Project Summary

Summer 2020

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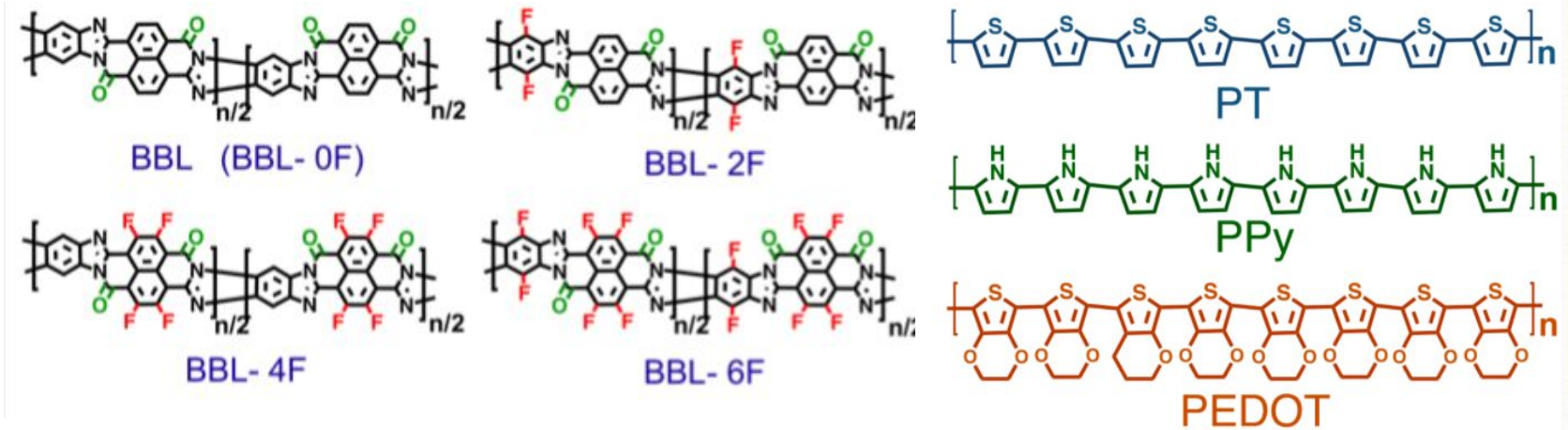
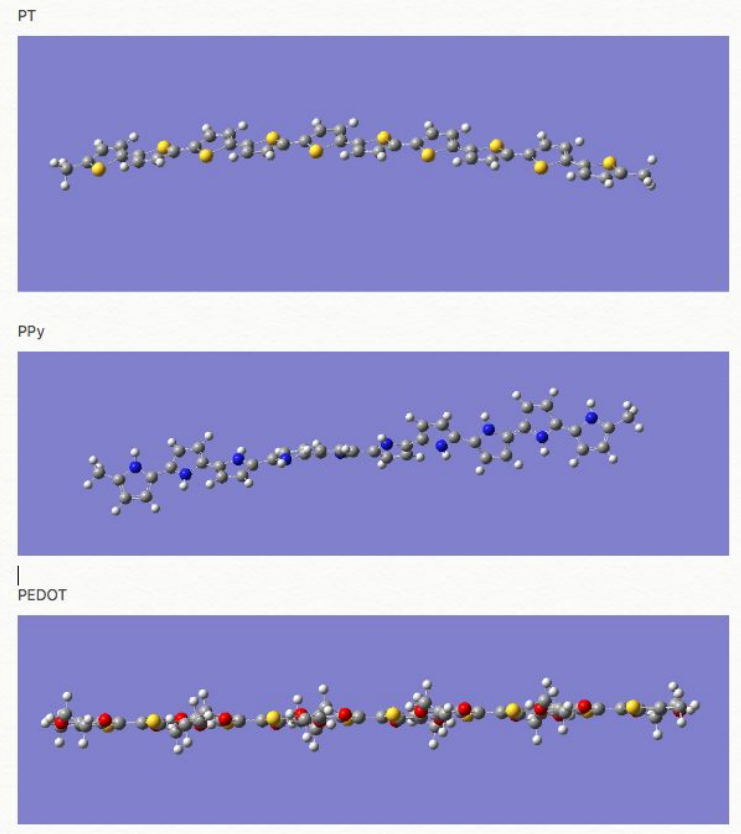
Introduction:

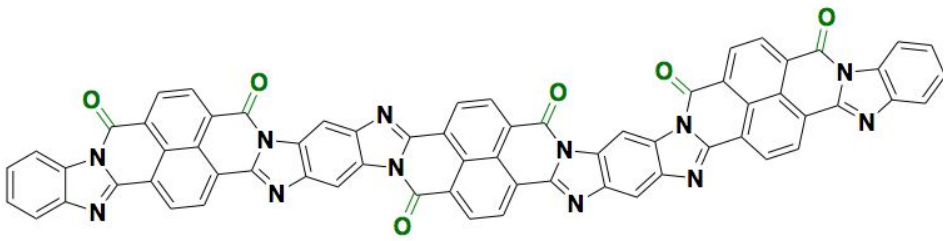
Goal: study fluorinated BBL derivatives to determine effects fluorination has on optical and electronic properties in the neat polymer and blends with both BBL and p-type polymers (polyethylenedioxythiophene (pedot) polypyrrole (PPy) and polythiophene (PT)



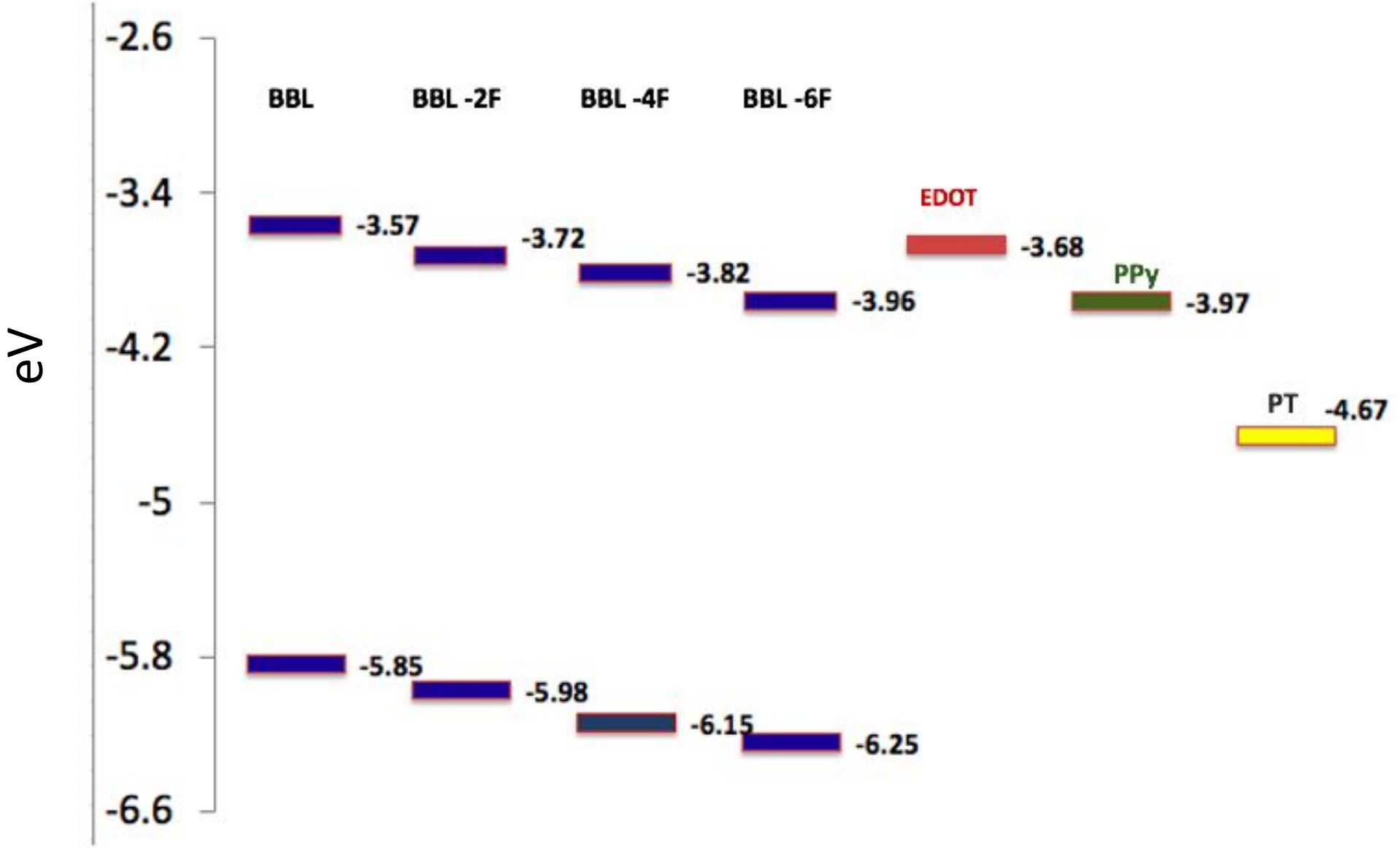


Methods

- DFT Calculations of the neat BBL derivatives and the Bilayer blends consisting of BBL derivatives and the p-type polymers
- Geometrically optimized in ground state using density functional theory (DFT) and in excited state using time-dependent DFT (TD-DFT) to determine optical and electrical properties
- Level of theory for all calculations: b3lyp
- Solved for 12 excited states in neat BBL, 6 for bilayers
- The p-type polymer chains consisted of ten monomer units (N=10)
- BBL chain consisted of three monomer units (N=3) in the cis/trans/cis conformation



