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

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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].

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