Organic Electronic Materials by Design: Finding a Needle Through the Haystack

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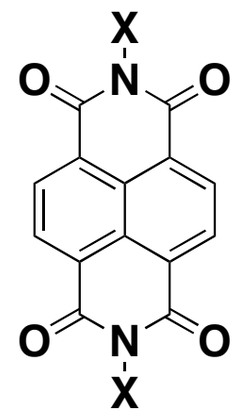
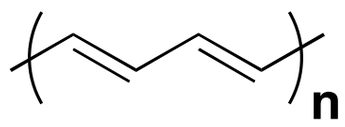
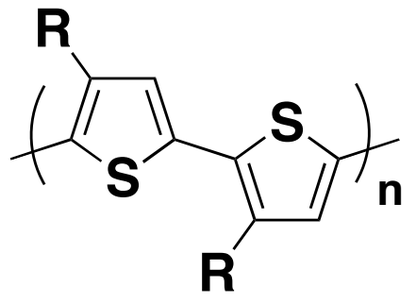
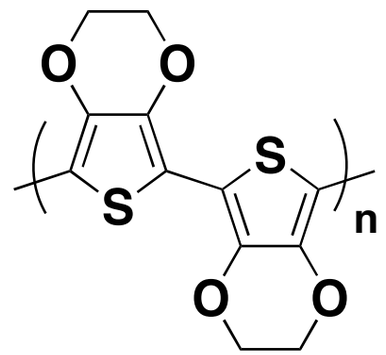
The Hutchison Group

Benefits of Organic Electronic Materials







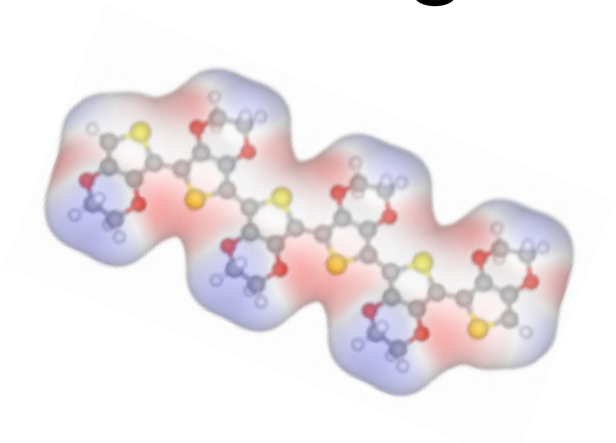


Key Benefits

- Synthetically Tailorable
- Soluble Inks / Dyes
- Flexible, Lightweight
- “Green” Materials
- Low Cost?

So What's Our Target?

Consider charge transport:



