

Abstract Submitted
for the DAMOP20 Meeting of
The American Physical Society

Resonant inter-Coulombic decay (ICD) of innershell photoexcitations in halogen@C₆₀ endohedral molecules¹ RUMA DE, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA — Considering halogen@C₆₀ endohedral molecules, we study the transfer-decay of photoinduced innershell vacancies of the atom or the fullerene through the “other” ionization continuum, that is, respectively, *via* the fullerene or atomic continuum. This process, driven by the Coulomb-type long range coupling between the members of the ‘dimer’ and augmented by various degrees of wavefunction hybridizations, is generally known as the inter-Coulombic decay (ICD). A density functional study is employed to model the ground state structure of the molecules and their ionization response to the radiation field is treated in a linear response framework [1]. Previous predictions of ICD based were reported for various noble gas endofullerenes [2,3]. The current research, on the other hand, investigates effects of open-shell structures of the halogen atoms on ICD resonances. Focus has also been given to observe how the ICD features evolve when a fullerene electron fills the halogen outer vacancy. Detailed results will be presented in the conference. [1] Madjet *et al.*, *Phys. Rev. A* **81**, 013202 (2010); [2] Javani *et al.*, *Phys. Rev. A* **89**, 063420 (2014); [3] De *et al.*, *J. Phys. B* **49**, 11LT01 (2016).

¹Supported by the National Science Foundation grant PHY-1806206

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Date submitted: 30 Jan 2020

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