Towards Low-Cost Solar Cells: Organic-based Materials for Light-weight, Flexible Photovoltaics

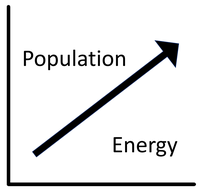
Joshua T Koubek and Alan Sellinger

Department of Chemistry, Colorado School of Mines, Golden, CO 80401

Background Information

Need for Solar

- Rapidly rising population
- Increasing demand for energy
- Rapidly rising amounts of green houses gases that are produced from fossil fuel based energy
- Energy demand projections indicate that there will be a large increase in more isolated areas around the world where large scale power plants are not appropriate



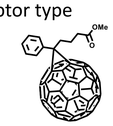
Why OPV

- Lightweight
- Flexible
- Transparent
- Low Production Cost Potential

Fullerenes

- Fully π-conjugated
- Three Dimensional
- High Purification Costs
- Poor material interfacing
- Only an acceptor type molecule

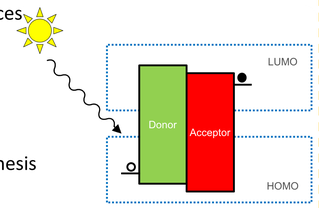
C_{60} : \$443/g



$PC_{61}BM$: \$742/g

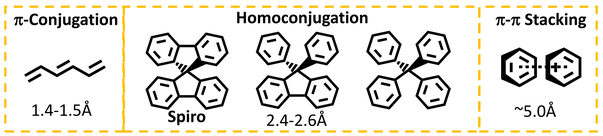
Premise of Research

- ↑ Efficiency
  - Improve exciton transfer to/from interface
  - Optimize HOMO, LUMO, and Band Gaps
  - Optimize Material Interfaces
- Keep Costs ↓
  - Easy to Process
  - Cheap Reagents
  - Simple High Yielding Synthesis



Homoconjugation (HC)

Definition: The interaction and stabilization of π-bonds with neighboring groups through transannular effects in which the neighboring groups are separated by a single non-conjugated atom. This can also be thought of as intramolecular π-π stacking with only a single atom spacer.



- HC has been accepted since the 1960s, yet limited research has been done
- Literature reports on the subject show that the geometry of the neighboring groups directly correlate with HC
- Many molecules have been synthesized with this type of molecular arrangements but they did not explore the HC impact on the system
- As shown above there is a clear decreasing of distance in HC molecules vs that of π-π stacking which would increase the potential of π orbital overlap
- Aside: the Spiro HC molecule (shown above) is known to have the most extreme geometry for HC and is considerably difficult to synthesize

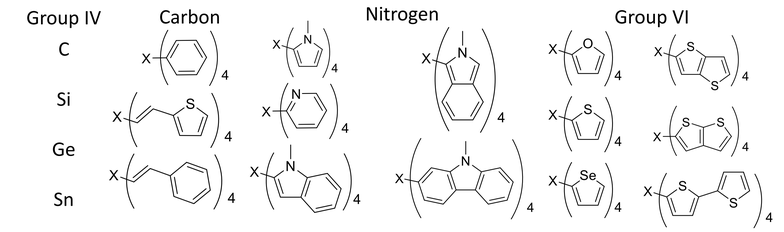
Density Functional Theory

Amsterdam Density Functional Computations

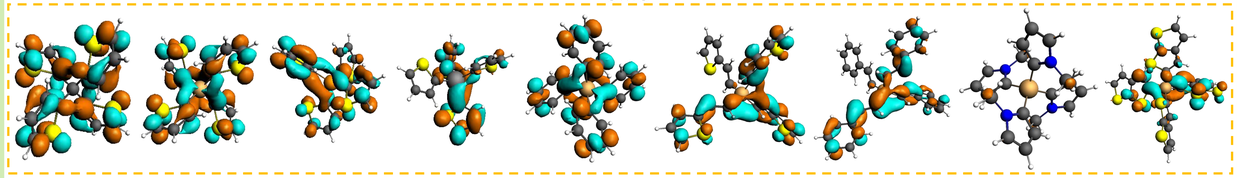
Conformers: 200-600 Universal Force Field (UFF)

Geometry Optimization: GGA:PBE, TZP, Large Frozen Core

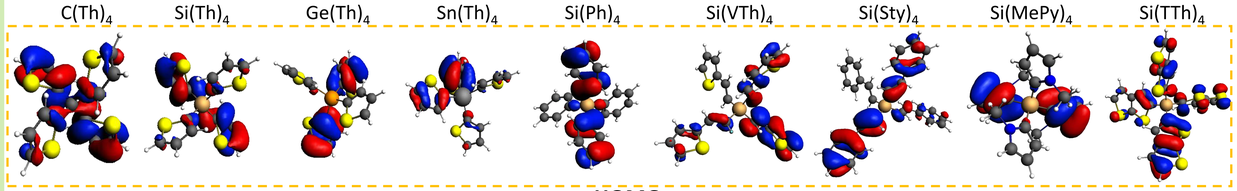
Single Point: Hybrid:B3LYP-D3, AUG/ATZ2P (Sn-QZ4P), No Frozen Core