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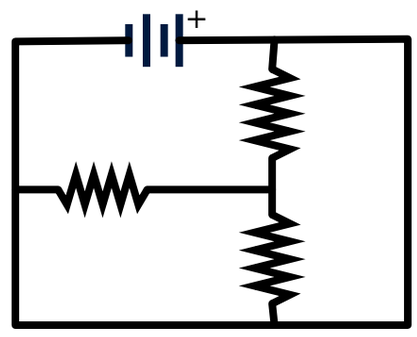
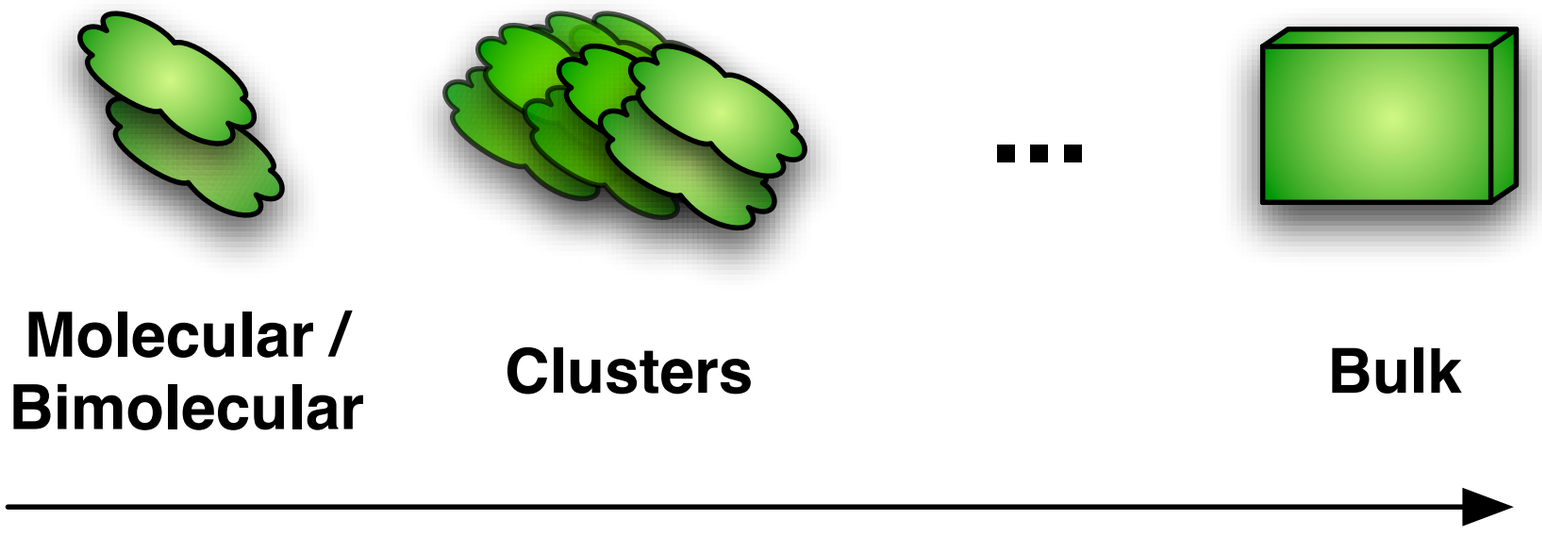
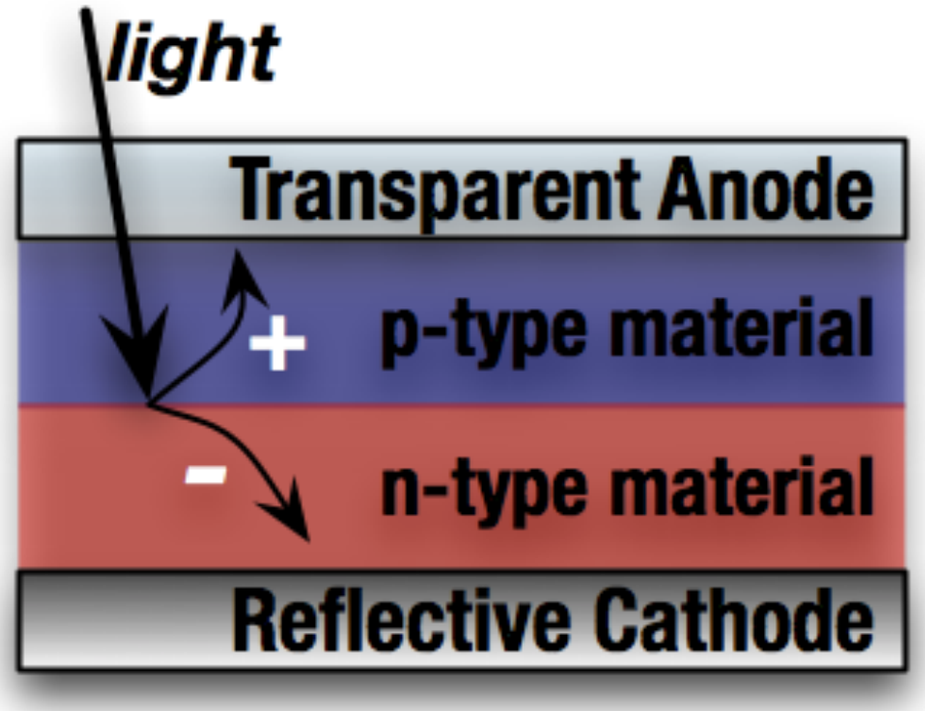


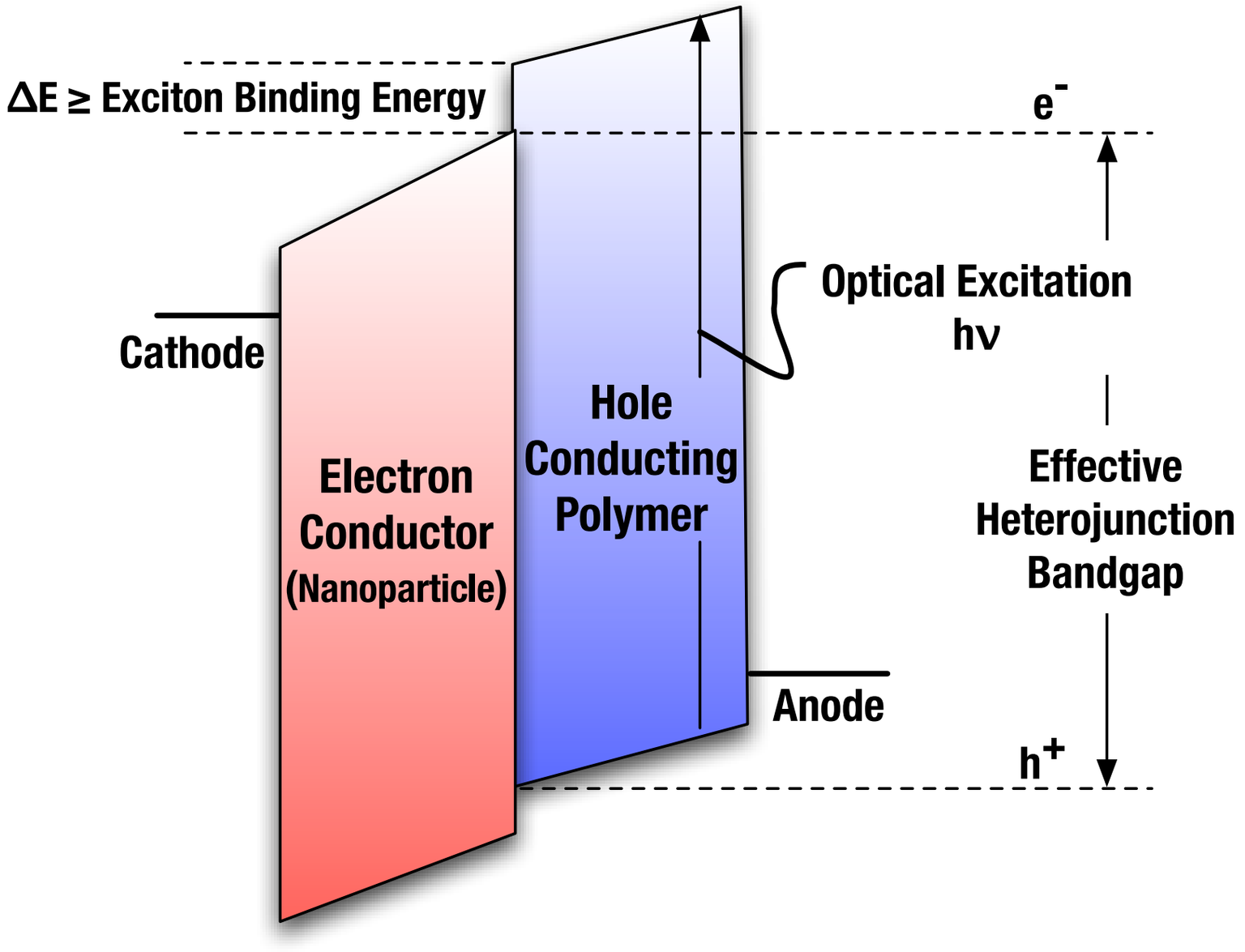


Defects, impurities, mechanisms ...
