Abstract Submitted
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Quantum-mechanical study of ionization and capture in proton-methane collisions[1] ARASH SALEHZADEH, TOM KIRCHNER, York University
— A recently developed method for first-principles calculations of electron removal from multicenter molecules subjected to ion impact [1] is applied to the proton-methane collision system in the 20 keV to few MeV energy regime. As in our previous work involving water molecules we use a spectral representation of the molecular Hamiltonian and a single-center expansion of the initially populated molecular orbitals to make the problem amenable to the two-center basis generator method for the solution of the time-dependent single-particle equations. Results for (net) capture and ionization are compared with available experimental data and with results obtained from the simple Bragg additivity rule according to which the molecular cross sections are obtained from adding atomic ones. We observe good overall agreement at high energies. At low and intermediate energies the situation is less clear: While our molecular method clearly outperforms the Bragg rule for capture, the latter seems to fare better in the case of ionization. A detailed comparison and analysis will be presented at the conference.

[1] M. Murakami *et al.*, Phys. Rev. A **85**, 052704 (2012).

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Tom Kirchner
York University

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