Work Plan

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Background: DFT method combined with B3LYP hybrid functional has been widely used to study the electronic structure and optical properties of organic. However, it is well known that the traditional DFT functionals tends to promote a delocalization of the system's wave function. This fact is a major challenge when modeling organic semiconductors, as it is known that localized quasiparticles are responsible for the charge transport in these systems. The recently developed range-separated hybrid functionals (RSH) with tuning range separation parameter has been successfully used to overcome this kind of difficulty.

Main Goal: We propose the use of RSH to obtain electronic and optical properties of organic molecules in a more precise and molecule customized fashion. Time dependent DFT (TDDFT) calculations with functional that includes long-range corrections considering globally tuned ω parameter dedicated to each system. We show how this procedure is observed to be superior to the standard DFT method as far as static and optical properties are concerned. We also propose to test different schemes, such as the optimization of the ω parameter using other schemes, such as by parametrization with highly correlated methods, such as Coupled-Cluster or Moller-Plesset (MP) theory.

Systems and Properties of Interest: The systems of interest are small to medium organic molecules designed of under investigation for use in Photovoltaic Cells or Light Emitting Diodes. The properties of interest are those related to the phenomena of light absorption, light emission and charge transport within these materials.