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Vibrational relaxation of hot carriers in C_{60} molecule[1] MOHAMED MADJET, QEERI, Hamad Bin Khalifa University, Doha, Qatar, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA
— Electron-phonon coupling in molecular systems is at the heart of several important physical phenomena, including the mobility of carriers in organic electronic devices [1]. Following the optical absorption, the vibrational relaxation of excited (hot) electrons and holes to the fullerene band-edges driven by electron-phonon coupling, known as the hot carrier thermalization process, is of particular fundamental interest [2]. Using the non-adiabatic molecular dynamical methodology (PYXAID + Quantum Espresso) based on density functional approach [3], we have performed a simulation of vibrionic relaxations of hot carriers in C_{60}. Time-dependent population decays and transfers in the femtosecond scale from various excited states to the states at the band-edge are calculated to study the details of this relaxation process. [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).

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