Quantum description of the photo-induced electron transfer in gold-organic nanomaterials

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The electron flow between a metallic aggregate and an organic molecule after excitation with light is a crucial step on which are based the hybrid photovoltaic nanomaterials. So far, designing such device with the help of theoretical approaches have been heavily limited by the computational cost of quantum dynamics models able to track the evolution of the excited states over time. In this contribution we present the first application of Time-Dependent Density Functional Tight-Binding (TD-DFTB) method [1] for an experimental nanometer-sized gold-organic system consisting in a hexylprotected Au_{25} cluster labelled with a pyrene fluorophore, in which the fluorescence quenching of the pyrene is attributed to an electron transfer from the metallic cluster to the dye. The full quantum rationalization of the electron transfer is attained through quantum dynamics simulations, highlighting the crucial role of the protecting ligands shell in the electron transfer, as well as the coupling with nuclear movement.[2] This work paves the way towards a fast and accurate theoretical design of optoelectronic nanodevices.

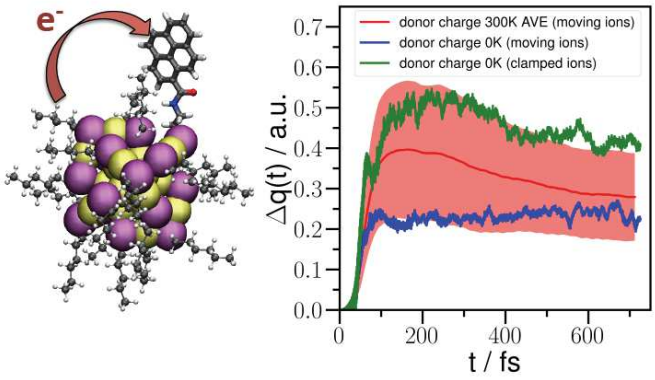

Figure 1. *Functionalized nanocluster under study and computed photoinduced electron flow.*

[1] Franco P. Bonafé, Bálint Aradi, Ben Hourahine, Carlos R. Medrano, Federico J. Hernández, Thomas Frauenheim, and Cristián G. Sánchez, J. Chem. Theory Comput. 2020, 16, 7, 4454–4469.

[2] A. Domínguez-Castro, C. R. Lien-Medrano, K. Maghrebi, S. Messaoudi, T. Frauenheim, and A. Fihey, *Nanoscale*, **2021**,*13*, 6786-6797.