Probing Unusual Hidden Electron Dynamics in Molecules of Biomedical Interest Using Soft PPS Radiation Signatures (RS) in the Framework of Attomechanics Models

Kresimir Rupnik[a,*]

[a] *Department of Chemistry Louisiana State University, Baton Rouge, LA 70803 USA* , chrupn@lsu.edu

Unbiased RS models were originally introduced to study ultrafast, relatively higher energy events in systems of biomedical interest [1]. That work continued with the study of causal relations between electron attodynamics and the interacting (driving) radiation by measuring characteristic electron RS, that is the observed signatures of such interactions. During the last decade our Polarization Phase Selective (PPS) High Magnetic Field (HMF) instrumentation and methods developed in the framework of new integrative attomechanics modeling significantly improved [2-3]. That allowed inclusion of *soft* HMF PPS RS for studies in the energy region of chemical reactions in large, complex and unstable bio-molecules, "far from equilibrium". Our main challenges are highly selective RS extractions from large sets of interfering components. Scientifically important question we address here is: can these methods probe electrons during protein synthesis and activity, or during interactions with other molecules, like radical SAM. Contrary to what has been suggested in literature, our magnetooptic studies already provide conclusive evidence about electron locations and actions in some studied enzyme reactions. However, some of our most important findings are related to the previously unseen electron dynamics and new protein configurations. Indeed, we can separate signatures from previously indistinguishable proteins that show small structural but paramount activity differences, and we can separate (symmetrical) signatures from recently discovered unusual and previously unseen electron spin-flips [4]. Such events can be hidden or "dark" due to the overlappings and interferences. We estimate that controlling window for such events starts at tens of femtoseconds or in some cases even shorter time.

References

1. K. Rupnik, et all. *J. Chem. Inf. Comput. Sci.* **34** (1994), 1054.
2. D. Shafir, Y. Mairesse, H. J. Worner, K. Rupnik, D.M. Villeneuve, P. B. Corkum and N. Dudovich, New Journal of Physics **12** (2010), 073032
3. K. Rupnik, "Variable Magnetic-Field (VMF) Ultrafast Polarization Phase Selective (PPS) Attomechanics Studies in the Areas of Fundamental Significance to Biochemistry/Biophysics: New Methods and Tools for Monitoring Electronic Processes in Biosystems", Published by NHMFL (December, 2018)
4. K. Rupnik et all., (submitted) (2019)

[*] *This work was a part of the UF-PPS Study Project (K. Rupnik PI) which is also performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490, and 0654118 and the U.S. Department of Energy.*