Abstract

Hydrogen and sodium titanates have attracted interest as possible photocatalysts for

energy conversion, storage and environmental remediation. Here, first-principles calcula-

tions based on density functional theory have been carried out to study their crystal and

electronic structures, their exfoliation behaviour and defect formation. In the hydrogen

titanate, half of the hydrogen forms water in the stoichiometric compound, and the crystal

cell has a lower symmetry with respect to its sodium counterpart. H2Ti3O7 and Na2Ti3O7

have electronic gaps of 2.96 eV and 3.13 eV, respectively. Hydrogen and sodium vacancies

are the defects with the lowest formation energies, making these compounds p-type semi-

conductors. Oxygen vacancy formation is suppressed with respect to titanium dioxide.

Finally, the two compounds have a low surface energy, promoting exfoliation of the bulk

and the formation of 2D materials and nanotubes.