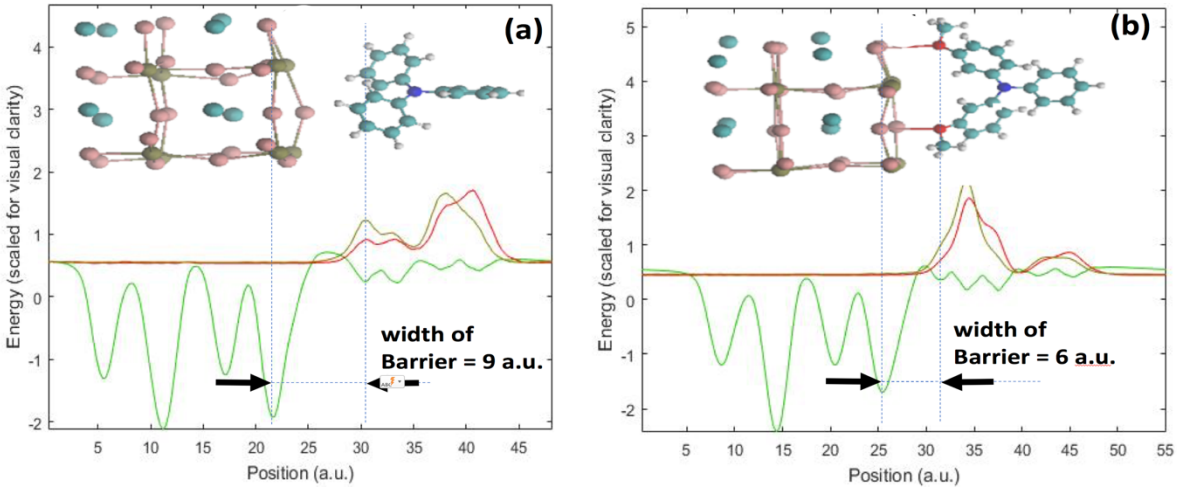
# Electron Dynamics at Cesium Lead Iodide Perovskite/Spiro-OMeTAD Interface

Landon Johnson[1], Aaron Forde[1], Dmitri Kilin[2]

1. Department of Physics, North Dakota State University, Fargo, ND 58108, United States
2. Department of Chemistry and Biochemistry, North Dakota State University, Fargo, ND 58108, United States

Perovskite based solar cells are gaining popularity in research due to the ease of their fabrication and high efficiency performance compared to other non-traditional solar cells; traditional cells being crystalline silicon photodiode cells. This research aims to explore the electron dynamics at two types of cesium lead iodide perovskite/spiro-OMeTAD inorganic-organic interfaces, "through-space" and "through-bond." The evolution operator is utilized to calculate the time progression of the electron wavefunction across the potential profile for each model. Dynamics are simulated in one dimension, where the local one-particle potential profiles are taken from *ab-initio* ground-state geometry optimization and are projected along the z-axis.[1] The simulation demonstrates that the "through-bond" model allows for greater electron transfer rates across the interface than the "through-space" model. This agrees with the principle of quantum tunneling, as the potential barrier across the interface in the "through-bond" model has both lower width and height than the "through-space" model, and therefore higher transmission probability.




*Snapshots of (a) "through-space" and (b) "through-bond" simulations. Insets represent atomistic models of* $Cs_nPb_nI_{3n}$, n=8, slabs interfacing tribenzenamine dye, which mimicks Spiro-OMeTAD. The *green curves represent the potential energies, while the red and tan curves represent different techniques of modeling the evolution of the electron probability distribution. The deep potential wells on the left model the perovskite while the shallow wells on the right model the spiro-OMeTAD dye. The first shallow well located at position 31.5 a.u. in (b) models the methoxy linker group.*

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.