Abstract Submitted
for the GEC18 Meeting of
The American Physical Society

Classical description of water molecules in collisions with fast ions[1] ALBA JORGE, MARKO HORBATSCH, York Univ, CLARA ILLESCAS, Universidad Autonoma de Madrid, TOM KIRCHNER, York Univ — The study of fast ions impinging on molecules of biological interest has become a field of interest in recent years. This is due to a need of atomic data for inelastic processes, involving specifically the water molecule, for hadron therapy. Different theoretical methods, historically used for ion-atom collisions, are being adapted to deal with molecular targets, such as the Classical Trajectory Monte Carlo (CTMC) method, which is being applied for this task using multi-center potentials. However, the non-degeneracy of the molecular orbitals (MOs) and the electron interaction with a non-central potential imply some differences with respect to the atomic approach which need a deeper study. In this work, classical calculations, taking into account the alignment of the initial distribution for each MO, are compared to the quantum-mechanical Two-Center Basis Generator Method and to experimental data, in order to shed light on these issues.

[1]This work has been supported by York Science Fellowship program

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Date submitted: 18 Jun 2018 Electronic form version 1.4