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Spin-density functional theory treatment of He^+-He collisions[1]
MATTHEW BAXTER, TOM KIRCHNER, York University, EBERHARD ENGEL, Goethe University Frankfurt — The He^+-He collision system presents an interesting challenge to theory. On one hand, a full treatment of the three-electron dynamics constitutes a massive computational problem that has not been attempted yet; on the other hand, simplified independent-particle-model based descriptions may only provide partial information on either the transitions of the initial target electrons or on the transitions of the projectile electron, depending on the choice of atomic model potentials. We address the He^+-He system within the spin-density functional theory framework on the exchange-only level. The Krieger-Li-Iafrate (KLI) approximation is used to calculate the exchange potentials for the spin-up and spin-down electrons, which ensures the correct asymptotic behavior of the effective (Kohn-Sham) potential consisting of exchange, Hartree and nuclear Coulomb potentials. The orbitals are propagated with the two-center basis generator method. In each time step, simplified versions of them are fed into the KLI equations to calculate the Kohn-Sham potential, which, in turn, is used to generate the orbitals in the next time step. First results for the transitions of all electrons and the resulting charge-changing total cross sections will be presented at the conference.

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