First Principles Study of Solar Cell PCE of Organic Molecules

Mary Catlett and Dr. Mario F. Borunda
Senior Project Presentation
Friday 12/14/2018

Power Conversion Efficiency (PCE)

- Ratio of the output energy to the input
- Important factor determining if a solar panel is marketable
  - Current consumer solar panels have PCE's starting at 15%

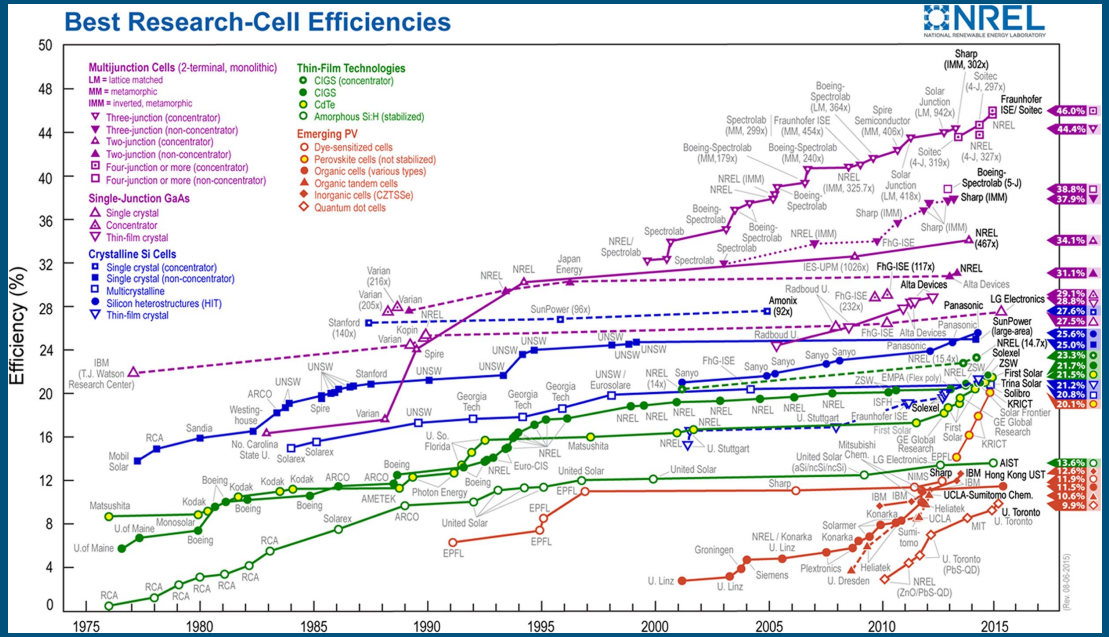
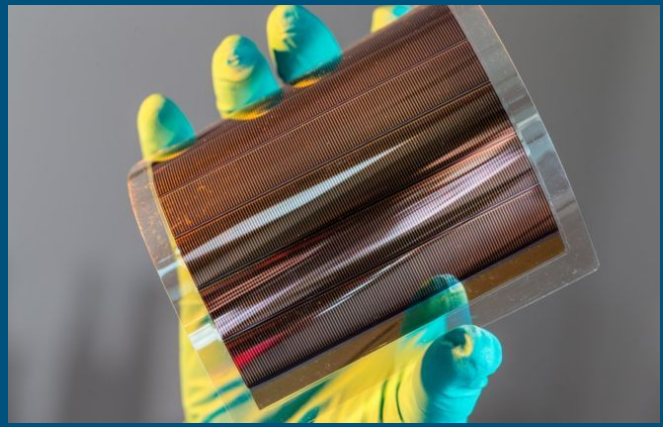


Image: http://www.nrel.gov/ncpv/

Central Motivation

- Organic Photovoltaics (OPVs) are low cost to manufacture due to roll-to-roll manufacturing process
- OPV PCE levels are increasing quickly
  - 2017: 14%*
  - 2018: 17.3%*
- Computational screening can contribute to increased performance
  - Identify and target high performing molecular families



