“Concept of atoms-in-compounds: application to study electronic structure of molecules and solids containing f- and d-elements”

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Capabilities of x-ray emission spectroscopy and other experimental methods in measuring properties of atoms-in-compounds as a way for non-destructive testing the physical-chemical state of heavy atoms are limited, first of all, by difficulties in interpretation of experimental data. Establishing a straight and unambiguous link between the measured characteristics and the effective states of an atom in a chemical compound [1-3] (material etc.) by modeling its electronic structure has obvious perspectives in applications. However, this connection is still not well exploited due to the extreme cost of modern schemes of the relativistic study of materials and other systems of practical interest. The numerical instability of theoretical estimates of the values of the chemical shifts etc., which are up to six orders of magnitude smaller than the energy of x-ray transitions, is the main problem. It is shown in [1-3] that rather economical calculation of the values of the chemical shifts of X-ray emission spectra for heavy-element compounds can be performed using the embedded cluster model developed in our lab [4].

In the talk our results of the embedded cluster calculations of characteristics of atoms-in-compounds on Th and U in xenotime, the Nb atom in the fersmite mineral (with basic formula CaNb2O6) with respect to the metallic Nb are presented and discussed. The calculations of the embedded cluster’s electronic structure for these structures are performed with using DFT and the generalized relativistic effective core potential method [5]. The values of the chemical shifts are obtained with using the methods developed in [1-5]. The results of optimization of Embedding potentials for ytterbium trifluoride relative difluoride ytterbium etc. are also presented and discussed.

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