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Ionization and fragmentation of complex molecules studied with a density functional theory based approach[1]

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Ion-impact induced ionization and fragmentation of complex molecules have important applications in many branches of science. If the molecule is H_2O an obvious topic to address is the radiobiological relevance of these processes, e.g. in the context of hadron therapy, to name just one example. From a more fundamental physics viewpoint ion-molecule collision systems constitute interesting many-body systems, whose analysis poses challenges to both experimentalists and theorists. This talk will describe a theoretical approach to ion-molecule collisions, which is based on density functional theory to describe the nonperturbative electron dynamics. The basis generator method applied in the past successfully to ion-atom collisions is adapted to deal with the multi-center problem one faces when one considers molecular targets [1]. Cross sections for single- and multiple-electron processes (capture and transfer to the continuum) are obtained directly from solving time-dependent Kohn-Sham-type orbital equations and using a Slater determinant based analysis. Fragmentation yields are predicted on the basis of a semi-phenomenological model which uses the calculated cross sections as input [2]. Results will be presented for various ions impacting on water molecules in the energy range of 10–5000 keV/amu and compared with experimental data and previous theoretical calculations where available. First applications of the model to collisions involving CH_4 molecules will also be discussed.

[1] M. Murakami *et al.*, Phys. Rev. A **85**, 052704 (2012);
[2] M. Murakami *et al.*, Phys. Rev. A **85**, 052713 (2012).

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