

Electron capture, excitation and ionization in collisions of Be, Ne_q⁺, Ar_q⁺ ions with proton

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The electron capture and excitation processes in H⁺-Be collisions are investigated by the quantum-mechanical molecular orbital close-coupling (QMOCC) method and by the two-center atomic orbital close-coupling (TC-AOCC) method in the energy range 1-1000eV/u and 0.5-100keV/u, respectively. Total, n-shell and state-selective electron capture and excitation cross sections are calculated with large expansion of MO and AO basis sets. In the overlapping energy range the results of the two sets of calculations are compared. Meanwhile, collisions of proton with Ne(1, 2)⁺ and Ar(1, 2)⁺ ions are studied using the time-dependent density-functional theory (TDDFT). The electron capture, electron loss and ionization cross sections are obtained in the energy range of 1-100keV/u and compared with data from other sources when available.

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