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Water adsorption on strontium titanate stepped surface.

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Recently synthesized strontium titanate (STO) multifaceted nanoparticles demonstrated promising for water-splitting properties. Combining facets with different topology, these nanoparticles provide favourable conditions for facet-targeted doping and therefore more efficient charge generation. Topologically different facets also reduce recombination of the generated charge.
There are two primary types of facet topologies for these nanoparticles – regular (001) surface and parallel to (110) stepped surface. The latter one is considered to be stepped with faces of the steps parallel to (001) and equivalent directions, as energetically more stable, than (110) surface.
Water molecule adsorption and dissociation modelling was performed on the stepped STO surface. The most energetically favourable adsorption sites and configurations were found. Based on the obtained data, water splitting rection mechanism was proposed.