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Ultrafast electronic dynamics driven by nuclear motion.¹ ORIOL VENDRELL, Center for Free-Electron Laser Science, DESY

The transfer of electrical charge on a microscopic scale plays a fundamental role in chemistry, in biology, and in technological applications. In this contribution, we will discuss situations in which nuclear motion plays a central role in driving the electronic dynamics of photo-excited or photo-ionized molecular systems. In particular, we will explore theoretically the ultrafast transfer of a double electron hole between the functional groups of glycine after K-shell ionization and subsequent Auger decay. Although a large energy gap of about 15 eV initially exists between the two electronic states involved and coherent electronic dynamics play no role in the hole transfer, we will illustrate how the double hole can be transferred within 3 to 4 fs between both functional ends of the glycine molecule driven solely by specific nuclear displacements and non-Born-Oppenheimer effects. This finding challenges the common wisdom that nuclear dynamics of the molecular skeleton are unimportant for charge transfer processes at the few-femtosecond time scale and shows that they can even play a prominent role.

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