AUGER TRANSITION PROBABILITIES AND ELECTRON EMISSION CROSS SECTIONS DURING 2pπ VACANCY DECAY IN Ne^+-Ne QUASIMOLECULE

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Abstract

The probabilities of Auger transitions are calculated when a vacancy is filled in the 2pπ orbital in the Ne^+-Ne quasimolecule, a short-lived system is formed during ion and atom collisions. For the first time ever, calculations were performed for various degrees of quasimolecule ionization. It was found that with the increase of collision energy and the decrease in distance of the closest particles approach the degree of ionization of the quasimolecule system increases very significantly (from 2 to 6), which should be taken into account when calculating different collisional processes, in particular the particle stopping in matter. The use of quantum-mechanical description with taken into account the collision dynamics made it possible for the first time to quantitatively describe the experimental spectra of Auger electrons for a complex many-electron quasimolecule.

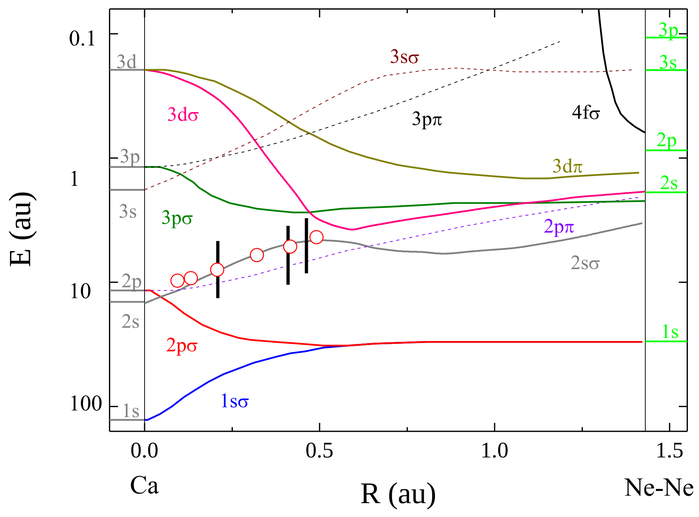

Fig. 1. The position of the effective term (point), which is obtained from the experiment [1,2], and the MO (Molecular orbital theory) diagram for Ne^{2+}-Ne [3].

The Auger transition probability per unit time can be obtained as:

$$W = \frac{2\pi}{\hbar}\left|\iint \chi_f^* \varphi_f^* \frac{e^2}{r_{1,2}} \chi_i \varphi_i d\tau_1 d\tau_2\right|^2$$

where χ_i, φ_i are the one-electron wave functions of two electrons in the atom located at excited levels, χ_f is the wave function of an electron in the $2p\pi$-orbital, φ_f is the wave function of an Auger electron (free electron leaving the atom). The operator $\frac{e^2}{r_{1,2}}$ - describes the Coulomb interaction of two electrons.

The filling of a vacancy at the 2pπ level can occur from the 3pσ orbitals (2 electrons in the orbital), 3dσ (2 electrons), 3dπ (4 electrons). We assume that the 3sσ, 3pπ and 3dδ orbitals do not contain electrons, because they are formed from unoccupied levels at large internuclear distances. The 4fσ orbital is emptied by the transitions of electrons to the continuum.

