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Time-resolving electron dynamics in molecules using strong laser fields: coherent probes of charge migration[1]

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When forced out of equilibrium, electrons in matter can respond exceedingly fast, leading to migration of charges on time-scales approaching the attosecond [1] and before the dynamic is impacted by the weaker coupling to a system "bath" with many degrees of freedom. This potentially complex quantum evolution can expose correlations between electrons and holes that are otherwise hidden in the static properties of the system. Probing the electronic structure and dynamics of molecules on the attosecond time scale is, however, a formidable challenge that requires state-of-the-art experimental setups and new theoretical tools and models. In this contribution, I will discuss time-resolving charge migration using strong laser fields and present a picture of charge migration that combines strong-field dynamics [2] with the quantum-chemistry-derived electronic structure of complex molecules [3]. Using a related set of molecules as examples, I will compare experimental measurements with the results of theoretical models and associated numerical simulations to unveil the time-dependent electronic structure [4]. [1] J. Phys. Chem. Lett. 8, 3991 (2017). [2] Phys. Rev. A 93, 043815 (2016); Phys. Rev. A 97, 043407 (2018). [3] J. Chem. Phys. 145, 094105 (2016). [4] Phys. Rev. A 98, 043425 (2018); Appl. Sci. 8, 1129 (2018).

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