

Abstract Submitted
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Role of electron correlation in femtosecond relaxation of photoexcited electrons in C₆₀¹ MOHAMED MADJET, QEERI, Hamad Bin Khalifa University, Doha, Qatar, ORIOL VENDRELL, Aarhus University, Aarhus, Denmark, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA — Electron-phonon coupled dynamics in molecules underpins many vital phenomena in matter, including the mobility and collection of carriers in organic devices [1]. Following the absorption of photons by a fullerene molecule, the relaxation of excited electrons to the band-edge via electron-phonon (e-p) coupling, transferring energy to the vibrational degrees of freedom, is of fundamental interest [2]. We simulate the relaxation dynamics in C₆₀ using two schemes: (i) Quantum Espresso software to describe the structure and the PYXAID package, which employs classical trajectory surface hopping for non-adiabatic (NA) e-p coupling [3], to describe the dynamics; this is effectively a single particle frame. (ii) Electronic structure calculated with the package GAMESS, describing the ground state at the Hartree-Fock level and the excited states at the Configuration Interaction Singles (CIS) level, followed by surface-hopping NA dynamics using Chemical Dynamics Tool Kit [4]. Comparisons indicate a dramatically faster decay induced by correlations. Such ab initio results will motivate and complement femtosecond measurements of relaxation processes in fullerenes via RABITT and streaking approaches. [1] Coropceanu et al, Chem. Rev. **107**, 926 (2007); [2] Ross et al, Nature Materials **8**, 208 (2009); [3] Madjet et al, Phys. Chem. Chem. Phys. **18**, 5219 (2016); [4] Madjet et al., J. Chem. Phys. **138**, 094311 (2013).

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