conferenceseries.com

Valérie Brenner et al., J Phys Chem Biophys 2018, Volume 8
DOI: 10.4172/2161-0398-C3-034

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland

Excited states deactivation in model proteins chains: nonadiabatic dynamics simulations and *ab initio* methods

Valérie Brenner[1], **T. Very**[1,2], **S. Hoya**[2], **N. Ben Amor**[2], **E. Gloaguen**[1] and **M. Mons**[1]
[1]Laboratory Interactions, Dynamics and Lasers-CEA Saclay, France
[2]Quantum Chemistry and Physics Laboratory-Paul Sabatier University, France

Following UV absorption, many biomolecular systems are endowed with mechanisms of excited-states deactivation that ensure their photochemical stability. One of the major goals of our research is to investigate conformer-selective dynamics of biologically relevant molecular systems by an original innovative computational strategy in order to document the basic physical phenomena controlling the lifetime of excited states, highlighting the link between electronic dynamics and structure. This innovative multi-step computational strategy allows to both characterize the first excited states of bio-relevant systems and model efficiently their potential energy surfaces, using, first, nonadiabatic dynamics simulations based on time-dependent density functional theory (NA-TDDFT) to provide hints about the critical motions that drive the deactivation, which will then be investigated at a better level with two families of methods: i) the standard approximate coupled cluster singles and doubles method (CC2) and ii) and multireference (MR) methods. Developed on small capped peptide models and always backed up by key conformation selective gas phase experiments carried out in our team at several timescales,[1,2] this innovative strategy is now applied to monohydrated capped peptides as well as capped dipeptides. We will present here the last results obtained on these systems. In addition, benchmark of the CC2 method on a set of model peptide chains (structure, energetic and vibrational frequencies of the first ππ* exited state)[3,4] as well as assessment of the CC2 method validity from comparison with MR methods[5] will be also reported.

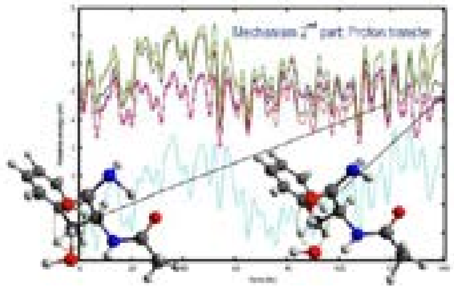

Figure: Illustration of a deactivation mechanism: Time dependence of the potential energy of the ground (blue) and four lowest excited states of NAPA-H_2O along a selected nonadiabatic trajectory.

Recent Publications:

1. Mališ M, Loquais Y, Gloaguen E., Biswal H S, Piuzzi F, Tardivel B, Brenner V, Broquier M, Jouvet C, Mons M, Došlić N, Ljubić I (2012) Unraveling the mechanisms of nonradiative deactivation in model peptides following photoexcitation of a phenylalanine residue. Journal of the American Chemical Society 134:20340-20351.
2. Mališ M, Loquais Y, Gloaguen E., Jouvet C, Brenner V, Mons M, Ljubić I, Došlić N (2014) Non-radiative relaxation of UV photoexcited phenylalanine residues: probing the role of conical intersections by chemical substitution. Physical Chemistry Chemical Physics 16:2285-2288.
3. Y. Loquais, E. Gloaguen, M. Allaudin, V. Brenner, B. Tardivel, M.Mons (2014) On the near UV photophysics of a phenylalanine residue: conformation-dependent ππ* state deactivation revealed by laser spectroscopy of isolated neutral dipeptides. Physical Chemistry Chemical Physics 16:22192-22200.
4. W. Y. Sohn, V. Brenner, E. Gloaguen, M. Mons (2016) Local NH–π interactions involving aromatic residues of proteins: influence of backbone conformation and ππ* excitation on the π H-bond strength, as revealed from studies of isolated model peptides. Physical Chemistry Chemical Physics 18:29969-29978.

Biography

Valérie Brenner is a theoretical chemical physicist specialized in non-covalent interactions modeling and quantum chemistry computations of medium-sized and large molecular systems. She has always been working closely with different experimental teams and has acquired a wide experience in studying the physical chemistry of medium-sized and large molecular systems. After a period devoted to both modeling of intermolecular interactions and exploration of the large molecular systems potential energy surfaces during which she developed “homemade” codes, she has been recently invested in a new research field, i.e. computation of excited states of large molecular systems, focusing on the mechanisms of non-radiative relaxation in model protein chains.

valerie.brenner@cea.fr

Notes: