Electronic properties of organic compound for solar cells

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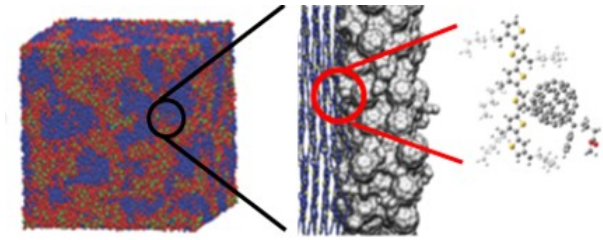
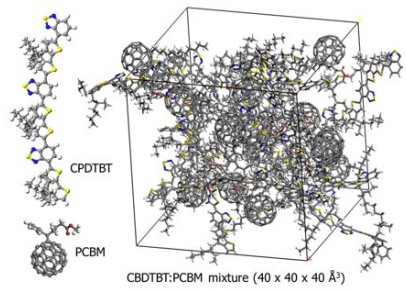
Clean/sustainable solar energy can be harvested at low cost by **organic photovoltaic cells** built with bulk heterojunction (BHJ) blends of **electron-donating** polymers and **electron-accepting** fullerene derivatives, but further improvement from the current efficiency (~10%) is hampered by lack of understanding of the blend morphology.

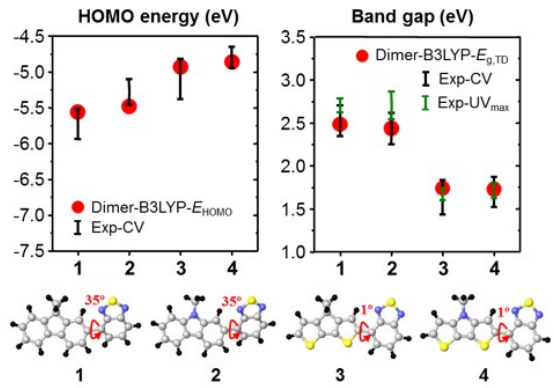
The purpose of this project is to gain a molecular-level understanding of **donor-acceptor nanophase morphology in BHJ** in order to **improve device performance** (>10%) by controlling the **electronic structure**, **molecular ordering**, and p**hase separation**. It will be done with a multi-scale modeling tool bridging quantum mechanics regimes and classical mechanics (all-atom or coarse-grained) regimes, a methodology applicable to other systems/processes exhibiting several length- and time-scales.



The multiscale approach



Classical MD simulation to study nanophase morphology.



QM calculations to design new compounds