*Science 2018, DOI:10.1126/science.aat2612

Image: https://www.bbc.com/news/science-environment-45132427

Purpose

- In this study, our goal is to compare PCE predictions proposed by Scharber to experimental data available in literature

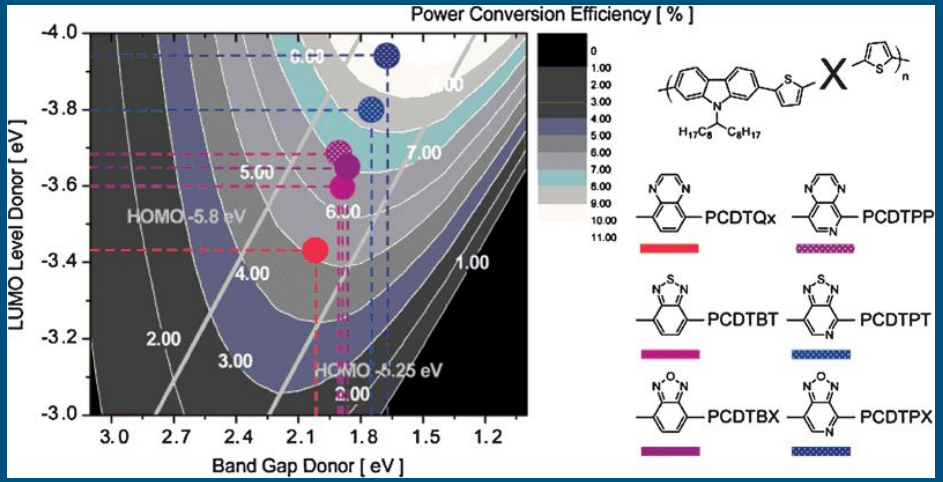


Image: https://pubs.rsc.org/en/content/articlehtml/2010/cs/b915995a

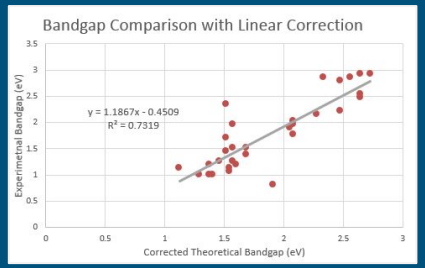
Project Outline

1. Built Molecules in Avogadro*

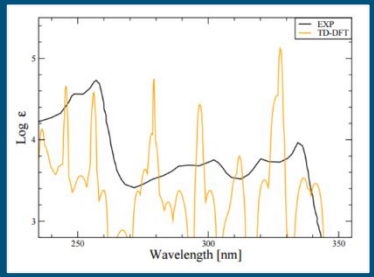
2. Basic Geometry Optimization in Avogadro*

3. Ground State Calculations in Octopus**

4. Geometry Optimization
1st attempt: Octopus
2nd attempt: Quantum Espresso



5. Optical Absorption Spectrum in Octopus



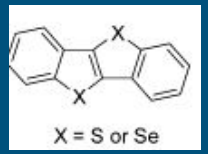
6. Convolute Absorption Spectrum with Solar Spectrum

7. Calculate the Quantum Yield for each molecule

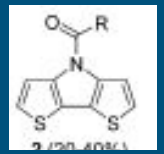
8. Compare calculations to the Scharber Model and experiment

Molecules

Set 1: 18 to 45 Atoms

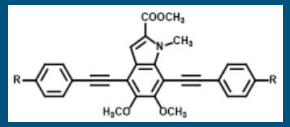


M5_1a
M5_1b
M5_2b



M13_a
M13_d

Set 2: 46 to 63 Atoms



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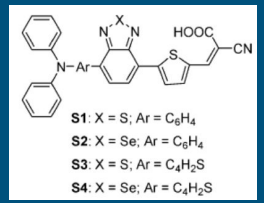
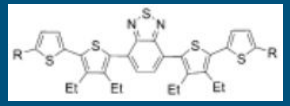
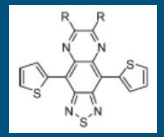