See PHYS Poster #477 Wed. Evening

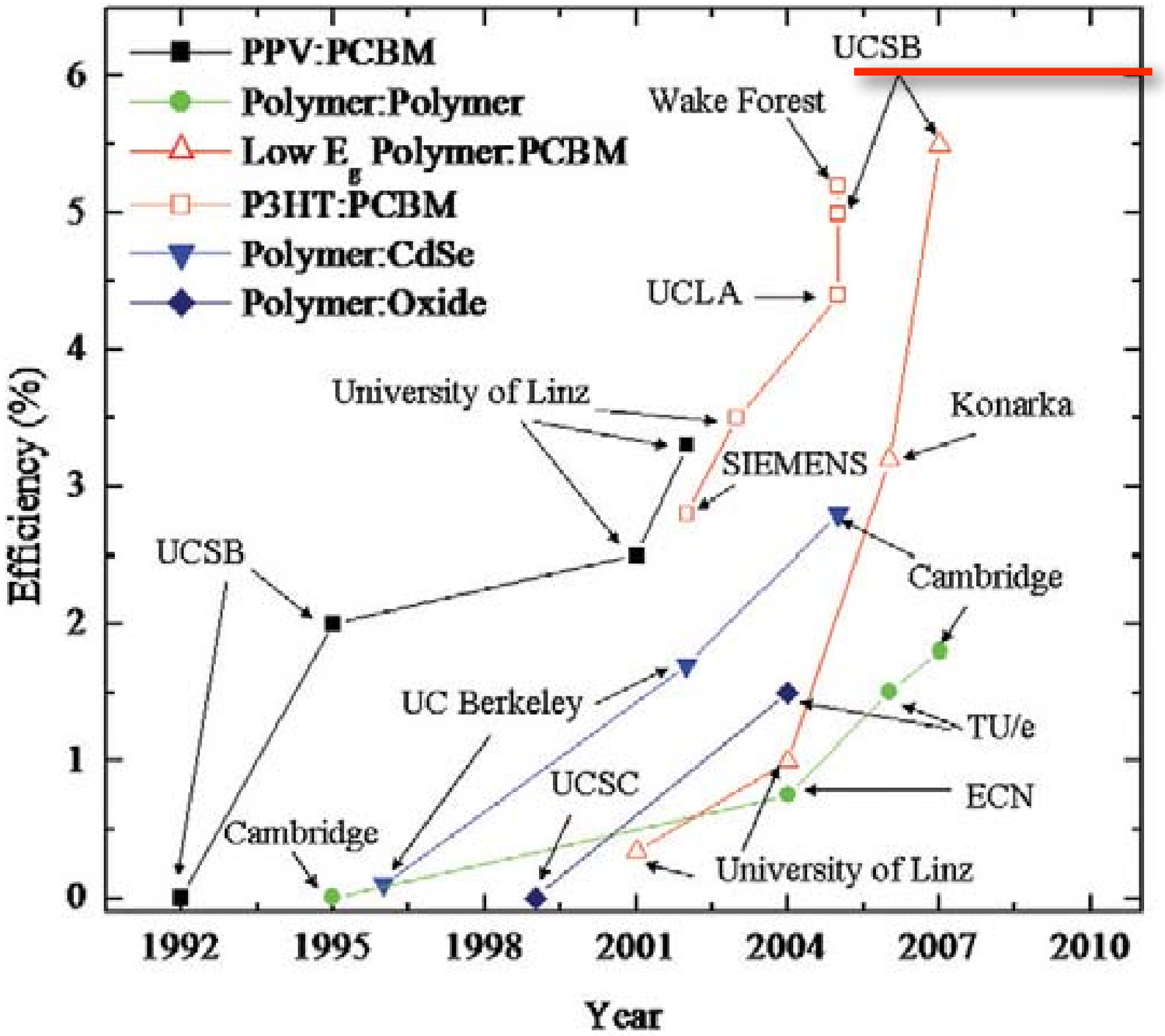
10^{120} Possible Molecules!

Organic Bulk Heterojunctions



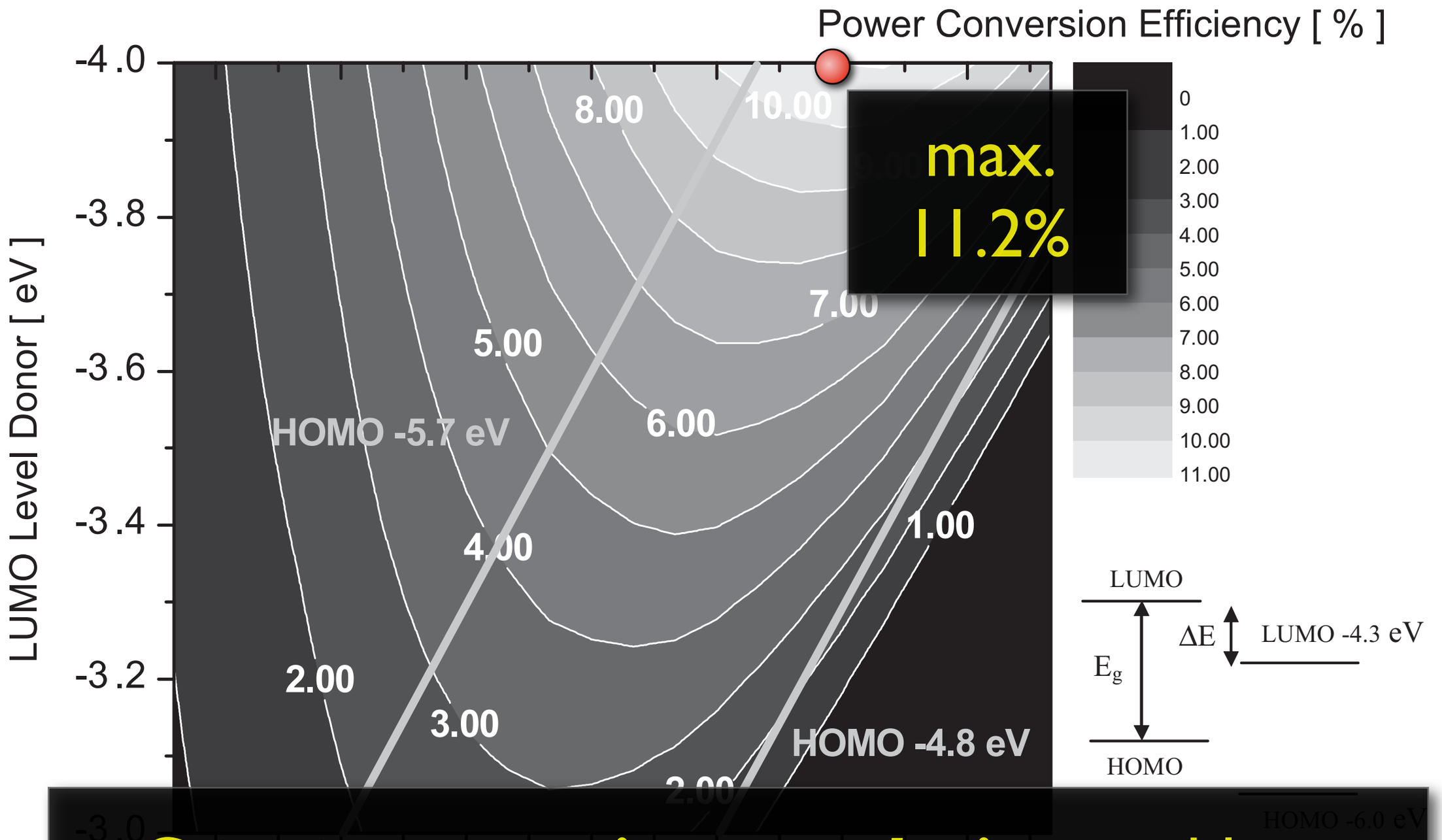


Experimental Progress (Slow)