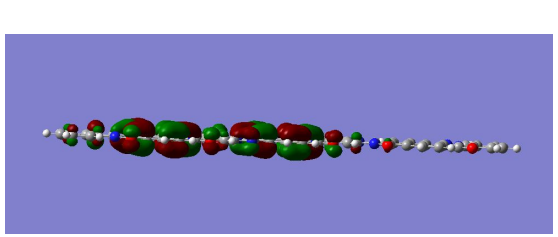
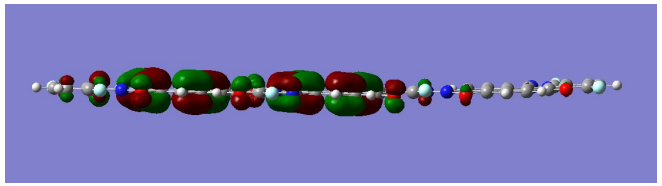
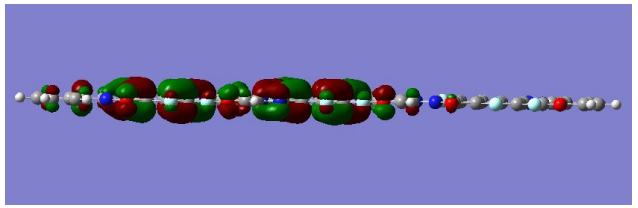
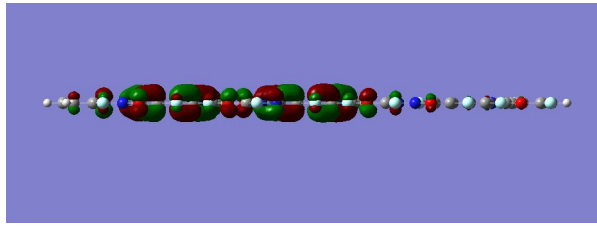
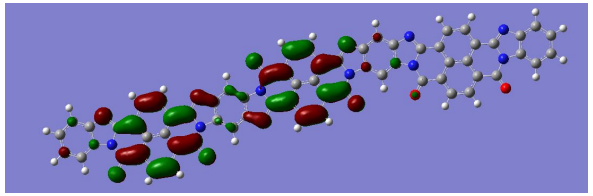
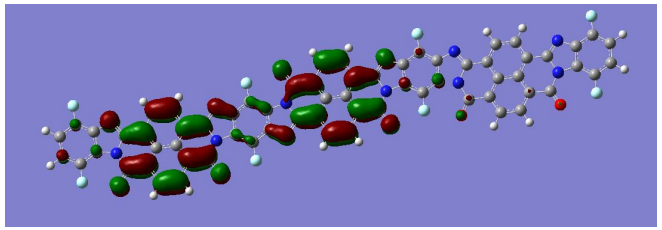
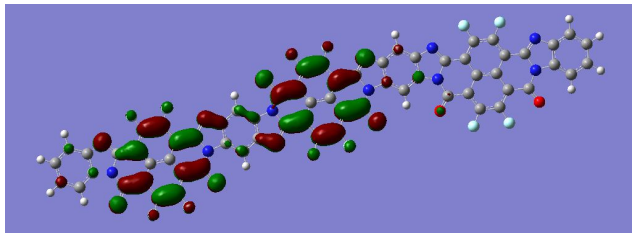
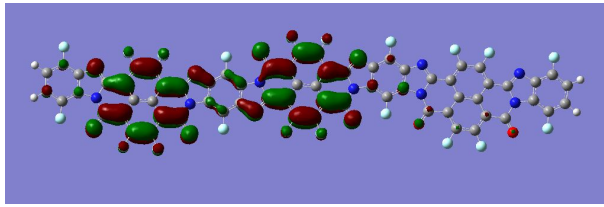
Results: Energy Levels (ground state)



- Decreasing LUMO of n-type polymer BBL as degree of fluorination increases
- Compared to HOMOs of p-type polymers

