Preparation and Optical Properties of Zirconia Sol-Gel Materials

Nina Petkova [1], Stoyan Gutzov [1], Ivelina Georgieva [2], Natasha Trendafilova [2], Stephen Dlugocz [3]

[1] Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria.
E-mail: npetkova@chem.uni-sofia.bg
[2] Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria.
[3] Institute of Physical and Theoretical Chemistry, Braunschweig University of Technology, Braunschweig, Germany.

The sol - gel technology is a low temperature method for preparation of different oxide materials like SiO_2, ZrO_2, Al_2O_3 or SnO_2 with interesting optical, electrical and mechanical properties from liquid precursors [1, 2]. In the present contribution the preparation and optical properties of sol-gel zirconia materials obtained via different schemes are described, which are potential candidates for doping with rare-earth complexes. The sol-gel materials are characterized with UV/Vis/NIR reflectance spectroscopy, SEM / TEM microscopy, IR and X-ray diffraction and molecular modeling with programs Gaussian09 and Turbomole. The use of chelating ligands like acetylacetone (AcAc) and acetic acid (AA) leads to transparent gels with high optical quality, materials prepared without modifying agents display a granule structure. Samples obtained with AcAc are yellow colored because of the formation of a complex between zirconium and AcAc with two characteristic peaks at 290 nm and 450 – 550 nm due to intra-ligand electronic transitions. The optical band gap of the prepared sol-gel glasses changes from 2.97 eV (AcAc addition) to 4.85 eV (preparation without chelating agents) depending on the doping conditions. Three potential Zr(IV)-AcAc complexes are modeled: $Zr(AcAc)_2(BuO)_2$, $Zr(AcAc)_2(OH)_2$ and $Zr(AcAc)_2(OH)_2{\cdot}2H_2O$ in order to understand their UV/Vis optical properties. The geometry optimizations and TDDFT calculations are performed at B3LYP/6-31++G(d) level and small effective core potential (SDD) for the Zr atom.

References

1. S. Gutzov, G. Ahmed, N. Petkova, E. Füglein, I. Petkov, *J. Non-Cryst Solids* **354** (2008) 3438.
2. G. Ahmed, I. Petkov, S. Gutzov, *J. Incl. Phenom. Macrocyclic Chem.* **64** (2009) 134.