McGehee, et. al. *Mater. Today* **(2007)** *10* p.28

Heeger Efficiency Criterion



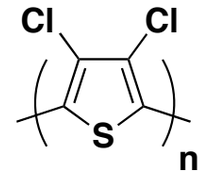
Criteria present ***inverse design*** problem:
What molecules to make?

Heeger, et. al. *Adv. Mater.* **(2006)** *18* p. 789

First Step.... "Diversity Library"

- Primitive level:
  Do we find *anything* which meets our target?
- Secondary:
  Key "structural features"
- And...
  Use these for further screening (new properties?)

In Silico Property Prediction



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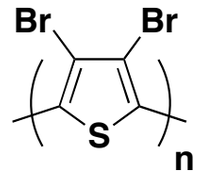

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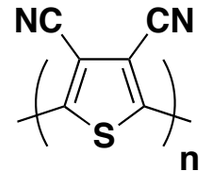

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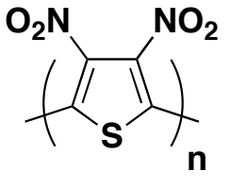

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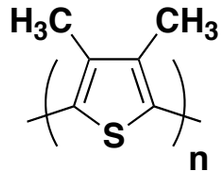

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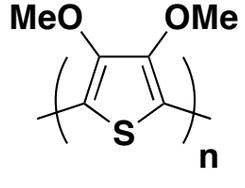

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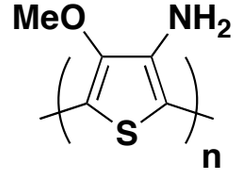

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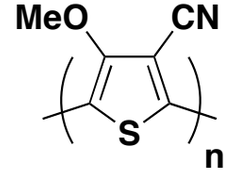

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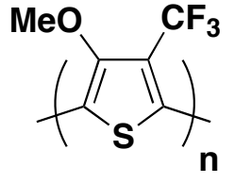

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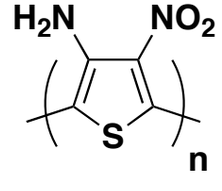

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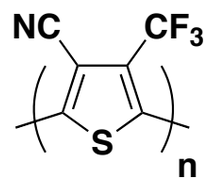

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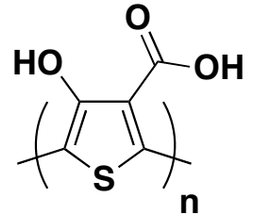

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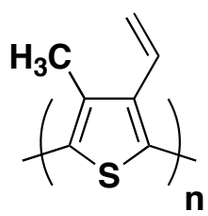

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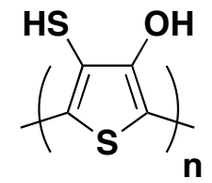

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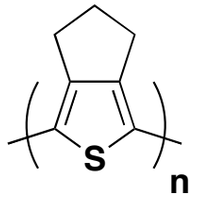

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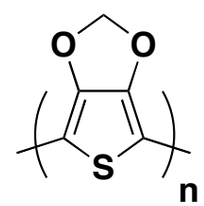

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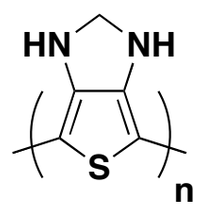

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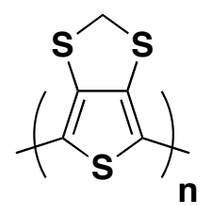

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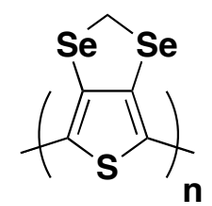