Molecular Orbitals- BBL Derivatives Molecular Orbitals- ground state

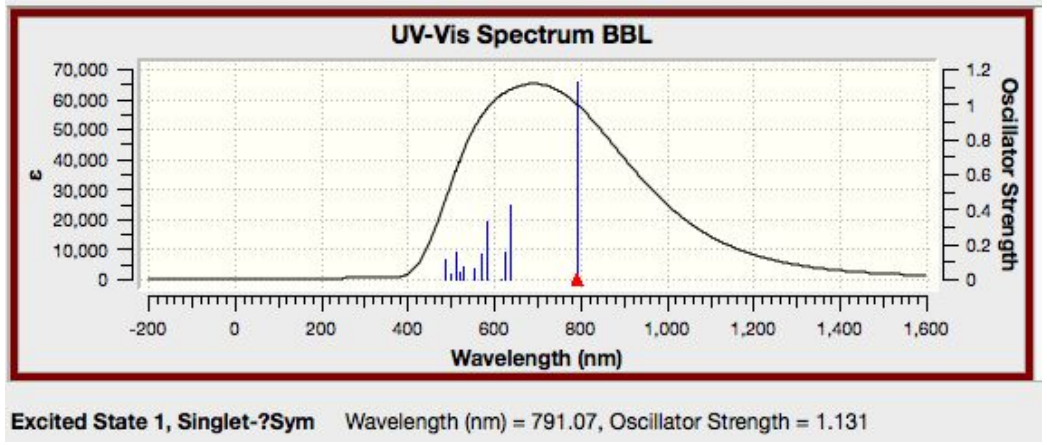
BBL **BBL -2F** **BBL -4F** **BBL -6F**

- BBL and BBL 4F more planar
- BBL 2F and BBL 6F have more torsion in the backbone possibly due to interactions between the F and O

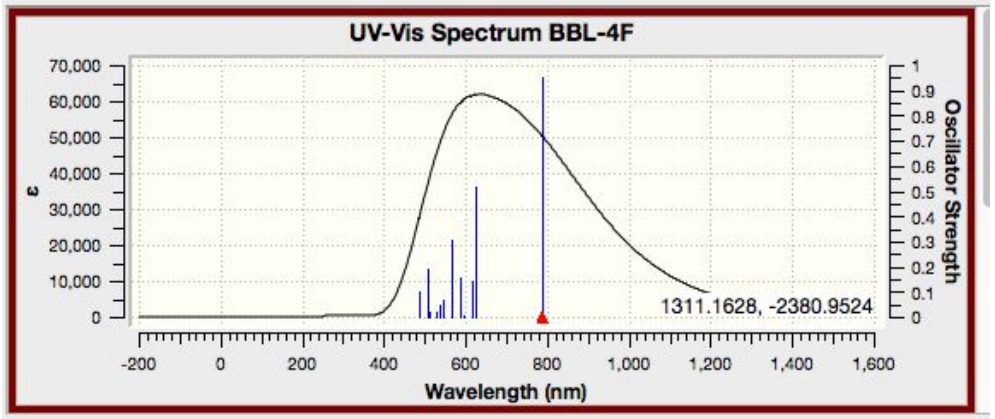
UV-Vis Spectra: TD-DFT calculations, n=3, 12 excited states

BBL: 791.07 nm



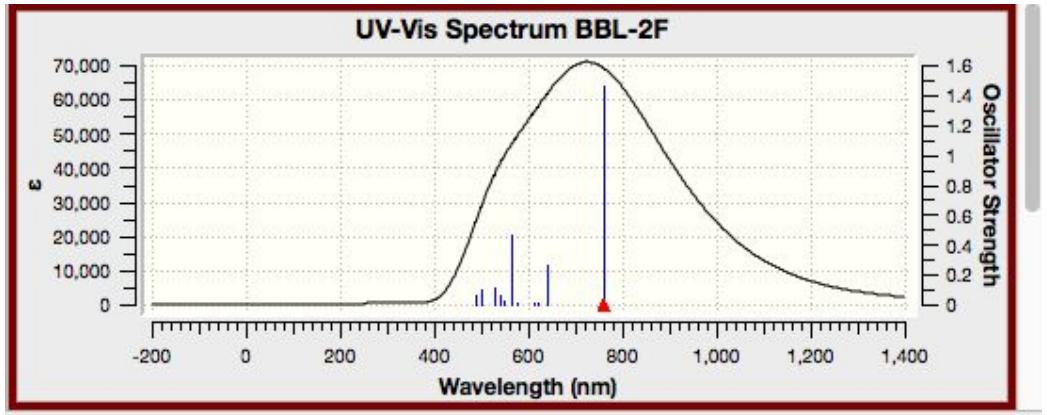
Excited State 1, Singlet-?Sym Wavelength (nm) = 791.07, Oscillator Strength = 1.131

BBL-4F: 786.93 nm



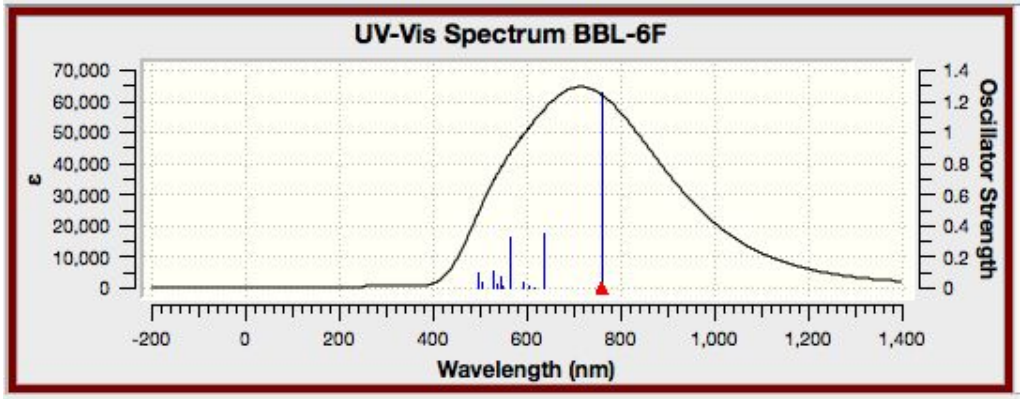
Excited State 1, Singlet-?Sym Wavelength (nm) = 786.93, Oscillator Strength = 0.9495