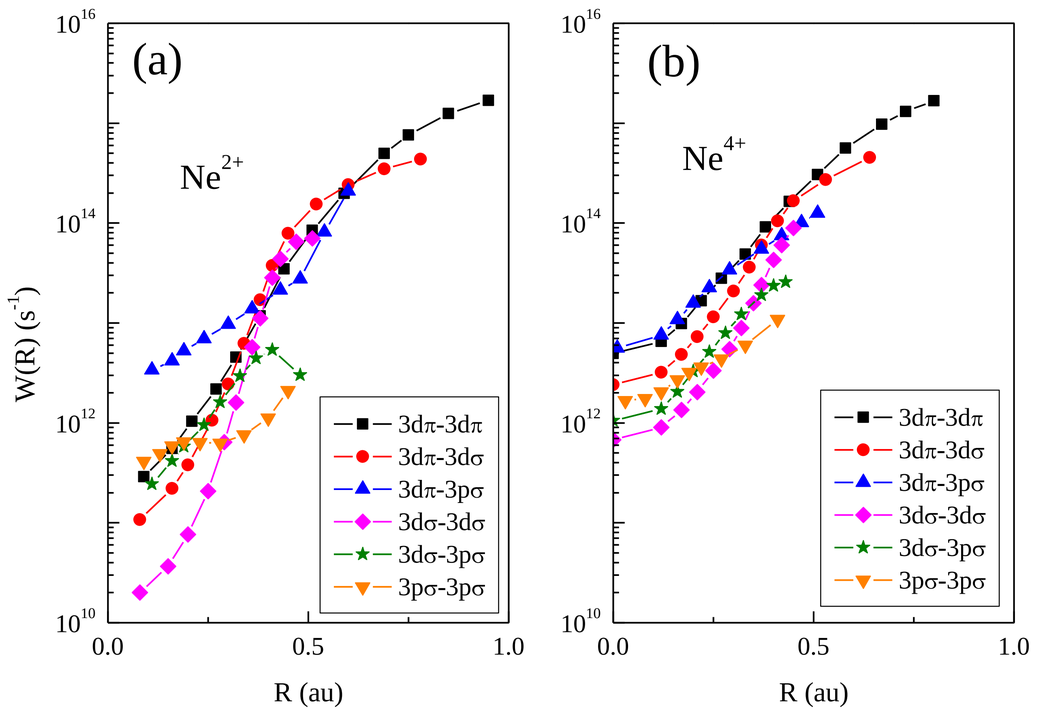

Fig. 2. Auger transitions probabilities for various channels in the Ne^{2+}-Ne (a) Ne^{4+}-Ne (b) quasimolecules as a function of the energy of the emitted Auger electron.

