Nanochemistry and Nanobiotechnology.

Di- and fourth-cores complexes of zirconium and hafnium in aqueous solutions – DFT analysis

Ł. Siepietowski[1]

[1] *Department of Inorganic, Analytical Chemistry and Electrochemistry, Faculty of Chemistry, Silesian University of Technology, B. Krzywoustego 6, 44-100 Gliwice, Poland.*
E-mail: Lukasz.Siepietowski@polsl.pl

A zirconium and hafnium salt solutions are precursors of nanooxides of zirconium and hafnium. If we want obtain a mixed hafnium-zirconium nanooxides, it could be a very interesting which mixed tetramers appear in the solutions.

In this paper are presented the results of DFT calculations for dimers and tetramers of hafnium and zirconium aqua-hydroxo-complexes. The B3LYP method with the potential of Douglas-Kroll, and the third row and including the presence of a solvent (Continuum Polarizable Model) was were used. In the considered ions, the multicenter orbitals localized on hafnium atoms with an energy corresponding to the level 1s of single hafnium atoms were observed. There was were no multicenter orbitals localized on zirconium atoms corresponding to 1s orbital of a single atom of these metals. Both hafnium and zirconium atoms contained in tetramers have multicentral orbitals corresponding to 2p and 3d orbitals of single atoms of respectively hafnium and zirconium respectively.

As a result, the calculation of the free energy of multicentral ions in an aqueous solution, the multicentral ions' molar free energy of creation, the molar free energy of polymerization to the tetramer, as well as the stability of the constants of polymerization were obtained.

1. *Zielen A . J., Connic R. E.// J. Am. Chem. Soc.- 1956- **78**(22), 5785-5792.*
2. *Devia D. H., Sykes A. G.// Inorg. Chem. -1981- **20**, 910-913.*