BBL-2F: 761.62 nm



Excited State 1, Singlet-?Sym Wavelength (nm) = 761.51, Oscillator Strength = 1.4654

BBL-6F: 760.89 nm

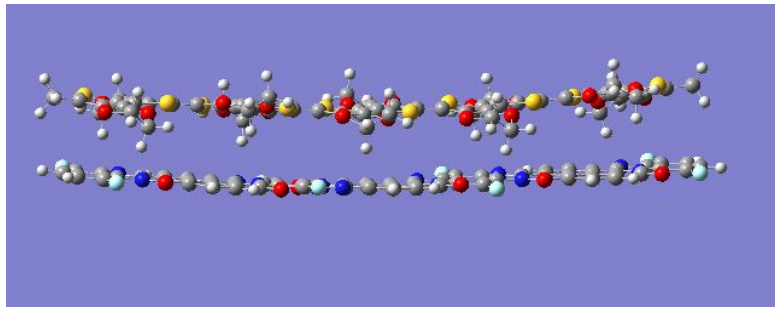


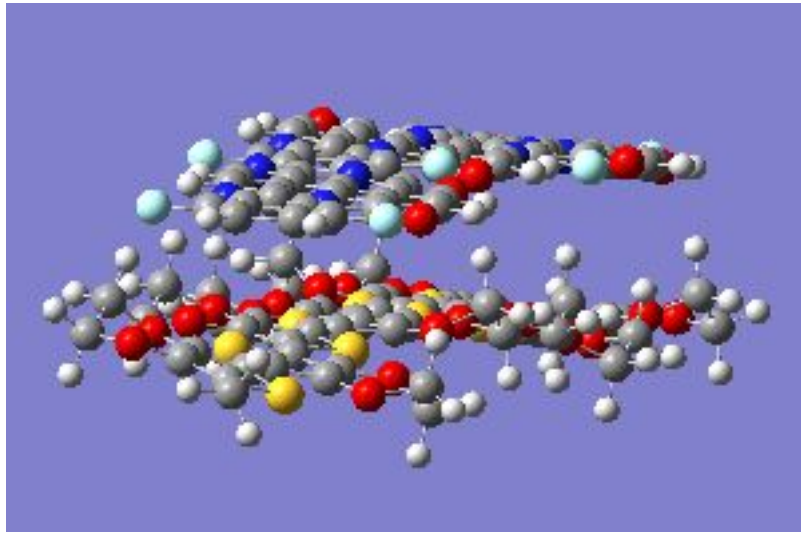
Excited State 1, Singlet-?Sym Wavelength (nm) = 760.89, Oscillator Strength = 1.2599

