Ultrafast Hydrogen Migration in a Photoionized Glycine by a Mixed Quantum-Classical Dynamics

KETY Kossi;[A] **GONZALEZ-VASQUEZ Jesús**;[B] **MITRUSHCHENKOV Alexander**;[A] **DECLEVA Piero**;[C] **JOUBERT-DORIOL Loïc**;[A] **CIREASA Raluca**;[D] **PELAEZ Daniel**;[D] **PALACIOS Alicia**;[B] **MARTIN Fernando**;[B] **GATTI Fabien**;[D]

A) Université Gustave Eiffel, Laboratoire de Modélisation et Simulation Multi-échelle MSME, F-77454 Marne-la-Vallée, France;
B) Departamento de Quimica, Modulo 13, Universidad Autónoma de Madrid, 28049 Madrid, Spain;
C) CNR IOM and Dipartimento di Scienze Chimiche e Farmaceutiche, Universitá di Trieste, 34127 Trieste, Italy;
D) Université Paris-Saclay, Institut des Sciences Moléculaires d'Orsay ISMO, UMR CNRS 8214, F-91405 Orsay, France.

kossi.kety2@univ-eiffel.fr

We have theoretically investigated the ultrafast intramolecular hydrogen migration in the glycine molecule ionized by XUV attosecond pulse train of duration 1.5 fs as experimentally observed by Castrovilli et al.[1]. Since the interaction of the pulse with the molecular system leads to ionization, standard quantum chemistry methods used to describe excited bound states break down and methods which accurately describe electronic continuum states are in order. We have used the correlated single channel approach as implemented in the Tiresia code[2] to calculate the dipole matrix elements, the cross-sections of a singly ionized glycine and the ionization probabilities are evaluated for a specific attosecond pulse train of duration 1.5 fs used in the previous experiment[1]. The coupled electron-nuclear dynamics is described by the Trajectory Surface Hopping (TSH) [3] method. We do observe a hydrogen migration as shown in the snapshots of the TSH dynamics displayed in figure 1. The migrations mostly occur when the active state reachs the cationic ground state. Further calculations are currently performed using the Heidelberg Multi-Configurational Time-Dependent Hartree (MCTDH)[4] package on a linear vibronic coupling model in order to study coherence effects which lack in the TSH method.

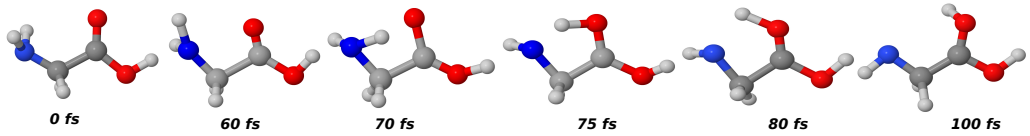

Figure 1: Snapshots of the geometries during the dynamics showing the hydrogen migration .

Keywords: Photo-ionization probability, hydrogen migration, trajectory surface hopping, glycine.

[1] Castrovilli et al. The Journal of Physical Chemistry Letters 9 (2018) 6012-6016
[2] P. Decleva, M. Stener, D. Toffoli, Molecules 2022, 27, 2026.
[3] Jesús González-Vázquez et al. Journal of chemical theory and computation, 7(5):1253-1258, 2011.
[4] M. Beck, A. Jäckle, G. Worth, H. D. Meyer, Physics Reports (2000) 324 (1) Elsevier BV: 1–105.