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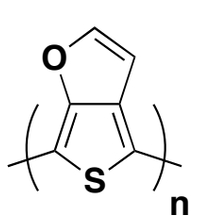

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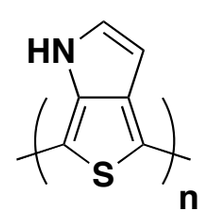

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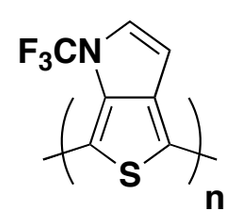

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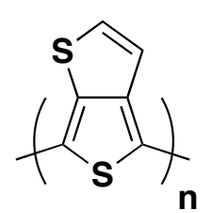

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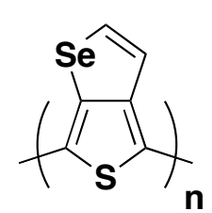

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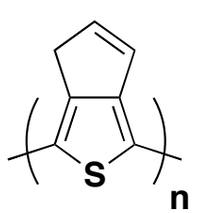

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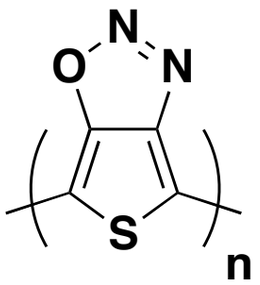
Some Hits, New Targets?



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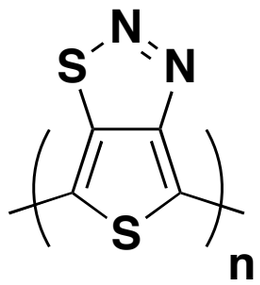

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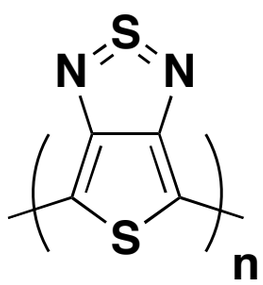

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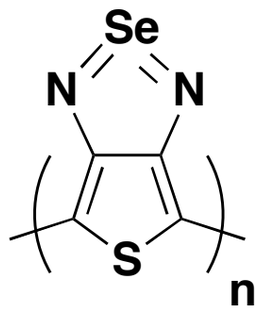

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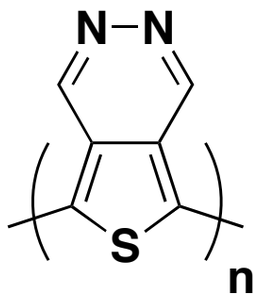

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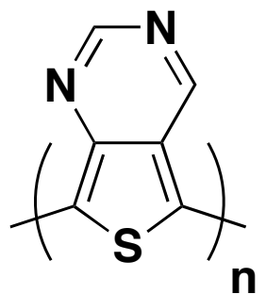

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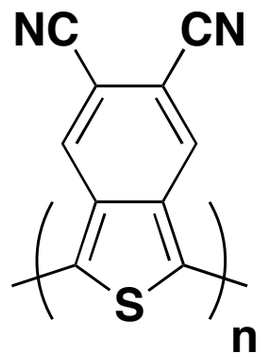

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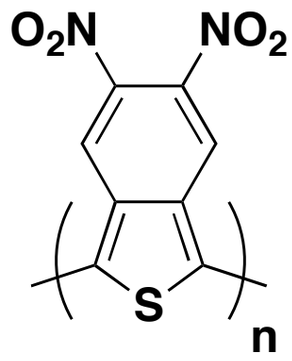

