Insights on photo-ionization of Uracil and its tautomers: Using Non-Dyson ADC(3) approach

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Uracil is one of the four nucleobases in the nucleic acid of RNA hence, plays a crucial role in genetic stability or segmentation and mutation, for example under radiation therapy. Photon induced ultrafast electron dynamics is precursor to the associated chemical kinetics and reaction pathways under irradiation. Under photo-ionization study as the coupling of electron dynamics lead to nuclear dynamics the study of the former is important. Using the single particle Green's function Non-dyson ADC(3) method, we study the ultrafast electron dynamics and femtosecond charge migration processes in tautomers of Uracil molecules. From the investigation of the migration of hole charge following the ionization of the system, the time required for onset of response to sudden ionization and creation of charge density is found to be 40-50 attoseconds. Our results demonstrate different charge transfer sites and electron density oscillations of two uracil tautomers under photoionization. Overall based on our study, it is possible to identify distinct features of charge migration and dissociative electron attachment from parent tautomer variety, utilisable for exploring new relaxation pathways and in design of new uracil derivatives using the laser irradiation.