SORBONNE UNIVERSITÉ

Sorbonne Université/ China Scholarship Council program 2021

Thesis proposal

Title of the research project: Theoretical investigation of X-ray emission from collision-induced highly-excited states of ions

Keywords: Atomic Collisions, *ab initio* simulation, theoretical chemistry

Joint supervision: yes (Yong WU, China)

Joint PhD (cotutelle): yes (Yong WU, China)

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Doctoral school (N°+name): ED 388

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Subject description (2 pages max):

1) Study context

The solar wind is a hot plasma, composed of charged particles, electrons and ions (around 92% of protons, 8% of helium ions and 0.1% of heavier elements) that may collide with atoms and molecules (H, O, OH, CO, CH_4, NH_3, H_2O,...) from solar-system bodies (planets and comets). X-ray emission induced by these collisions [1] can be detected and used to determine the structure and dynamics of the solar wind plasma. In particular, heavy ions from the solar wind (mostly multi-charged oxygen) can capture electrons from the molecules into highly-excited electronic states which then deexcite radiatively emitting the X-ray photons [2]. This scenario, called the Solar Wind Charge-Exchange (SWCX) mechanism seems to be the most probable process for the X-ray emission of comets [3].

Elaborate models have been developed to simulate the X-ray emission due to the SWCX mechanism [2,4]. In practice, charge-exchange cross-sections from highly-excited multi-charged ions are needed as input data of these models. Accurate *ab initio* calculations of these data are complicated tasks. In the impact energy range (around 0.1 keV/amu) relevant for the solar wind diagnosis, all electronic channels (excitation, ionization and electron-transfer) are open and more importantly are strongly coupled. Thus, a non-perturbative approach coupling all these processes must be used to obtain correct charge-exchange cross-sections. The PhD project aims therefore at developing a state of the art *ab initio* code for the theoretical description of relevant ion-molecule collisions and to employ the codes to obtain accurate data for atomic and molecular processes during these collisions. These data are necessary to model X-ray emission from comets and planets due to the interaction with the solar-wind plasma. Based on these accurate data, a better knowledge of the solar-wind composition are expected.

2) Details of the proposal

To calculate the charge-exchange cross-sections in keV ion-molecule collisions, we will extent our current code, that has been used succesfully to describe ions colliding with one and two-active-electron atoms and molecules [5-10], to larger target systems. Our code relies on a non-perturbative approach which couples all open-electronic processes and thus allows a numerically exact description of the charge-exchange [11,12]. This approach is accurate but very demanding on computer resources (CPU-time and RAM) due to the matrix elements computations and storage. It has been so far, applied only to rather small systems such as H, H^-, He and H_2. We recently modify the code such that the target systems can be described using Hartree-Fock molecular orbitals, opening the way to employ the quantum chemical tools available. We plan to implement a Configuration Interaction approach for the description of the electronic dynamics during ion-molecule collisions, which will allow us to study relevant molecular systems that are currently out of reach. The PhD student will participate to the development of the code and will employ it to investigate X-ray emission from collision-induced highly-excited states of ions.

3) References

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4°) Profile of the Applicant (skills/diploma…)

The applicant should have a master degree in Chemistry or Physics. She/He should have some knowledge in programming, numerical methods and theoretical chemistry approaches.

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