Dynamics of processes involving atoms or molecules and superfluid ^{4}He nanodroplets

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Although the study of chemical reactions in superfluid ^{4}He nanodroplets (ND) is a very interesting topic and has been the subject of some experimental efforts, until now little attention has been paid to this problem from a theoretical perspective [1]. Here, we will present the most recent developments achieved in our laboratory on the quantum dynamics of a selection of relevant chemical and physical processes involving one or two impurities and a superfluid ^{4}He ND (T≈0.37 K). Thus, e.g., to investigate the photodissociation dynamics of diatomic molecules in ^{4}He ND, a hybrid quantum mechanical theoretical approach that combines time dependent DFT (helium) and QM dynamics (molecule) has been developed [2]. This method has been applied to the study the Cl_2 photodissociation arising from the B←X transition, considering $Cl_2(v=0,X)@(^4He)_N$ doped nanodroplets of different sizes (N=50-500) [2]. In addition to the analysis of this interesting system, where the initial Cl-Cl chemical bond is broken, we will also present a rather wide set of results comprising, e.g., the $(^4He)_N$ relaxation process occurring in the after photodissociation time period, and other relevant processes (atomic pick up and chemical reaction). In all cases, the dynamic properties and microscopic mechanism have been examined considering a wide set of initial conditions. We hope that these results will encourage the experimentalists to investigate the dynamics of this kind of systems.

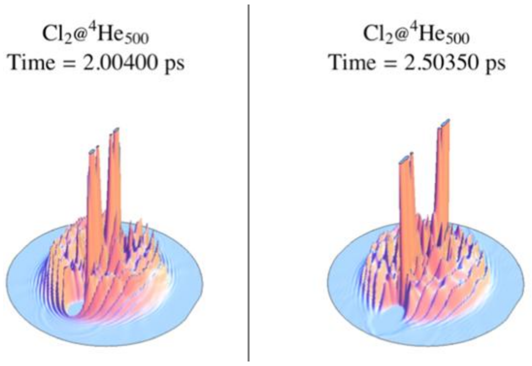

Fig. 1. Snapshots showing the helium density (xz plane), during the final of the $[Cl_2(B)@(^4He)_{500}]^*$ photodissociation. The z axis corresponds to the Cl-Cl bond axis.

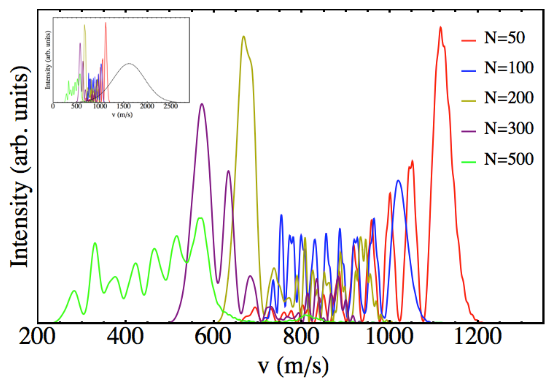

Fig. 2. Velocity distributions of the Cl photofragment for different ND sizes. The gas phase result (black line) is given in the small figure.

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References

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