Bilayers – BBL **2F**

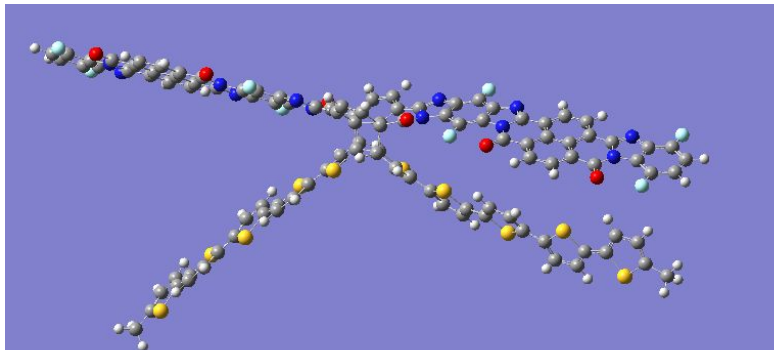
*Bend in BBL 2F/PT

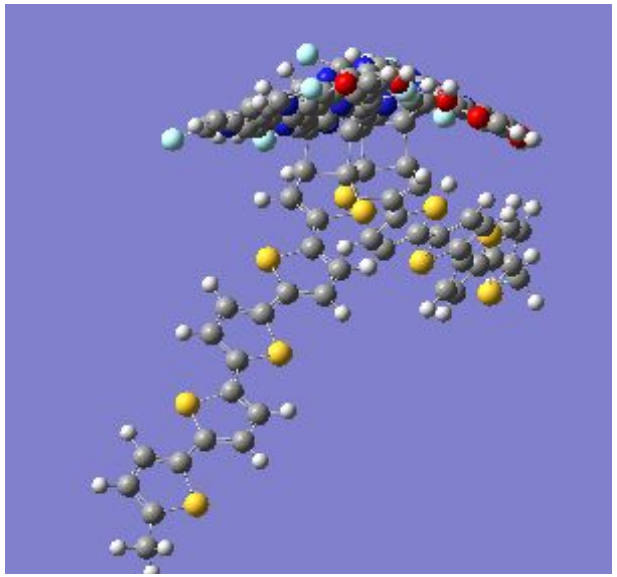
BBL2F/ edot



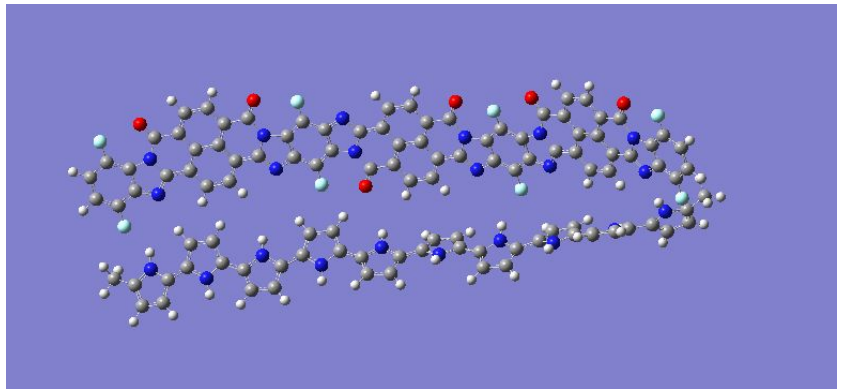


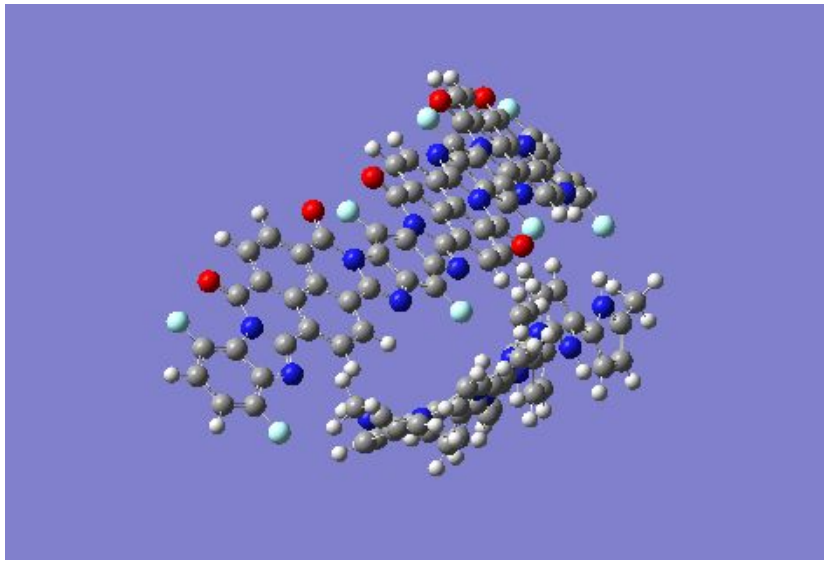
BBL 2F/ PT*





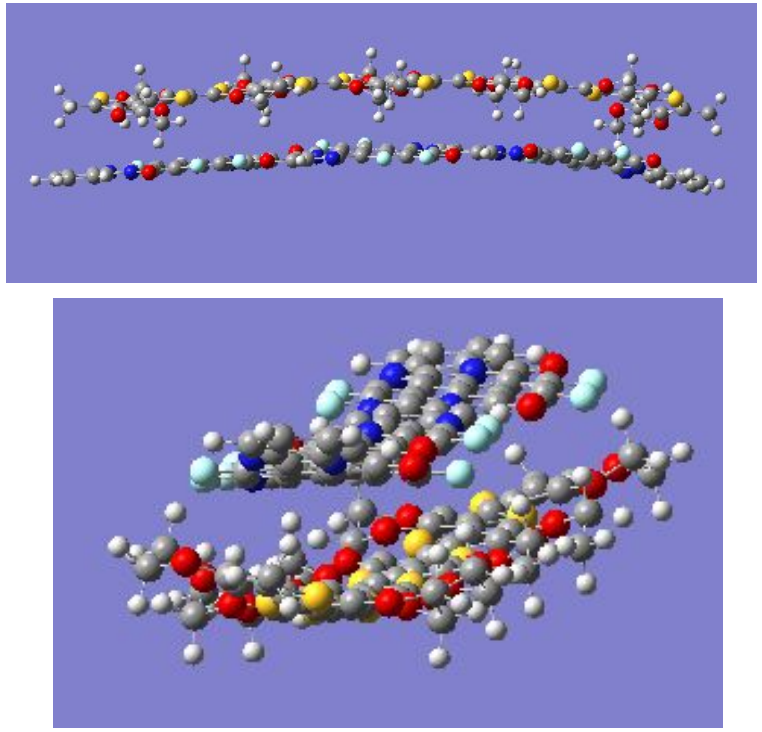
BBL 2F/ PPy



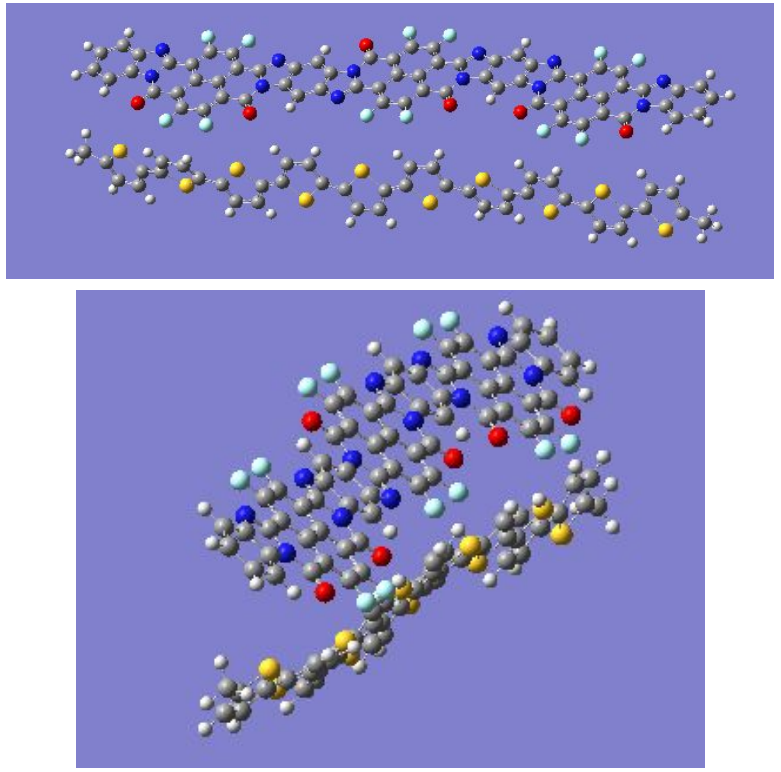