M1_S1
M1_S2
M1_S3
M1_S4

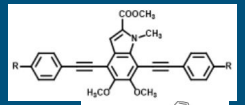


M6_3



M7

Set 3: 64 to 99 Atoms



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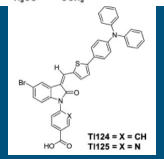
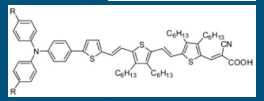


M2_24
M2_25



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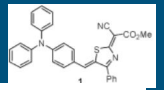

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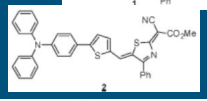

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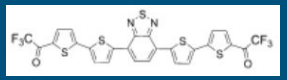

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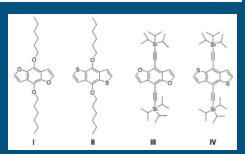
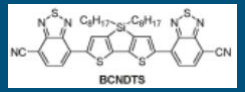


M9_3
M9_4
M9_III
M9_IV



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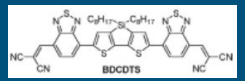
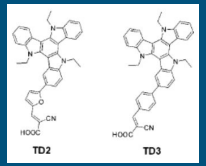


M11_2

M12_2
M12_3



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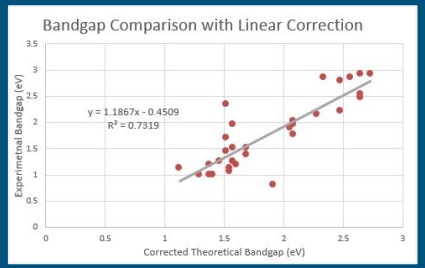

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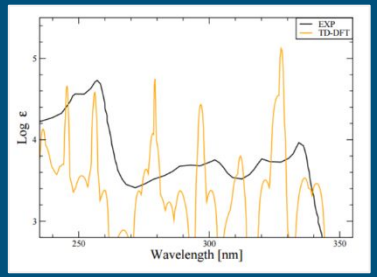


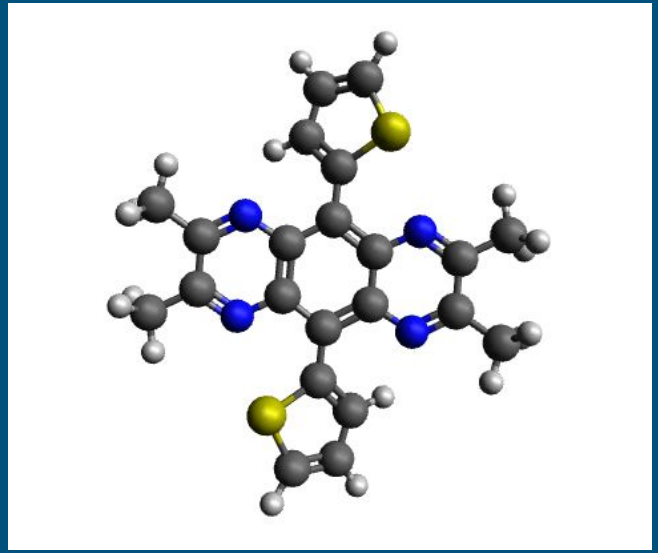
6. Convolute Absorption Spectrum with Solar Spectrum

7. Calculate the Quantum Yield for each molecule

8. Compare calculations to the Scharber Model and experiment

Building Molecules

- We manually constructed a model of each molecule from the papers in Avogadro
- We used the “optimize geometry” feature to optimize the molecule’s structure using molecular mechanics.
    - This step was a way to reduce the amount of time for subsequent calculations.



