CFEL SCIENCE

SEMINAR

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CFEL – Building 99, seminar room II and III (ground floor)

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Computational molecular spectroscopy: from atmospheres of hot exoplanets to the optical control of molecules

Over the past years there have been a rapid improvement in nuclear motion approaches to solving spectroscopic problems, which has been described as the fourth age of quantum chemistry. The methodology which is commonly attributed to the spectroscopy from first principles is in fact a combination of high level ab initio (electronic structure) calculations, high level nuclear motion (variational) calculations and empirical refinement to the highly accurate experimental data (e.g. line positions). This methodology is increasingly competitive with experiment allowing in many cases a more reliable determination of various molecular data.

We apply this methodology to generate huge lists of transitions for molecules, important for modelling atmospheres of hot objects, such as exoplanets and cool stars. There is a major demand from astrophysics and elsewhere of comprehensive line lists for molecules important in these hot atmospheres environments, including evaporating or lava planets with atmospheres of molten rocks. The line lists we produce provide the input for models of radiative transport through hot atmospheres and are useful for a variety of terrestrial applications. Our group at UCL is the world leader in providing spectroscopic data for hot atmospheric and industrial applications.

The description of physical processes involved in the interaction of molecules with the radiation in these environments have much in common with the description of processes involved in the laser control of motion of small molecules. The same methodology used for exoplanetary studies can be efficiently applied to controlling molecular orientation through radiative rotational transitions by electric fields.

In this talk, I will discuss the current state-of-the-art of the computational molecular spectroscopy, show examples of exoplanetary applications, where efficient and accurate solutions of the nuclear motion Schroedinger equation can help in characterization of alien atmospheres and optical control applications, where the motion and orientation of polyatomic molecules can be efficiently controlled by lasers.

Host: Jochen Küpper/ CFEL Molecular and Ultrafast Science Seminar