Abstract Submitted
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**Photo-Electron Injection into TiO2: Quantum Dot vs. Graphene**[1] RUN LONG, University College Dublin — We presented a detailed comparison on the similalaries and differences of the ultrafast photoinduced electron transfer (ET) from two kinds of donor species, namely PbSe quantum dot (QD) and graphene, into the acceptor $TiO_2$ surface via *ab initio* time domain density functional theory simulations. The main diffrences stem from the size and dimensionality of the donor species and donor-acceptor bonding characteristics. For exmaple, the QD is localized species and composed by heavy atoms that connected to $TiO_2$ surface via chemical bonds. In contrast, the graphene layer is delocalized two-dimensional object that attached to $TiO_2$ substrate by van der Waals interaction and partial chemical bonds. The ET mechanism depends on the dimensionality of the donor and donor-acceptor chemical bonding. The injection from the localized donor states of the QD is dominatly adiabatic. In contrast, the injection from the two-dimensional graphene into $TiO_2$ exhibits prominently nonadiabatic (NA) component. The NA mechanism is efficient for the graphene/$TiO_2$ composites because it is delocalized over two dimensions and is able to couple with a dense manifold of delocalized $TiO_2$ conduction band states and weak coupling as well. The high density of acceptor states in this case favors the NA mechanism.

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