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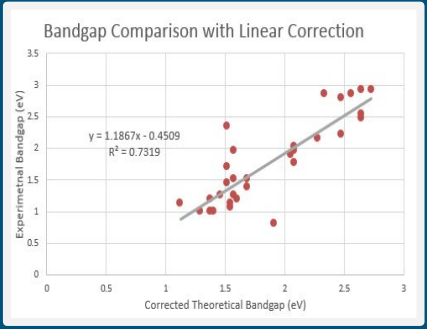

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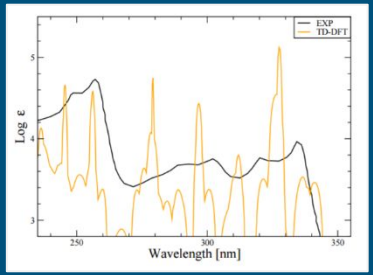

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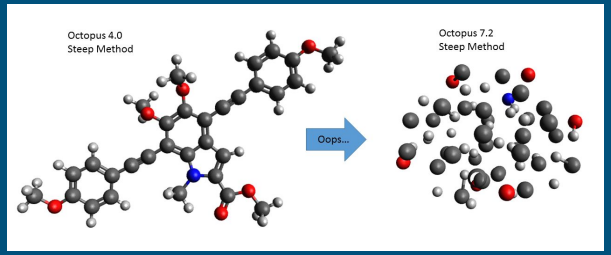
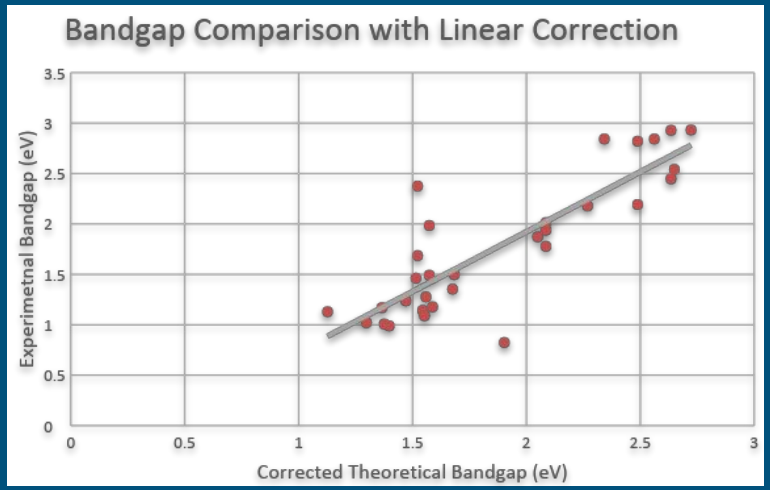
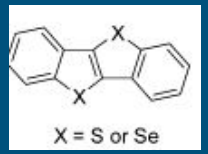
Previous Optimization Study

- Tried to use Octopus Software
  - There were a lot of bugs
  - Data was not very accurate
- Only the 6 smallest molecules converged

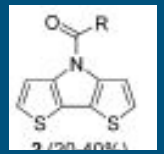




Converged Molecules (RED)



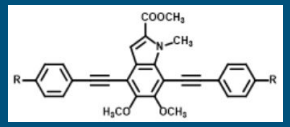
M5_1a
M5_1b
M5_2b



M13_a
M13_d

Convergence Criteria:

- Maximum Force: 0.01 eV/Angstrom



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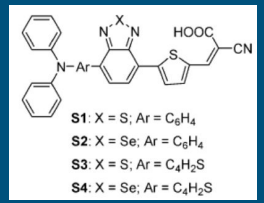
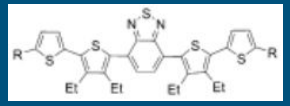


M1_S1
M1_S2
M1_S3
M1_S4



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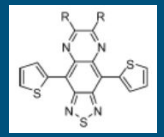

