Abstract Submitted
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**Quantum versus classical description of inelastic processes in charged-particle collisions with the water molecule.**[1] ALBA JORGE, MARKO HORBATSCH, York University, CLARA ILLESCAS, Universidad Autonoma de Madrid, TOM KIRCHNER, York University — Inelastic processes following the impact of fast ions on molecules of biological importance have received a lot of attention in recent years. Special interest has been focused on the ionization of the water molecule due to its relevance in hadron therapy. The well known Classical Trajectory Monte Carlo (CTMC) method, commonly used for describing the initial state and time evolution of atomic systems, can be applied to the characterization of molecular ones as well, e.g., through multi-center potentials. A classical description of molecular orbitals (MOs) poses, however, some important differences compared to atomic orbitals, such as the non-degeneracy of the MOs and the electron interaction with a non-central potential. The $Li^{3+}$ + $H_2O$ collision system has been studied theoretically with the quantum-mechanical Two-Center Basis Generator Method (TC-BGM), reporting cross sections which agree with measured data. A detailed comparison of these two methodologies on the level of orientation-dependent results for individual MOs sheds light on the accuracy of the classical description of the water molecule. This comparison will be presented at the conference.

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