

## A time-dependent picture of the charge transfer process in the $S^{3+} + H$ collision.

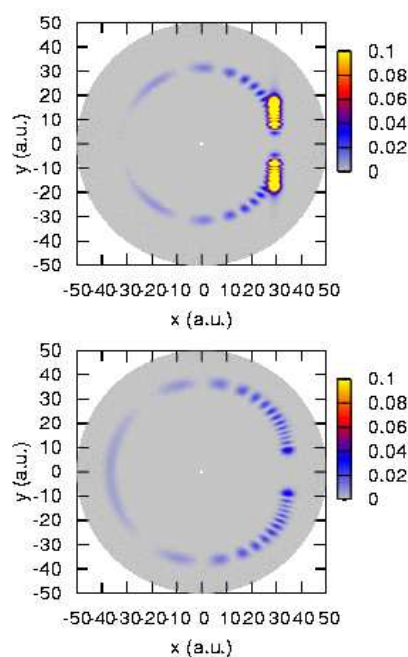
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**Synopsis** In this work we observe for the first time the evolution of the electronic charge density in a collisional system. The model used is system  $S^{3+} + H$  over the range of relative ion kinetic energies from [1-10] eV. To this aim, *ab initio* potential energy surfaces and non-adiabatic couplings together with wavepacket propagations have been used.

Charge transfer is one of the most important processes that occur in collisions between multiply charged ions and atoms or molecules at low energy. As such, multiply charged ions in collision with atomic and molecular targets like  $H$ ,  $H_2$  is a longstanding domain of interest [1]. In this presentation, the collisional system  $S^{3+} + H$  is studied in a time-dependent wave packet formalism which allow us calculating the explicit time evolution of the electronic charge. Based on previous theoretical investigations on this system [2,3], an *ab initio* molecular calculation of the potential energy surfaces and non-adiabatic couplings has been set up with CASSCF-MRCI methods. The ultrafast nature of the nuclear collision is studied in the range of energy [1-10] eV. Time-dependent wave packet methods are applied in the diabatic representation using the split operator technique [4]. The calculations were carried out in one-(1D) and two-dimensions (2D). As a test calculation, the 1D collision model only considers the internuclear distance between the incident hydrogen atom and the sulphur ion taken as the origin of electronic coordinates (with the impact parameter  $\vec{b}=0$ ). The 2D calculations are performed including the distance  $\vec{R}$  and the scattering angle  $\theta$ , which allows to consider impact parameters between [0-20] a.u. As an example, snapshots at  $t=75$  fs of the wavepacket in 2D for the ion kinetic energy 10 eV are presented in the Fig. 1.

Time-dependent wave packet methods provide a clear and direct physical insight into the dynamics of the ultrafast (few fs) character of the charge transfer process even at very low energies [5,6]. From this point of view, the study of ion-atom collisions is a perfect test case for the development of efficient numerical techniques which can be used afterwards in more complex reactions such these of biological meaning.



**Fig. 1.** 2D snapshots at  $t=75$  fs of the wavefunctions in the entry channel with  $S^{3+}(3s^2 3p)^2P^o + H$  configuration (top) and the  $S^{2+}(3s^2 3p 3d)^3P^o + H^+$  state (bottom).

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### References

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