**ATOMIC K-SHELL DOUBLE HOLE CREATION DUE TO ELECTRON CAPTURE AND PHOTOIONIZATION**

Kiselev M.D.1,2,3, Gryzlova E.V.3, Grum-Grzhimailo A.N.3

*1Faculty of Physics, Lomonosov Moscow State University, Moscow, Russia;*

 *2Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia;*

*3Laboratory for Modeling of Quantum Processes, Pacific National University, Khabarovsk, Russia*

E-mail: md.kiselev94@gmail.com

Double core hole (DCH) states could be created in two different mechanisms. The first is core subshell electron capture by the nucleus and subsequent shake-process of an electron from the same subshell either to the high unoccupied state (shake-up) or to the continuum (shake-off) mostly due to instant changing of the nucleus charge by unity. Another way is photoionization, when one electron is “knocked out” from the subshell and the residual one undergoes shake-process resulting from changing in screened potential. Physics of the DCH currently attracts interest stimulated by new possibilities of their creation by X-ray free electron lasers and advanced synchrotron sources. Furthermore, DCHs might become a new tool for chemical analysis [1] and plasma diagnostics [2].

In this theoretical contribution we compare the two mechanisms of producing the DCH: K-electron capture and K-shell photoionization. General theoretical approaches to both problems are known, but we are not aware of such a comparison based on up-to-date models for many-electron atoms. We focus on DCH states in K-shell of 7Be and 37Ar (isotopes with natural electron capture radioactivity). The goal is to determine double K-vacancy production probability in both described channels. Also, we analyze shake-off electron spectra and compare the results with different theoretical approaches and experiment.

Our model is based on sudden approximation with the use of fully non-orthogonal sets of electron orbitals in initial and final states, accounting for *j*-splitting of the subshells. Expansions for transition matrix elements are obtained with ZAP\_NO package [3]. Radial wave functions are constructed within the multiconfigurational Hartree-Fock method [4]. Photoionization calculations are performed with the use of B-spline R-matrix (BSR) software complex [5].

This research was funded by the Russian Ministry of Science and Education grant No. 075-15-2021-1353. The work of M.D.K. is supported by the Ministry of Science and Higher Education of the Russian Federation (project No. 0818-2020-0005) using resources of the Shared Services “Data Center of the Far-Eastern Branch of the Russian Academy of Sciences”.

1. M. Nakano *et al.*, Phys. Rev. Lett. 110, 163001 (2013).

2. A.Ya. Faenov *et al.*, Laser and Particle Beams 33, 27 (2015).

3. O. Zatsarinny, Comput. Phys. Comm. 98, 235 (1996).

4. C.F. Fischer, T. Brage and P. Jonsson, Computational Atomic Structure: An MCHF Approach (Bristol: IOP Publishing, 1997).

5. O. Zatsarinny, Comput. Phys. Comm. 174, 273 (2006).