

Intramolecular vibrational redistribution in the non-radiative excited state decay of uracil in the gas phase: an ab initio molecular dynamics study.

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An atomistic description of the Intramolecular Vibrational Redistribution of Uracil in gas phase is presented¹. This analysis is based on molecular dynamics simulations on the ground state of Uracil, following UV excitation, from the conical intersection (CI) point between the ground state and the $\pi\pi^*$ excited state (which is situated at about 1 eV below the Franck-Condon point).

To this aim we have performed several ground state Ab initio Molecular Dynamics simulations, by exploiting the accurate PBE0 functional, comparing the results obtained when starting from the CI point with 0eV and 1eV of extra kinetic energy. The analysis of the variation of Uracil structural parameters and of the redistribution of the total kinetic energy among the different vibrational modes provide an interesting picture of the IVR process, which can provide insights not only on the photo activated dynamics in the gas phase but also on the Vibrational cooling process in solution.

1. P. Carbonniere, C. Pouchan, R. Improta, *Phys. Chem. Chem. Phys.* **2015**, DOI: 10.1039/C4CP05265J.