

Dr. Laurent Bonnet

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CNRS Research Director

Theoretical Chemistry Group

Email: l.bonnet@ism.u-bordeaux1.fr

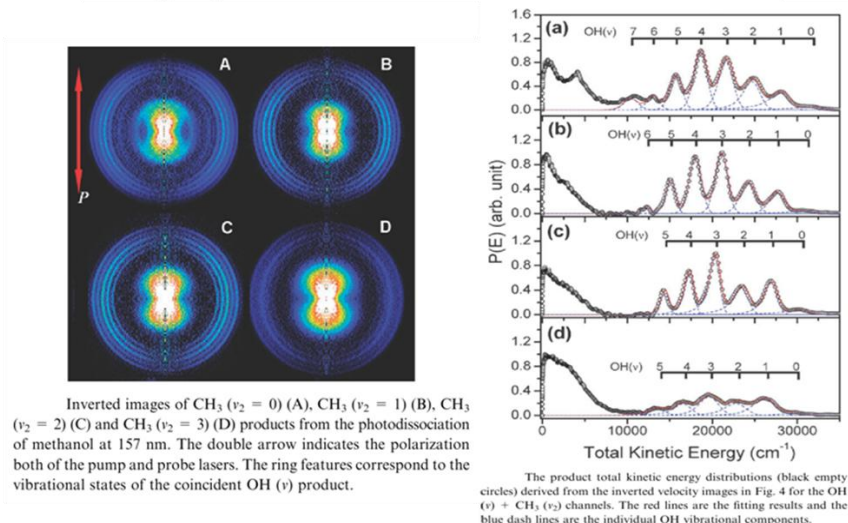
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New perspectives in the mixed quantum-classical treatment of photodissociation dynamics

Modern molecular beam and spectroscopic technics allow the measurement of state-correlated translational energy distributions between photodissociation products with an amazing level of precision, as illustrated in Fig. 1 (for more details, contact me). Product quantum state distributions can then be extracted from these data. Accurate

Product pair correlation in CH_3OH photodissociation at 157 nm: the $\text{OH} + \text{CH}_3$ channel

Zhichao Chen,^{ab} Andre T. J. B. Eppink,^b Bo Jiang,^a Gerrit C. Groenenboom,^c Xueming Yang^{*a} and David H. Parker^{*b}



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theoretical descriptions of the mechanics of molecular fragmentation are thus needed to reproduce and rationalize these data, or predict them when experiments cannot be performed. Beyond their fundamental interest, photodissociation dynamics studies provide very useful data to specialists of planetary atmospheres or interstellar clouds, and they form a branch of molecular physics which has continuously generated technological progress for more than a century.

For about three decades, accurate experimental studies were mainly focused on triatomic photodissociations, but nowadays, modern methods like the velocity imaging technics allow the accurate study of polyatomic processes. Ideally, one would like to describe the observables by rigorous quantum mechanical approaches. However, such methods are very hard to apply to polyatomic processes, for they often lead to prohibitive calculations, despite the power of modern computers.

The alternative approach consists in treating nuclei as if they were classical objects, Hamilton equations being much easier to numerically solve than the Schrödinger equation. More often than not, however, strong quantum effects show up in the dynamics, and one must include quantum constraints in the classical description. This operation is performed in the light of the fascinating semiclassical mechanics of molecular collisions of Miller, Marcus, Heller and others and the trajectory surface hopping method of Tully to deal with possible non adiabatic transitions between electronic states. The Bordeaux reaction dynamics group has international expertise in these approaches.

The primary goal of the thesis will be to apply these theoretical tools to the photodissociation of the polyatomic species CH_3I in a first step, and CH_3OH in a second step. The candidate will interact with two colleagues (Dr. P Larregaray and Dr. Ph. Halvick) in addition to me. As far as the second process is concerned, the work will also be done in collaboration with the group of Prof. Hochlaf, at Paris Est University, who is specialized in electronic structure calculations. The candidate must like theoretical developments and FORTRAN programming.

Do not hesitate to contact me for more details on the work.