Na uptake at TiO_2 anatase surfaces under electric field control: a first-principles study

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Anatase nanoparticle (TiO_2) is an efficient Na-ion battery negative electrode, but its activity depends on the exposed crystalline facets. Hence, we propose here a DFT+U study of Na^+ adsorption and insertion at (101), (100) and (001)-TiO_2 surfaces under the influence of external electric fields, which are simulated by adding a sawtooth-like electrostatic potential to the bare ionic potential. Our results highlight the high-energy (001) surface to be the most active, for both directions of external fields, proving its activity to be exerted reversibly. Besides further insights, these outcomes pave the route for further exploration and design of electrode materials by simulation of battery *in operando* conditions.