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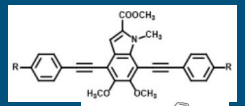

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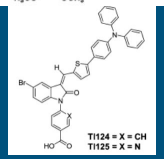
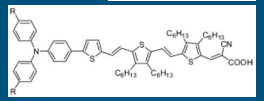


M2_24
M2_25



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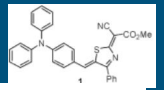
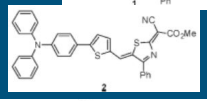


M4_1



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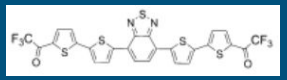

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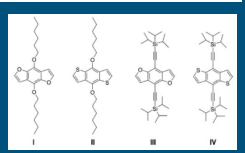
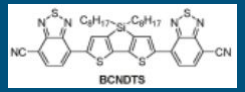
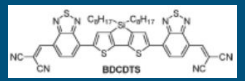


M9_3
M9_4
M9_III
M9_IV

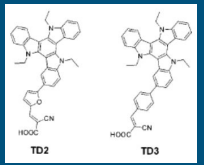


M11_1



M11_2

M12_2
M12_3



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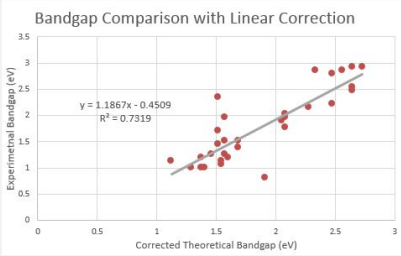

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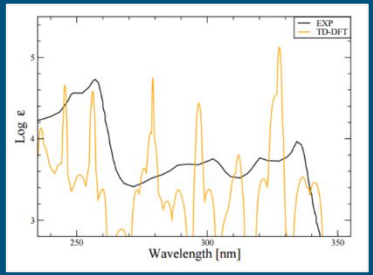

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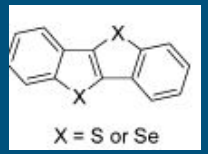
Calibrating System

- This semester, project calculations were transitioned to Quantum Espresso
- We split the molecules into three sets based on size, to better optimize computing resources.
- Set 1: 18 to 45 Atoms
  - WTL: .5 to 2 days
  - System, Size: +10 Angstrom in x, y, z
  - Hardware: 1 node (32 GB RAM), 12 processors
- Set 2: 46 to 63 Atoms
  - WTL: 3 to 5 days
  - System Size: +15 Angstrom in x, y, z
  - Hardware: 2 nodes (64 GB RAM), 24 processors
- Set 3: 64 to 99 Atoms
  - WTL: between 1 and 5 days
  - System Size: +20 Angstrom in x, y, z
  - Hardware: 1 BigMem node (256 GB RAM), 12 processors

Converged Molecules



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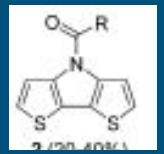

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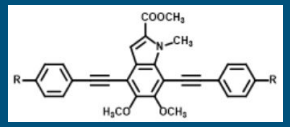

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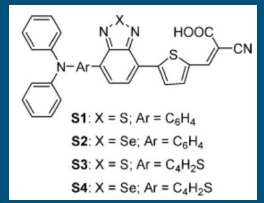
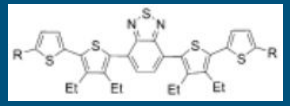
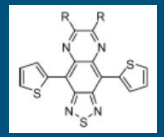


M1_S1
M1_S2
M1_S3
M1_S4



M6_3



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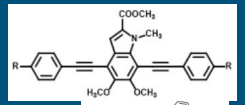

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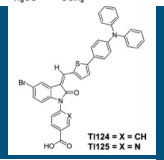
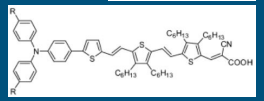


M2_24
M2_25



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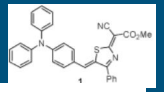