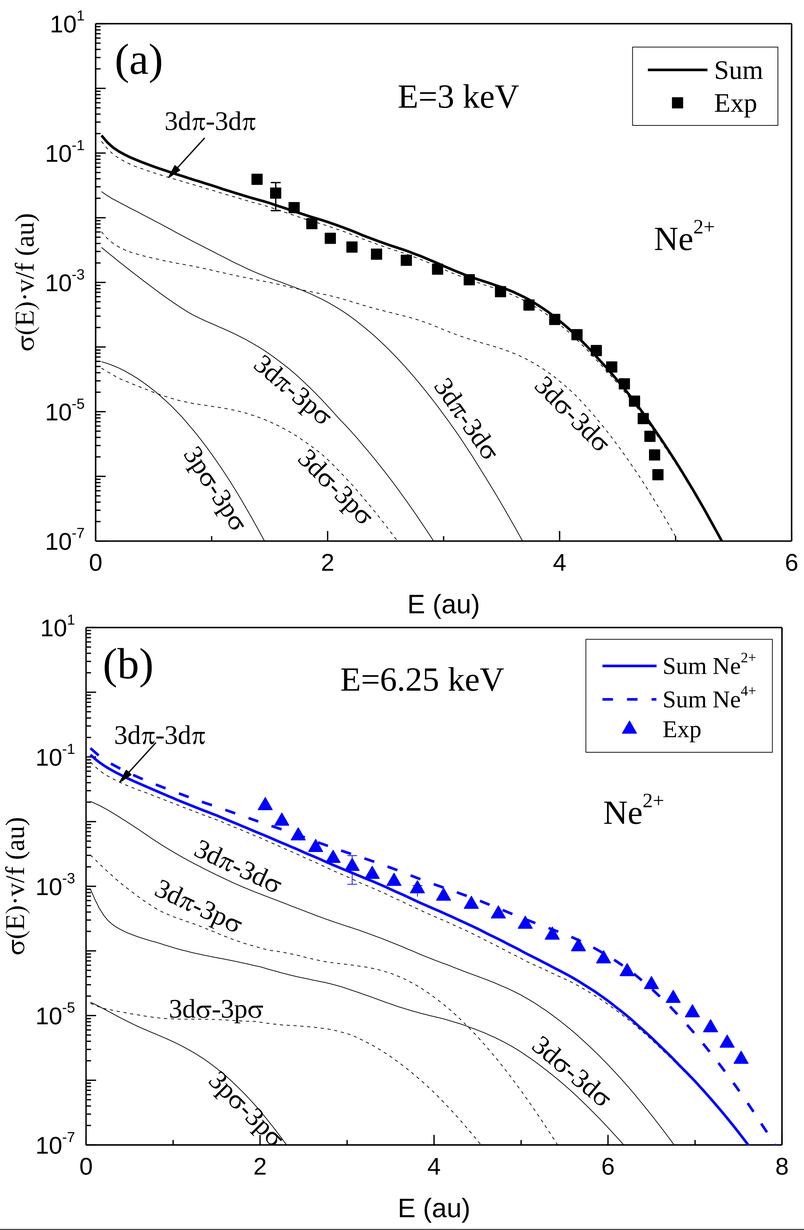

Fig. 3. Comparison of the experimental spectra with our calculations. In the lower left corner, the contribution of various channels for a 2pπ-vacancy decay. Bold curves are the total contribution of all channels. For an energy of 6.25 keV, a calculation is presented for the Ne^{4+}-Ne and Ne^{2+}-Ne systems .

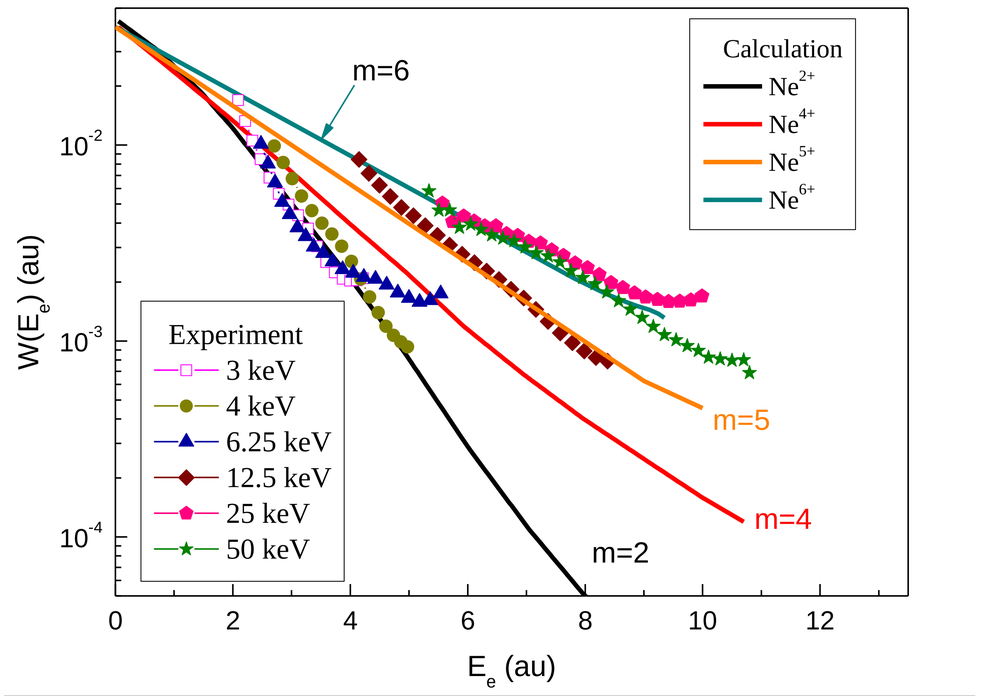

Fig. 4. Comparison of the calculated Auger transition probability for the dominant $3d\pi^2$-$2p\pi\varepsilon$ channel at different ionization degrees (m) of the system with the values obtained from the experiment at different collision energies.

CONCLUSIONS

For the first time ever for a multielectron quasimolecule Ne-Ne, the probabilities of Auger decay of vacancies during a collision were calculated for different degrees of ionization of the quasimolecule and were compared with experiment.

The dominant contribution of the transition from the initial 3dπ-3dπ state to the 2pπ-orbital is established from the whole variety of possible Auger decay channels.

References

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