Abstract Submitted
for the GEC10 Meeting of
The American Physical Society

Quantum-mechanical capture and ionization calculations for ion-water-molecule collisions[1] TOM KIRCHNER, York University, HANS JUERGEN LUEDDE, Goethe-Universitaet, MITSUKO KOROBKIN, MARKO HORBATSCH, York University — We elaborate on a nonperturbative quantum-mechanical approach to ion collisions from molecular targets introduced recently. Its key ingredients are an expansion of the initially populated molecular orbitals in terms of a single-center basis and a spectral representation of the molecular Hamiltonian. The approach amounts to a separation of molecular geometry and collision dynamics and offers the possibility to use well-established ion-atom methods with relatively minor modifications. We have extended our basis generator method to deal with the collision dynamics and address ionization and fragmentation of water molecules by ion impact in the few-keV to few-MeV regime. We consider different geometries and study the variation of the results with respect to the orientation of the molecule. In order to compare the results with experimental data and other calculations we have performed a (partial) average of the orientation-dependent cross sections. The results for net electron transfer and ionization in proton-water-molecule collisions are in remarkably good agreement with measurements. Furthermore, fragmentation cross sections will be presented. The results indicate a stronger dependence on the molecular geometry than found in the case of the net ionization and transfer cross sections.

[1]This work is supported in part by NSERC, Canada

Tom Kirchner
York University

Date submitted: 11 Jun 2010 Electronic form version 1.4