiO₂ systems.

A recent self-consistent-charge density-functional tight-binding (SCC-DFTB) set of parameters for Ti-X pairs of elements (X = Ti, O, Li) has been developed. The performance of this set has been validated with respect to TiO2 bulk polymorphs and TiO2 nanotube systems. It has been found that the band structures and geometric parameters of anatase, brookite and rutile and polymorphs are in good agreement with the reference computational data and with experiment. These set of parameters were also tested on lithiated bulk TiO2 and nanotubes.
Most computational simulation has been performed at CHPC (Lengau) for our systems using 24 cores. However, the duration of nanotubes simulation was a challenge, since each job has a time limit of 96 hours using HPC resources. The performance of SCC-DFTB parameters set has been validated on TiO2 systems within materials studio. The current DFTB module is a suitable tool for future in-depth investigation of chemical processes occurring on the TiO2 polymorphs and nanotubes as well as for other processes of physicochemical interest.

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