

Abstract Submitted  
for the GEC12 Meeting of  
The American Physical Society

**Calculations for ion-impact induced ionization and fragmentation of water molecules**<sup>1</sup> TOM KIRCHNER, MITSUKO MURAKAMI, MARKO HORBATSCH, Department of Physics and Astronomy, York University, Toronto ON M3J 1P3, Canada, HANS JÜRGEN LÜDDE, Institut fuer Theoretische Physik, Goethe-Universitaet, D-60438 Frankfurt, Germany — Charge-state correlated cross sections for single- and multiple-electron removal processes in proton-water-molecule collisions are calculated by using the non-perturbative basis generator method adapted for ion-molecule collisions [1,2]. A fragmentation model is then applied to calculate the yields of  $\text{H}_2\text{O}^+$ ,  $\text{OH}^+$ ,  $\text{H}^+$ , and  $\text{O}^+$  ions emerging after  $\text{H}_2\text{O}^{q+}$  formation [3]. A detailed comparison is made with experimental data from three groups covering the energy range from 20–5000 keV. It is found that multiple electron processes with  $q \leq 3$  play an important role at the lower end of this range and are calculated accurately within an independent particle model. We are currently completing the analogous analysis for  $\text{He}^+$ - $\text{H}_2\text{O}$  collisions for which the presence of the projectile electron poses some additional challenges.

[1] H.J. Lüdde et al, Phys. Rev. A 80, 060702(R) (2009)

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

[3] M. Murakami et al, Phys. Rev. A 85, 052713 (2012)

<sup>1</sup>Supported by SHARCNET and NSERC/Canada.

Tom Kirchner  
Department of Physics and Astronomy,  
York University, Toronto ON M3J 1P3

Date submitted: 19 Jun 2012

Electronic form version 1.4