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Scientific Report

Theoretical study of the charge transfer mechanism in the C^{2+}+OH collision

Theoretical investigation of charge transfer mechanism in collisions of multiply charged ions with molecular targets is an essential ingredient to study radiation effects in biological systems. In the present collaboration we focus on the charge exchange reaction $C^{2+} + OH \rightarrow C^{+} + OH^{+}$. In particular, we perform *ab initio* quantum chemical computations of the quasi-molecule COH^{2+} in order to reveal the adiabatic potential energy surfaces of various excited states and the respective nonadiabatic couplings which induce transitions between the molecular states, and then we also investigate the dynamical mechanism of the collision.

During the visit we discussed in depth several essential points of the quantum chemical calculations, in particular, how to choose the proper basis set and the active space of the molecular orbitals, and also how to read off the electron configuration from the CI vector. We clarified the symmetry properties of the system, and we managed to identify the entry channel and the relevant excited states. We made some test calculations by using the program-package MOLPRO. In the figure below the adiabatic potential energy curves of the ten lowest-energy states of COH^{2+} are shown at the collinear attach in the B_1 irreducible representation of the symmetry group C_{2v} at the CASSCF level in the minimal basis set VDZ. These curves correspond to the entry channel (uppermost curve in the asymptotic region) and to the exit channels, which may be relevant in the charge exchange process. In the near future we aim at a thorough investigation and as a result a complete understanding of this particular reaction.