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Vibrational relaxation of photoexcited electrons in fullerenes[1]
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Electron-phonon coupling in stimulated molecular systems underpins the mobility and collection of carriers in organic devices [1], finds applications in radiation damage or astrochemistry, besides fundamental interests [2]. We study the vibrational relaxation dynamics of photoexcited electrons to the fullerene band-edge driven by electron-phonon coupling. Time dependent density functional approach in the frame of non-adiabatic molecular dynamics (MD) [3] is used for simulations. MD with fewest switches surface hopping technique versus solving Schrodinger equation will be compared. Transition dipole moments, non-adiabatic electron-phonon couplings, and ultrafast time-dependent population decays from initially populated excited states will be presented. The work may motivate and complement recent interests [2] in ultrafast relaxation measurements in molecules by attosecond XUV pulses.
[1] A. V. Akimov and O.V Prezhdo, *J. Chem. Theory Comput.* **9**, 11 (2013); [2] Marciniak *et al., Nature Comm.* **10**, 337 (2019); [3] Madjet *et al., Phys. Chem. Chem. Phys.* **18**, 5219 (2016).

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