Porous silicon partly filled with water molecules: crystal structure, energy bands and optical properties from first principles

Ya. Shchur[a], A.S. Andrushchak[b], S. Vitusevich[c], O. Pavlyuk[d] and A.V. Kityk[e]

[a] *Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine, E–mail: shchur@icmp.lviv.ua*

[b] *Lviv Polytechnic National University, 12 S. Bandery str., 79013, Lviv, Ukraine*

[c] *Institute of Bioelectronics (ICS-8), Forschungszentrum Juelich, D-52425 Juelich, Germany*

[d] *Ivan Franko National University of Lviv, 6 Kyryla and Mefodia str., 79005 Lviv, Ukraine*

[e] *Faculty of the Electrical Engineering, Czestochowa University of Technology, Al. Armii Krajowej 17, 42-200, Czestochowa, Poland*

We present the *ab initio* study of band structure and optical properties of porous silicon partly filled with water molecules. Our research is aimed at elucidating the evolution of the main electron structure properties of Si going from ordinary bulk three-dimensional material to porous state with ordered pores of a nanosize level. We are also interested in water structuring properties in the small Si pores, on the one hand, and the water impact on the energy band structure and optical properties of such nanocomposite compound represented by porous Si with water molecules inside the pores, on the other hand.

We investigated several periodic space morphologies of porous Si filled with water molecules as a function of pore diameter ranging from 7.5 to 15 Å, containing 8 to 24 H_2O molecules and the supercell including totally 91 to 211 atoms, respectively. Energy bands, density of states, high-frequency dispersion of dielectric permittivity, refractive indices, extinction coefficients and absorption spectra were calculated. We established that the energy band gap of porous Si mostly increases with increasing pore diameter. An embedding of water molecules into the pores of Si has insignificant impact on the energy band gap of such nanocomposite. However, we revealed significant changes in refractive indices and extinction coefficients when pores were filled with water. In general, the filling the pores with water molecules results in reduction of the tetrahedral space anisotropy of electron structure inherent to nanoporous Si.