PhD GRANTS 2024

PhD project title: Theoretical study of the photodesorption of mixed ice of interstellar interest

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PhD project summary (max. 20 lines):

The anomalous abundance of the gas phase in cold, dense regions of the interstellar medium can be explained by the process of photodesorption of interstellar ices due to VUV radiation. During this process, an ice molecule absorbs a photon, and transforms its electronic energy into internal and translational energy that is redistributed within the ice. If energy transfer extends to the surface, it could cause molecule desorption, which would in turn enhance the gas phase. To consolidate this hypothesis, a collaboration between research groups at the University of Lille (PCMT/PhLAM) and the Sorbonne University (LERMA), using a combined experimental and theoretical approach based on VUV laser experiments and Ab Initio Molecular Dynamics simulations, has achieved a significant breakthrough in identifying and characterizing the mechanism involved in the photodesorption of pure carbon monoxide (CO) ices[1]. The remarkable agreement obtained between theory and experiment signifies that this result is a first step towards a better understanding of the impact of the photochemistry of molecular ices on the physical chemistry of the interstellar medium.

In the thesis work proposed here, we plan to go a step further and focus on simulating the photodesorption of mixed ices of interstellar interest, such as CO/N_2 or CO/NO ices. We propose to combine the advantages of Ab Initio Molecular Dynamics (AIMD) [2,3] with the power and flexibility of high-dimensional potential energy surfaces (NN-SEP) [4-7], obtained from machine learning methods (atomistic neural networks), to simulate the photodesorption process. The aim is to determine the desorption probabilities and energy distributions of the desorbed molecules. The results of this theoretical study will be directly compared with experiments carried out by the LERMA team at the Sorbonne.

References

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Key Words :

Photodesorption, VUV ray, interstellar ice, internal and translational energy distributions, *ab initio* molecular dynamics, (AIMD), density functional theory (DFT), Machine Learning (ML), High Dimensional Atomistic Neural Network PES (ANN-PES)