A DFT STUDY OF THE EFFECT OF SO_4 GROUPS ON THE PROPERTIES OF TiO_2 NANOPARTICLES

O. Miroshnichenko[1,2], S. Posysaev[1,2] and M. Alatalo[1]

[1] University of Oulu, Theoretical Physics Research Unit, P.O. Box 3000, FI–90014 Oulu, Finland
[2] Peter the Great St. Petersburg Polytechnic University, Department of Theoretical Mechanics, Polytechnicheskaya 29, 195251 St. Petersburg, Russian Federation
email: Olga.Miroshnichenko@oulu.fi

Titanium dioxide is one of the most investigated and most widely used semiconductor metal oxides. Such popularity comes from its countless applications in an enormous number of industry and technology fields with an increasing interest in nanosized TiO_2 clusters. The properties of small particles are different from the bulk, which is very important in, for example, light scattering measurements, where the refractive index is needed. The optical and electronic properties of titanium dioxide nanoparticles have shown to be strongly dependent on the structure and size of the particle[1, 2]. Besides these size and shape dependent changes, in the case of small particles, the effects of adsorbates become increasingly important, because in the applications, the nanoparticles often reside in water or other, more complicated solutions. Therefore, it is essential to understand the properties of TiO_2 nanoparticles in more detail and to extend the earlier results to realistic conditions, where adsorbates such as hydroxyls [3] and SO_4 groups are present on the surface of the clusters.

We have performed density functional theory (DFT) and time-dependent DFT calculations for titanium dioxide nanoparticles covered with varying number (1-4) of SO_4 groups. We find that SO_4 groups significantly affect the structure of nanoparticles and also change the photoabsorption characteristics. Moreover SO_4 groups influence the structure during the particle growth at the early stages of sulfate manufacturing method, allowing the particle to form in anatase structure instead of rutile.

[1] S. Auvinen, M. Alatalo, H. Haario, J.-P. Jalava, R.-J. Lamminmäki, J. Phys. Chem. C **115**, 8484 (2011).
[2] S. Auvinen, M. Alatalo, H. Haario, E. Vartiainen, J.-P. Jalava, R.-J. Lamminmäki, J. Phys. Chem. C, **117**, 3503 (2013).
[3] O. Miroshnichenko, S. Auvinen, M. Alatalo, Phys. Chem. Chem. Phys., **17**, 5321-5327 (2015).