

Abstract for an Invited Paper  
for the DAMOP09 Meeting of  
The American Physical Society

**Ab initio calculations of dissociative attachment and dissociative recombination of electrons and polyatomic species<sup>1</sup>**

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Interactions of free electrons with neutral and positively charged molecular species play a role in various physical systems. In interstellar space, reactions such as dissociative recombination determine the balance of various charged and neutral species. In a laboratory equipped with an apparatus like a COLTRIMS device, the dissociative attachment process can be used as a microscope to study polyatomic molecular dynamics. We discuss the theoretical and numerical methods used to calculate dissociative attachment and dissociative recombination of electrons with larger molecules from first principles. Studies using these methods are complimentary to other methods that yield more approximate reaction rates at greatly lesser numerical cost; they may yield precise information about the dissociation dynamics, product distribution, and differential cross section that approximate methods cannot. We discuss calculations performed to date on the target species  $\text{H}_2\text{O}$ ,  $\text{NO}_2$ , and  $\text{LiH}_2^+$ . We discuss the scaling of our numerical methods with the number of atoms, and the prospects of applying them to tetra-atomics.

<sup>1</sup>This work has been supported by the DOE and NSF