Abstract Submitted
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Hot carrier dynamics in endohedral compounds[1] MOHAMED MADJET, MARCELO CARIGNANO, QEERI, Hamad Bin Khalifa University, Doha, Qatar, ORIOL VENDRELL, Institute of Physical Chemistry, Heidelberg, Germany, ESAM ALI, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA — Using time-dependent density functional theory in combination with non-adiabatic molecular dynamical simulations [1,2], the carrier dynamics in photoexcited endohedral fullerene is investigated. In order to identify the effect of many electron correlations, we performed two sets of simulations. The first one is based on a single particle approach [1,3] that allows the study of large molecular and periodic systems. The second set is based on calculations performed taking into account many-body correlations only in the molecular systems [4]. Results on electronic properties, optical excitation and ultrafast hot electron relaxation dynamics will be presented. The effect of different exchange-correlation (XC) functionals will be discussed. The advantages and drawbacks of the two methods will be outlined. [1] A. V. Akimov and O.V Prezhdo, *J. Chem. Theory Comput.* **9**, 11 (2013); [2] Madjet *et al.*, *J. Phys. Chem. Lett.* **8**, 18 (2017); [3] Zapata *et al. J. Chem. Inf. Model.* **59**, 3191 (2019); [4] Madjet *et al. J. Chem. Phys.* **138**, 094311 (2013).

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