Bilayers- BBL 4F ground state, no methyl groups added

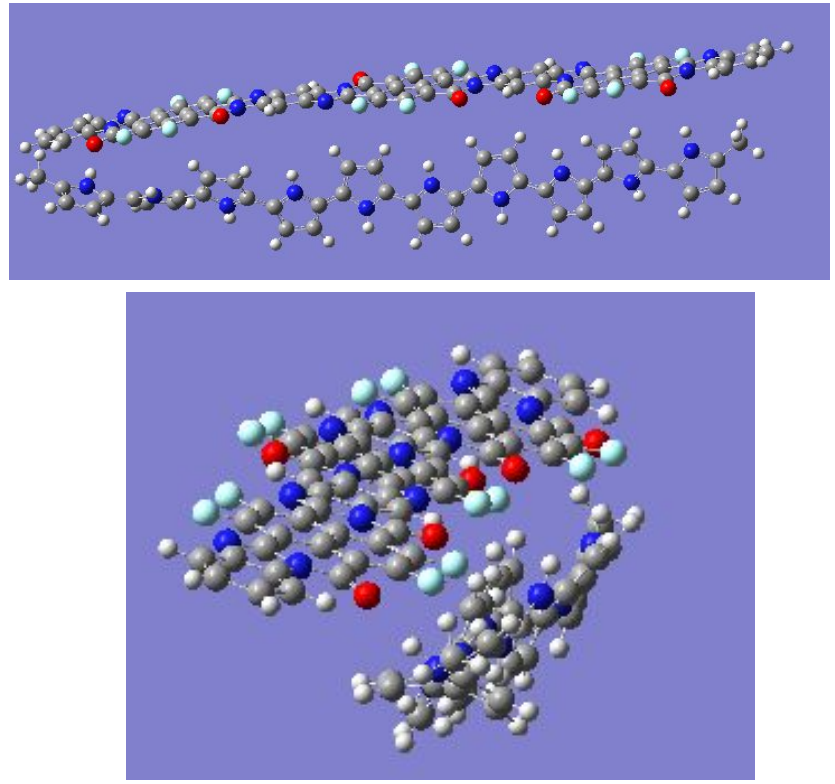
BBL 4F/ edot



BBL 4F/ PT



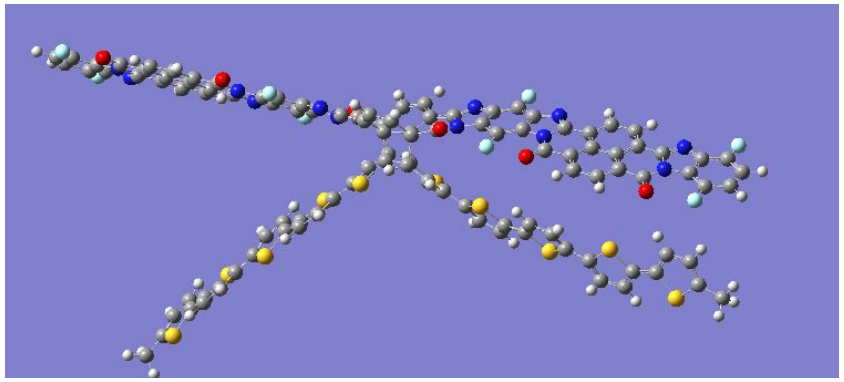
BBL 4F/ PPy

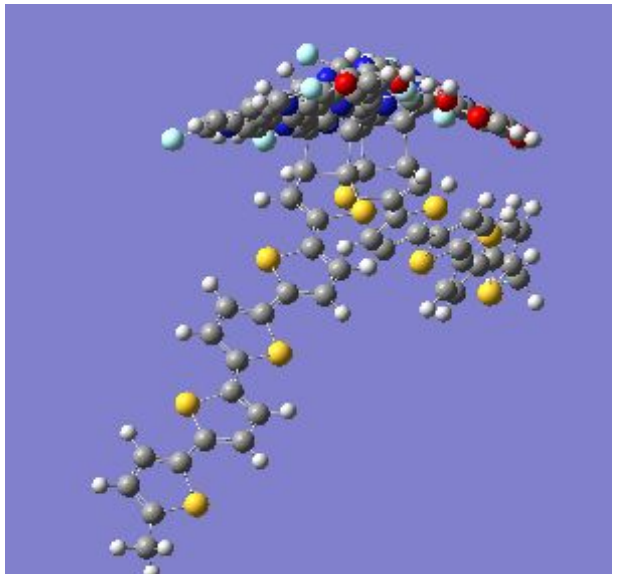


- Possibly Hydrogen bonding between oxygen on BBL and H from p-type polymer… avg bond length ~2.6 A
- Similar results for BBL 2F and BBL 6F

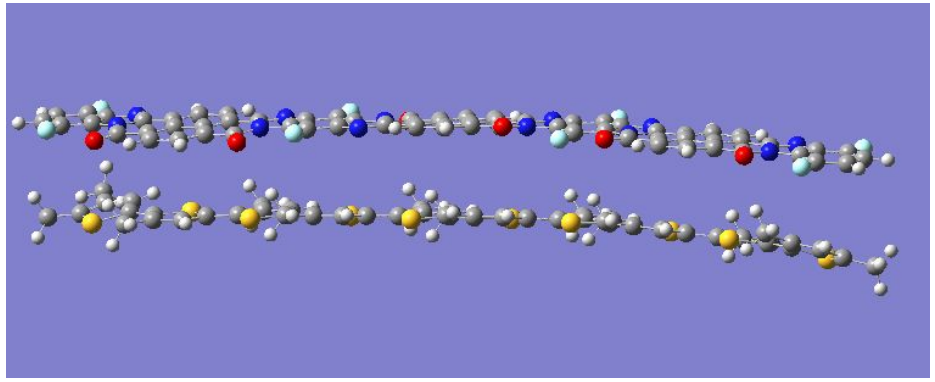
