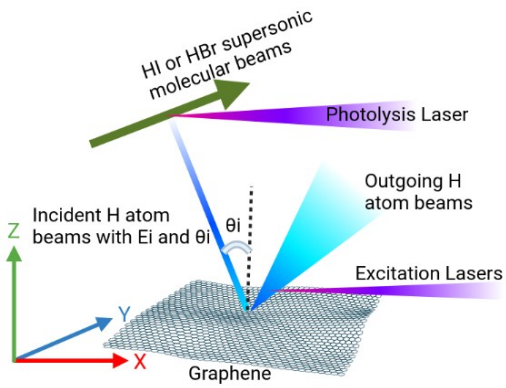
Internship master 2

Quantum Dynamics simulation for H atom scattering from graphene surface

For students very interested in quantum physics/Chemistry and its concrete applications and who want to interact with top-level groups outside France.

The adsorption of hydrogen atoms onto a graphene surface has garnered significant attention due to its wide-ranging applications in fields such as astrophysics, hydrogen storage, semiconductor manufacturing and a promising model system for studying intramolecular vibrational energy redistribution reactions. A recent breakthrough has permitted to measure very precisely the formation of the C-H bond and the exchange of energy from the H –atom to the grapheme (group of A. Wodtke of Göttingen, *Science* 2019). The number of degrees of freedom exerts a profound influence on quantum molecular dynamics computations.

To interpret these experiments including all the quantum effects, one of the most effective approaches involves employing the Multi-Configuration Time-Dependent Hartree (MCTDH) method developed in the group of L. Cederbaum/O. Vendrell in Heidelberg.



Recently, we executed with MCTDH full-dimensional (75D) simulations to enable us to directly compare the theoretical simulation results with experimental observations for this system. Based on the viability of this high-dimensional quantum dynamic simulation, we propose in this internship to conduct simulations under alternative initial conditions where quantum effects are anticipated to be much more pronounced. The work will be performed in strong interaction with the groups of Göttingen and Heidelberg.

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