Journal of Physics: Conference Series **388** (2012) 082054 doi:10.1088/1742-6596/388/8/082054

Ultrafast charge transfer dynamics induced by low energy collisions. Application to ion-atom and ion-molecule systems.

Marta Łabuda*[1], Jesús González –Vázquez† [2] and Leticia González‡ [3]

* Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Narutowicza 11/12, 80233, Poland
† Instituto de Química Física Rocasolano, CSIC, C/ Serrano 119, 28006 Madrid, Spain
‡ Institute for Physical Chemistry, Friedrich-Schiller-Universität, Helmholtzweg 4, 07743 Jena, Germany

Synopsis: In this work, we present a quantum dynamical study of the charge transfer process in the simple S^{3+} + H and complex C^{2+}-Uracil collisions at low energies using a time-dependent wavepacket approach.

Low energy charge transfer (CT) is one of the most important process that occurs in collisions between multiply charged ions and atoms or molecules. The main focus of this work is to examine, from a theoretical point of view, the mechanism of CT process in a molecular collision, taking place in the femtosecond (*fs*) time scale. The investigation of such a mechanism in real time is a pioneer application especially with respect to the complex ion-biomolecule interactions. In particular, such studies are essential for the understanding of radiation effects in biological systems, where e.g. highly charged carbon ions are used for cancer radiation therapy, cell killing and repairing [1-3].

Recently [4], we have developed new computational tools and have combined them with state-of-the art *ab initio* quantum chemistry methods to investigate the chemistry arising during CT process in simple S^{3+}-H collision [5]. For this model, we present the quantum wave packet calculations which have been carried out for the kinetic energies of the projectile of [1-10] eV in one- (1D) and two- (2D) dimensions. In a first step, the study of the CT mechanism necessitates the calculation of the potential energies of the states involved in the process, as well as the couplings between these states. These are obtained using high CASSCF/MRCI quantum chemistry methods. In the second step, the time-resolved aspects of the ultrafast collision are studied using time-dependent wave packet formalisms. In 1D, nuclear wave packet has been propagated in diabatic representation by using Split Operator technique. We have identified main channels involved in the CT process and calculated the CT probabilities over a given collision energy range. The evolution of the wave packet illustrates how the electronic charge evolves over different electronic states and shows interference effects. Additionally, 2D wave packet movies showing the evolution in *fs* scale have been prepared for different kinetic energies and impact parameters. Then, we can obtain the time-dependent probability distribution and time-independent angular distribution of the wave packet defining the scattering mechanism. This simple system serves to observe the nuclear and electron motions in the *fs* range, before more complex models or polyatomic targets were investigated.

The methodology used in ion-atom system has been applied to the complex model, the collision of carbon ion C^{2+} with the RNA base Uracil. Here, in the low-energy range, the collisional process is described as the evolution of a quasi-molecule formed from the ion-molecule system in which the reaction coordinate corresponds to the distance *R* between the centre of mass of Uracil and the colliding carbon ion. We will present the first results of molecular structure and ultrafast low energy dynamics of CT in this system. Such simulations allow a direct investigation of the dynamics for the complex system and provides a detailed picture of the CT mechanism.

Acknowledgments: This research was supported by a Marie Curie European Reintegration Grant (M.Ł) within the 7th European Community Framework Programme as well as by the COST action CM0702 "Chemistry with Ultrashort Pulses and Free-Electron Lasers" and the 645/N-COST/2010/0 grant.

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[1] E-mail: marta@mif.pg.gda.pl
[2] E-mail: jgv@tchiko.quim.ucm.es
[3] E-mail: leticia.gonzalez@uni-jena.de