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Interplay between protein folding and its physicochemical properties probed by VUV and X-ray action spectroscopy[1]

ALEKSANDAR MILOSAVLJEVIC, Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Understanding the correlation between proteins folding and its electronic structures and physicochemical properties could possibly lead to a more efficient prediction of protein functions in living organisms. We report on the recent experimental results obtained from both VUV and X-ray gas-phase action spectroscopy of multiply protonated protein ions formed by electrospray. The experiment has been performed by coupling a commercial linear quadrupole ion trap, fitted with an electrospray ion source (ESI), to the DESIRS (VUV) and PLEIADES (X-ray) beamlines at the SOLEIL facility, France. The series of charge states that could be formed by ESI for different proteins have been studied both in the valence shell and around the C-, N- and O-edges, with some control on their three-dimensional structure provided by their level of protonation. We found that both valence and core ionization energies of a protonated protein are strongly correlated to its tertiary structure, which influences its effective Coulomb field. On the other hand, the electronic core-to-valence shell transition energies are not markedly affected by the unfolding of the protein.

[1]In collaboration with Milos Rankovic, Christophe Nicolas, Francis Canon, Laurent Nahon, Alexandre Guliani