Contribution ID: **288** Type: **Poster**

Application of the two-step approach to investigaion of chemical shifts and other electronic properties determined by core region of heavy atoms

Monday, 12 May 2014 17:15 (1h 30m)

Modeling of electronic structure and properties of actinide compounds is of considerable importance for modern radiochemistry. However, reliable and accurate estimates are a great challenge for quantum chemistry of actinides due to strong relativistic and correlation effects in such compounds. A development of theoretical approaches to this problem will stimulate application of a number of experimental techniques of analytic chemistry such as the method of chemical shifts in X-ray emission spectroscopy (XES).
We report application of the theoretical method of generalized relativistic effective core potential [1] followed by the method of one-center nonvariational restoration [2] of valence electron wave function in the vicinity of heavy atoms to calculation of different properties of compounds containing heavy elements including actinides. Basing on the developed atom-in-compound (AiC) concept we demonstrate a possibility to use XES to control a number of properties that are determined by the core region of valence wavefunction. We show its applicability to provide a unified tool for indirect and independent accuracy check of the evaluated AiC characteristics. This is of great importance to the cases where an experimental check is difficult or even impossible [3].

The work is supported by the SPbU Fundamental Science Research grant from Federal budget #0.38.652.2013 and RFBR grant 13-03-01234-a. L.S. is also grateful to the President of RF grant no 5877.2014.2 and to the Dmitry Zimin “Dynasty” Foundation.

1. N.S. Mosyagin, A.V. Zaitsevskii, and A.V. Titov, Rev. At. Mol. Phys. 1, 63 (2010).
2. A.V. Titov et al., Int. J. Quant. Chem., 104, 223 (2005).
3. L.V. Skripnikov, A.N. Petrov, A.V. Titov, J. Chem. Phys. 139, 221103 (2013).

Primary author: Mr SKRIPNIKOV, Leonid (St. Petersburg State University, Petrodvoretz, Russia; Petersburg Nuclear Physics Institute, Gatchina, Russia)

Co-authors: Mr TITOV, Anatoly (St. Petersburg State University, Petrodvoretz, Russia; Petersburg Nuclear Physics Institute, Gatchina, Russia); LOMACHUK, Yuriy (St. Petersburg State University, Petrodvoretz, Russia; Petersburg Nuclear Physics Institute, Gatchina, Russia)

Presenter: Mr SKRIPNIKOV, Leonid (St. Petersburg State University, Petrodvoretz, Russia; Petersburg Nuclear Physics Institute, Gatchina, Russia)

Session Classification: Poster Session - Nuclear Analytical Methods

Track Classification: Nuclear Analytical Methods