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Study of electron capture and ionization in proton collisions with N_2 using *ab initio* methods.

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Synopsis Electron capture cross sections in collisions of protons with the nitrogen molecule are obtained with two semiclassical *ab initio* methods: one uses multireference configuration interaction wavefunctions while the other is based on monoelectronic wavefunctions and the independent particle approximation. The accuracy and usefulness of this last, simplified, approach is discussed in view of its applicability to study larger systems.

Ion-molecule collisions are ubiquitous events in different environments including interstellar clouds, planetary atmospheres, comets, magnetic fusion reactors and radiation damage of living tissues. One of the important processes that take place in these events is charge transfer (CT), which leads to molecular ionization and the possible production of fast neutrals. In particular, proton collisions with nitrogen molecules take place at the polar regions of the Earth atmosphere due to the incoming flux of the solar wind, in which the typical energies of the protons are of the order of a few keV. Proton collisions with N_2 may also be relevant in the edge of tokamak plasmas, as N_2 is a suggested scavenger for ITER.

In a recent work [1], we have performed a high-level *ab initio* calculation of the first 6 electronic states of the super-molecule $(HN_2)^+$, and the corresponding non-adiabatic couplings between them, and applied the semiclassical eikonal collisional equation to obtain state-selected and total CT cross sections.

In this work, we apply the method presented in [2] to calculate CT and single ionization (SI) cross sections. Within this method, the molecular target is represented by a monoelectronic pseudopotential and the scattering wavefunction is expanded in terms of asymptotically frozen molecular orbitals (AFMO). The anisotropy of the target molecule is accounted for by performing calculations with three different target orientations with respect to the projectile trajectory. The multielectronic analysis is performed using an independent particle interpretation.

Total CT and SI cross sections are obtained in the energy range that goes from 0.1 to 30 keV. The accompanying figure shows these cross sections compared with experimental [3, 4, 5] and other theoretical [6] works.

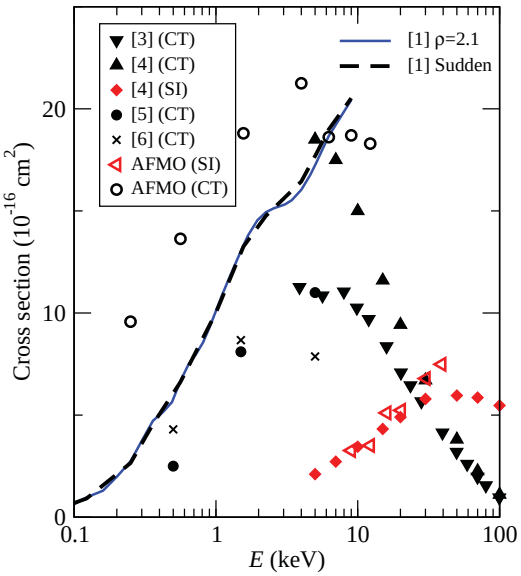

Figure 1. Total charge transfer (CT) and single ionization (SI) cross sections in collions of H^+ with N_2. Our results: lines [1] and empty symbols. Experimental data: [3, 4, 5]. Other calculations: [6].

References

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