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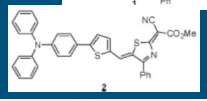

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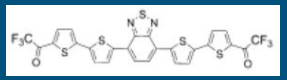

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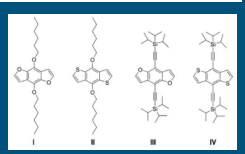
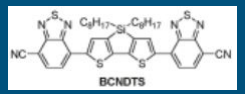


M9_3
M9_4
M9_III
M9_IV



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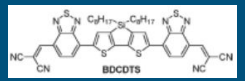
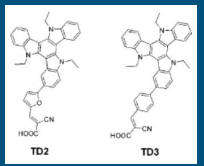


M11_2

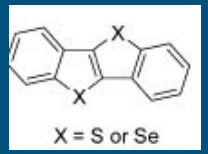
M12_2
M12_3



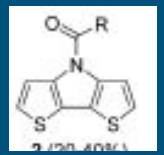
Convergence Criteria:

- Maximum Force: 0.0005 Ry/Bohr = 0.0125 eV/Angstrom

Non Converged Molecules



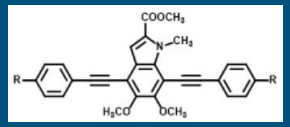
M5_1a
M5_1b
M5_2b



M13_a
M13_d

Convergence Criteria:

- Maximum Force: 0.0005 Ry/Bohr = 0.0125 eV/Angstrom



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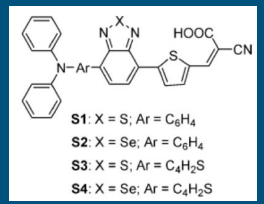
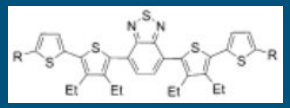


M1_S1
M1_S2
M1_S3
M1_S4



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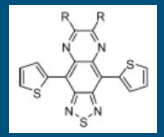

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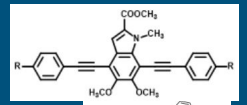

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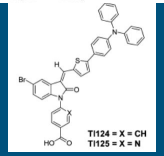
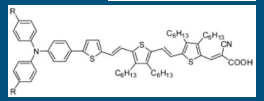


M2_24
M2_25



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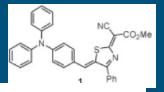

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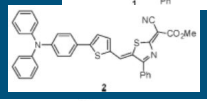

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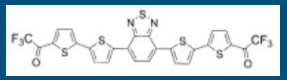

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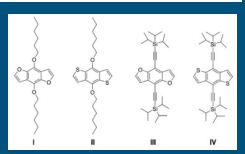
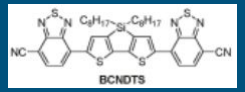


M9_3
M9_4
M9_III
M9_IV



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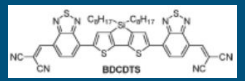
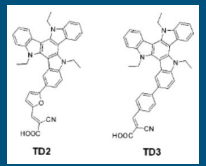


M11_2

M12_2
M12_3



Trends

- Smallest molecules converged first
  - Some larger ones did as well
- Larger molecules containing Flourine, Sulfur, and Silicon have not converged

Computing Time Comparison

Molecule	Octopus Convergence Time	Quantum Espresso Convergence Time
M5_1a	~150 hours	~1 hour
M5_1b	~175 hours	~1.5 hours
M5_2b	~200 hours	~4 hours
M7	200+ hours	~17 hours
M13_a	200+ hours	~5 hours
M13_d	200+ hours	~26 hours

