Helium nanodroplets: a Path Integral Molecular Dynamics study of the electron transfer Cs_2-He_N@C_{60} → $Cs_2^+C_{60}^-$@He_N,

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Electron transfer from a heliophobic $Cs_2(^3\Sigma_u)$ dimer, located on the surface of a He droplet, to a heliophilic, fully immersed C_{60} molecule is studied through PIMD simulations in the NVT (2K) and NVE ensembles to provide real-time dynamics. After electron ionization mass spectroscopy measurements [1] this spatially quenched reaction was characterized as a long-range electron transfer in a high-level ab initio study [2]. A droplet size of 2090 atoms is assumed to account for spatial hindrance on reactivity, see Figure 1. By increasing the number of beads in the simulations, the relevance of quantization is studied without an implicit assumption of superfluidity. Reaction probability increases with the level of quantization, and proceeds showing a rotational motion of cesium dimer which involves a substantial displacement of helium, as shown in Figure 2. It raises the issue of whether the interacting species are driven out-of-equilibrium after impurity uptake, since reactivity is strongly quenched if a full thermal equilibration is assumed. The results of this study have been recently published [3].

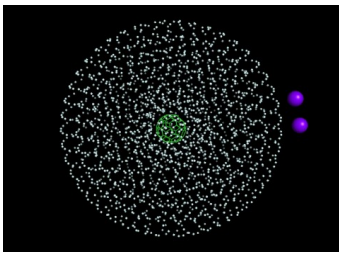

Figure 1: *Initial configuration involving 2090 He atoms.*

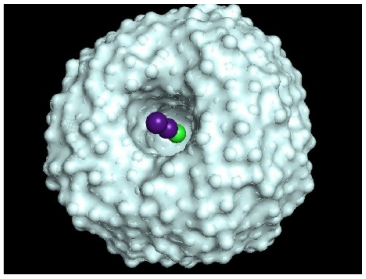

Figure 2: *Final arrangement after reaction.*

Index Terms: Path Integral Molecular Dynamics, Charge Transfer Reactions, Helium Nanodroplets.

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