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Migratory resonances and Wigner timers in the photoionization of fullerene class of molecules¹

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Empty fullerenes and atom-encaging endofullerenes are quintessential symmetric molecules exhibiting near stability in the room temperature. This property endows them with the quality to be tested for spectroscopic information otherwise inaccessible with regular atoms and molecules. Probing the response of fullerenes and endofullerenes to electromagnetic radiations is one classic way to accomplish this. Conventional spectroscopy of determining the photoelectron count and kinetic energy, as the frequency of the incoming photons varies, predicts varieties of resonances for such molecules. These resonances fundamentally originate from either the correlated electronic motions leading to plasmons [1,2] or from the molecule's structural symmetry inducing diffractions [3] or even from the mixing of both these effects in tandem [4]. A particularly exotic class of these resonances, which will be emphasized in the talk, includes photoexcitation at one site of the molecule but its subsequent decay at a different location [5], as well as a coherent admixture of this mechanism with localized Auger processes [5,6]. The other part of the talk will be devoted to connect to a more contemporary form of spectroscopy by evaluating the time-of-flight of the photoelectron, starting from its production at the molecule to the detector. This utilizes a Wigner clock based on the knowledge of energy-dependent photoelectron quantum phase. It will be shown that the information that can be obtained from the knowledge of this time is often consistent with the underlying electron correlative dynamics, both at the energy region of the giant plasmon resonance [7] and at the generic Cooper-type minima (or anti-resonances) [8,9]. A selection of the results will be presented which are computed by the density functional approximation. The ground state of the molecule is described in a local density approximation (LDA) framework with accurate exchange correlation potential [1]. And a linear-response variant of LDA (TDLDA) is utilized to describe the interaction with the photon [1,10]. Future research questions will be posed. Besides two postdocs, a PhD student, and the external collaborators, the program involved a large number of undergraduate students. [1] Madjet et al, *J. Phys. B* **41**, 105101 (2008); [2] Madjet et al, *Phys. Rev. Lett.* **99**, 243003 (2007); [3] Potter et al, *Phys. Rev. A* **82**, 033201 (2010); [4] Maser et al, *Phys. Rev. A* **86**, 053201 (2012); [5] De et al, *J. Phys. B Letter* **49**, 11LT01 (2016); [6] Javani et al, *Phys. Rev. A* **89**, 063420 (2014); [7] Barillot et al, *Phys. Rev. A* **91**, 033413 (2015); [8] Dixit et al, *Phys. Rev. Lett.* **111**, 203003 (2013); [9] Magrakvelidze et al, *Phys. Rev. A* **91**, 053407 (2015); [10] Choi et al, *Phys. Rev. A* (2017) (accepted) arXiv:1610.00346 [physics.atm-clus]

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