

DOUBLE CORE HOLE PRODUCTION IN ELECTRON K-CAPTURE AND ATOMIC PHOTOIONIZATION

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Double core hole (DCH) states enclose two vacancies in the electronic K-shell of atoms and molecules. This object currently attracts close attention and DCHs might become a new tool for chemical analysis [1] and plasma diagnostics [2]. DCHs are efficiently created by high-brilliance X-ray free-electron lasers in double ionization by two sequentially absorbed γ -quanta [3]. On another side, the DCHs were first detected many years ago in the process of K-electron capture by an atomic nucleus [4], when the nuclear charge is reduced by unity, and the second electron is shaken-up from the K-shell mostly due to the sudden change of the atomic potential. Using bright synchrotron radiation sources, the DCHs are observed in photoabsorption of the X-ray photon by the K-shell electron, with simultaneous shake of the second K-electron [5], similar, in a sense, to the case of the K-electron capture, but with the nuclear charge remaining the same.

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 also believe that theoretical predictions for the shake process in the K-capture, made decades ago, may be improved by using these models. Here we focus on the DCH states in ^{7}Be and ^{37}Ar isotopes with natural electron capture radioactivity and determine the relative DCH production probability P_{KK} . Furthermore, we analyze the relative probability of shake-up and shake-off, when the second K-electron is excited to a discrete state or is ionized, respectively. The shake-off electron spectra in the K-capture are obtained and compared with the results of different theoretical approaches and experiment. The photoionization calculations were performed by the R-matrix method with B-splines, as realized in the BSR package [6]. The non-orthogonality between electron wave functions in the initial and final states, which is crucial in treating ionization from the inner shell, was fully taken into account. The electron wave functions for the bound states were obtained in the multi-configuration Hartree-Fock approximation. The model for the K-capture is based on conventional sudden approximation and is utilizing codes from the same BSR package. Detailed results will be presented at the conference.

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