LUMO



$C(Th)_4$ $Si(Th)_4$ $Ge(Th)_4$ $Sn(Th)_4$ $Si(Ph)_4$ $Si(VTh)_4$ $Si(Sty)_4$ $Si(MePy)_4$ $Si(TTh)_4$



HOMO

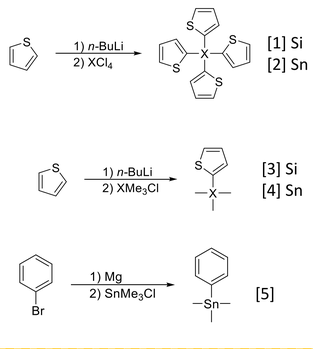
	$C(Th)_4$	$Si(Th)_4$	$Ge(Th)_4$	$Sn(Th)_4$
From Center	~1.5Å	~1.9Å	~2.0Å	~2.2Å
Between Arms	~2.5Å	~3.0-3.1Å	~3.2-3.2Å	~3.5-3.6Å

Spacing between Groups

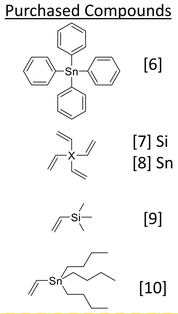
Potential for HC

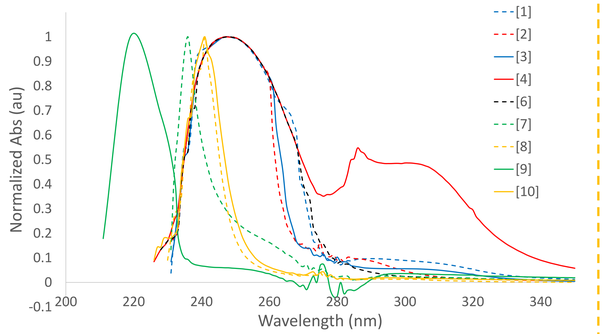
Experimental Results

Core Structure Synthesis & Analysis

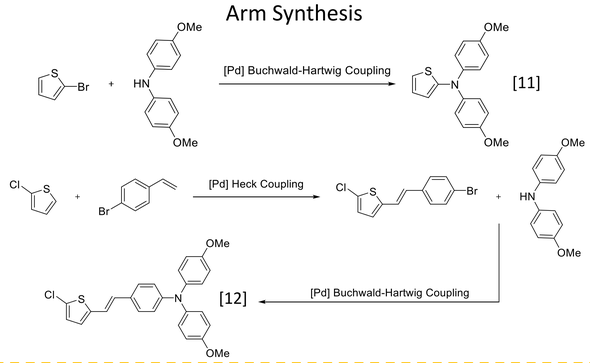


Purchased Compounds

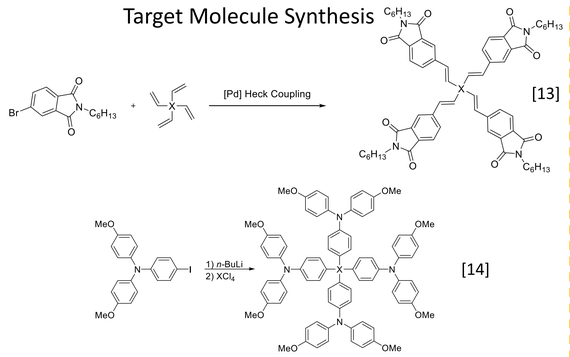




Arm Synthesis



Target Molecule Synthesis



Conclusions

Density Functional Theory

- ✓ Shows that all potential groups examined that geometrically should have HC, have varying degrees of potential when qualitatively analyzing the frontier orbitals
- ✓ A higher potential of HC as you go up the period
- ✓ More donating arms have a greater potential for HC

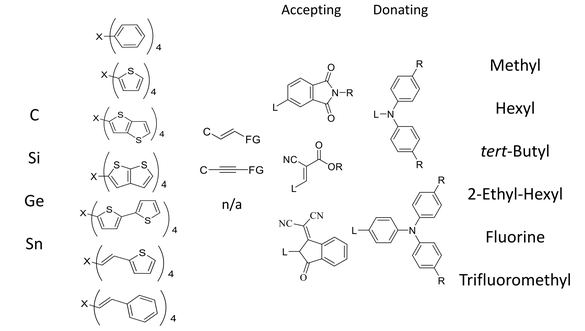
Experimental Results

- ✓ UV-Vis of Compounds [1-10] shows that there might be a correlation between HC and distance to the Arms as seen in the vinyl molecules but aromatic compounds show no noticeable difference
- ✓ Synthesis of arms and desired products (compounds [11, 12, & 14] show simple high yielding steps
- ✓ Compound [13] is a minor product in the reaction as the vast majority appears to be octa-substituted

Future Work

General Scheme: X—(C—L—FG—R)$_n$ Me_{4-n} n=1-4

X: Group IV; C: Core; L: Linker; FG: Functional Group (Accepting, Donating); R: Tuning Group



- Explore other variations or HC molecules as shown above by using the above general scheme of design
- Determine the impact of L,FG, and R groups on HC
- Work with the Lusk research group at CSM to run Molecular Dynamics computations to determine the possible charge transport ability
- Have devices solution processed with help from the Shaheen research group at CU Boulder for PCE.
- Explore the possibilities of using these materials as charge transport materials for perovskite solar cells.

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