Factors Affecting Time Differences

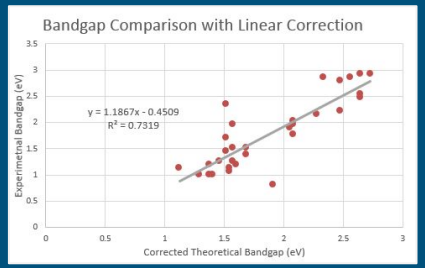
- Changing software being used
- Use of parallel computing when made transition to Quantum Espresso
- Newer supercomputer hardware at time of transition
- Last set of coordinates from Octopus runs for each molecule was used as starting point for Quantum Espresso calculations

1. Built Molecules in Avogadro

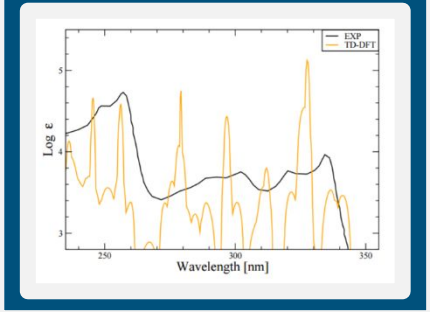
2. Basic Geometry Optimization in Avogadro

3. Ground State Calculations in Octopus

4. Geometry Optimization
1st attempt: Octopus
2nd attempt: Quantum Espresso



5. Optical Absorption Spectrum in Octopus



6. Convolute Absorption Spectrum with Solar Spectrum

7. Calculate the Quantum Yield for each molecule

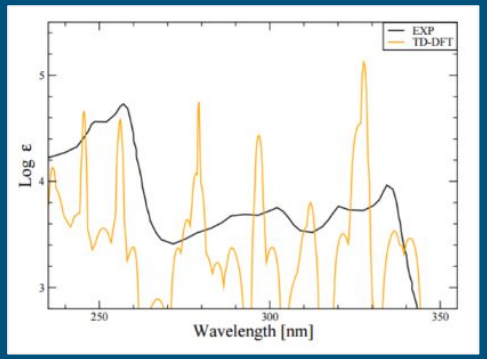
8. Compare calculations to the Scharber Model and experiment

Absorption Spectrums

Method:

- Time Dependent Density Functional Theory (TD-DFT)
- delta kick function in Octopus

Previous Attempt:



Future Attempts:

- Plan to decrease the oscillation discrepancy between experiment and theory by matching temperatures of systems

Conclusions

- Don’t use Octopus for geometry optimizations
  - Quantum Espresso is more efficient for that set of calculations
- To complete geometry optimizations
  - Maximum number of SCF cycle steps need to be changed

Next Steps

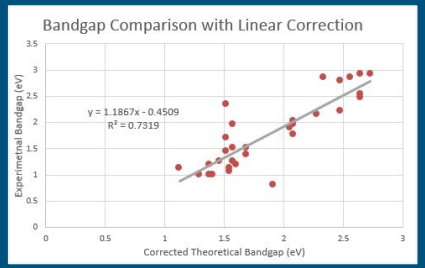
- Complete Geometry Optimization and Absorption Spectrum Calculations
  - Change maximum SCF steps allowed per calculation cycle
- Complete comparison of data to Scharber Model and experimental data

1. Built Molecules in Avogadro

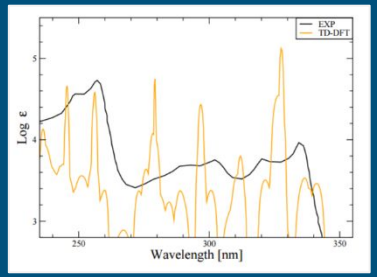
2. Basic Geometry Optimization in Avogadro

3. Ground State Calculations in Octopus

4. Geometry Optimization
1st attempt: Octopus
2nd attempt: Quantum Espresso



5. Optical Absorption Spectrum in Octopus



6. Convolute Absorption Spectrum with Solar Spectrum

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8. Compare calculations to the Scharber Model and experiment

Acknowledgments

- The Borunda Group
- Okstate High Performance Computing
- OSU Physics Department
- OK-LSAMP and McNair Scholars research grant programs

Molecule References

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