Study of Dye-Sensitized Cesium Lead Halide Perovskite Photovoltaics through Marcus Theory

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Perovskites have been around for a while, but recently have been started to be used in solar photovoltaic cells and radiative chemistry. The perovskite by itself is not capable to run solar reactions but coupled with an organic dye a solar cell can be constructed to harvest the energy from the sunlight. The specific perovskite used is Cesium Lead Halide perovskite and the organic dye used was a un functionalized tribezenamine and a functionalized tribezenamine with alcohol groups. The study of this donor of the perovskite and the acceptor of the dye is to see what kind of interaction happens between them and which scenario is better. There are two possibilities in how the electron can be transported between this acceptor and donor pairs. The first is a chemical bond formed through hydrogen bonding of the functionalized tribezenamine. In this scenario, the charge travels through the bond that is formed. This will give more favorable conditions for the transfer to happen due to the lowering of the activation barrier. The second scenario is a phis absorption between the tribezenamine and the perovskite.[1] Instead of having a bond form the charge must travel through empty space between the donor and acceptor. This will have a larger activation barrier due to no bond but the distance between the acceptor and donor is shorter. This gives for a possibility for the transfer to occur. To study these interactions a parameterization of electron-nuclear interaction has been made in the fashion similar to Marcus theory. This allows to study the transfer of the electron with the difference potential energy surfaces of the acceptor and donor. The quantized dynamics of coupled electronic and nuclear degrees of freedom was propagated in time using evolution operator technique. What was found is that the phis absorption requires lower activation energy to transfer the electron, but the hydrogen bond has higher reaction yields then the phis absorption but requires larger activation energy to achieve it.

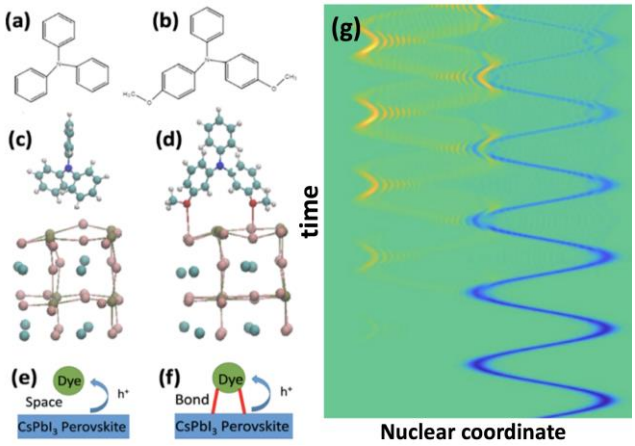

Figure 1. Figure 1 a, b) The structure of the tribezenamine functionalized and unfunctionalized. c, d) The scenarios of the chemical bond and the phis absorption. e, f) A diagram of the electron transfer in the two scenarios Panel (g) Shows the electron probability over time when the transfer occurs between the acceptor and donor.

1. Forde, A.; Kilin, D., Hole Transfer in Dye-Sensitized Cesium Lead Halide Perovskite Photovoltaics: Effect of Interfacial Bonding. *The Journal of Physical Chemistry C* **2017,** *121* (37), 20113-20125.