Methylated BBL 2F/ PT Bilayer

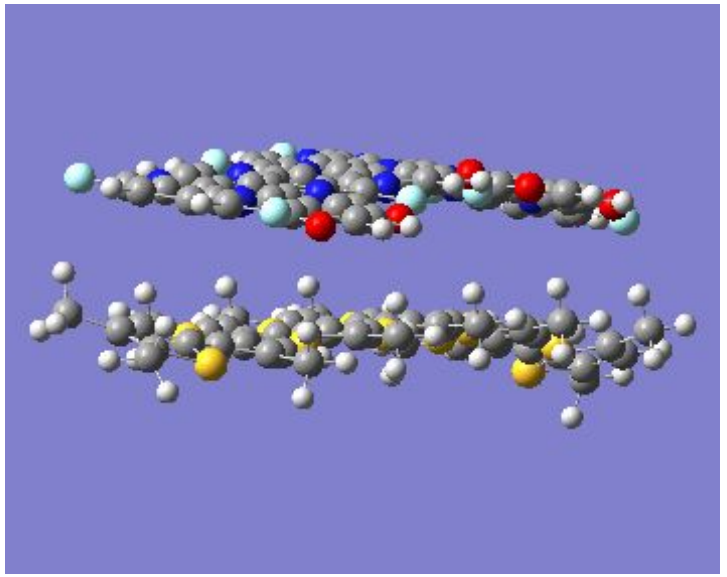
No methyl groups added: bend





Methyl groups added: no bend





Continuing paths

- Finishing ground state DFT bilayers with methyl
- TD-SCF calculations to solve for excited states with the bilayer blends
- Charge states in neat BBL films also will be studied using TD-DFT