Relativistic evaluation of inner-shell vacancy-production probabilities in low-energy ion-atom collisions

Y.S. Kozhedub[1], I.I.Tupitsyn[1], V.M. Shabaev[1], G. Plunien[2], S. Hagmann[3], Th. Stöhlker[3]

[1]*Department of Physics, St. Petersburg State University, Ulianovskaya 1, Petrodvorets, St. Petersburg 198504, Russia*
[2]*Institut für Theoretische Physik, Technische Universität Dresden, Mommsenstrasse 13, D-01062 Dresden, Germany*
[3]*Gesellschaft für Schwerionenforschung, Planckstrasse 1, D-64291 Darmstadt, Germany*
kozhedub@pcqnt1.phys.spbu.ru

The previously developed relativistic technique for evaluation of charge-transfer and electron-excitation processes in low-energy ion-atom collisions [1,2] based on active-electron approximation is extended for describing many-electron processes. The method employs the independent particle model, where the effective many-particle Hamiltonian is approximated by a sum of single-particle Hamiltonians reducing the electronic many-particle problem to a set of single-particle equations for all electrons in the collision system. The many-electron wave function is constructed from Slater determinants with single-electron wave functions. Time-dependent single-particle equations are solved using the coupled-channel approach with atomic-like Dirac-Fock-Sturm orbitals, localized at the ions (atoms). Interaction with other electrons is effectively described by the screening density-functional theory potential. Many-particle probabilities are calculated in terms of single-particle amplitudes employing the formalism of inclusive probabilities [3,4]. The developed method is applied to evaluations of the probabilities of many-particle processes. In particular, the K-vacancy-production probability in the Ne–$F^{6+}(1s^2 2s)$ collision at the projectile energies 230 keV/u and 530 keV/u is investigated in details and compared with experimental data and calculations based on the one-active-electron approximation [1]. The K-vacancy production probability is also calculated for the Xe-$Xe^{51+}(1s^2 2s)$ collision. The role of the relativistic effects is analyzed.

References:

[1] I.I. Tupitsyn, Y.S. Kozhedub, V.M. Shabaev, A.I. Bondarev, G.B. Deyneka, I.A. Maltsev, S. Hagmann, G.Plunien, and Th. Stöhlker, Phys. Rev. A **85**, 032712 (2012).

[2] Y.S. Kozhedub, I.I. Tupitsyn, V.M. Shabaev, S. Hagmann, G.Plunien, and Th. Stöhlker, Phys. Scr., in press.

[3] H. J. Lüdde and R. M. Dreizler, J. Phys. B **18**, 107 (1985).

[4] P. Kürpick, H. J. Lüdde, Comput. Phys. Commun. **75**, 127 (1993).