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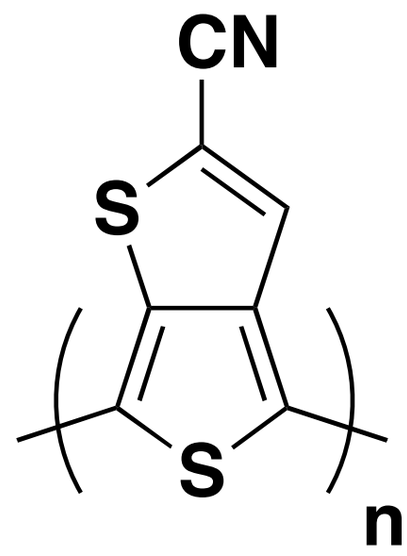
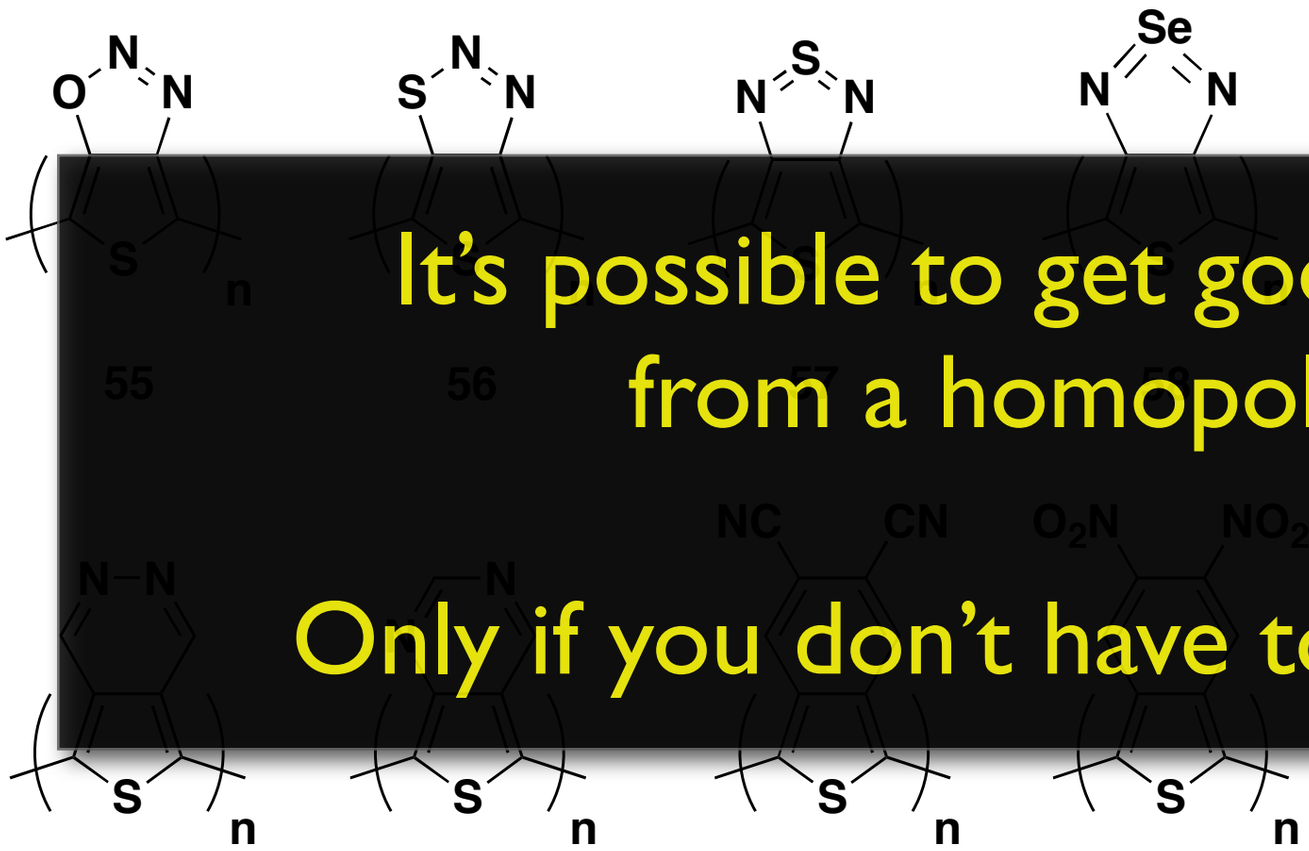


Some Hits, New Targets?



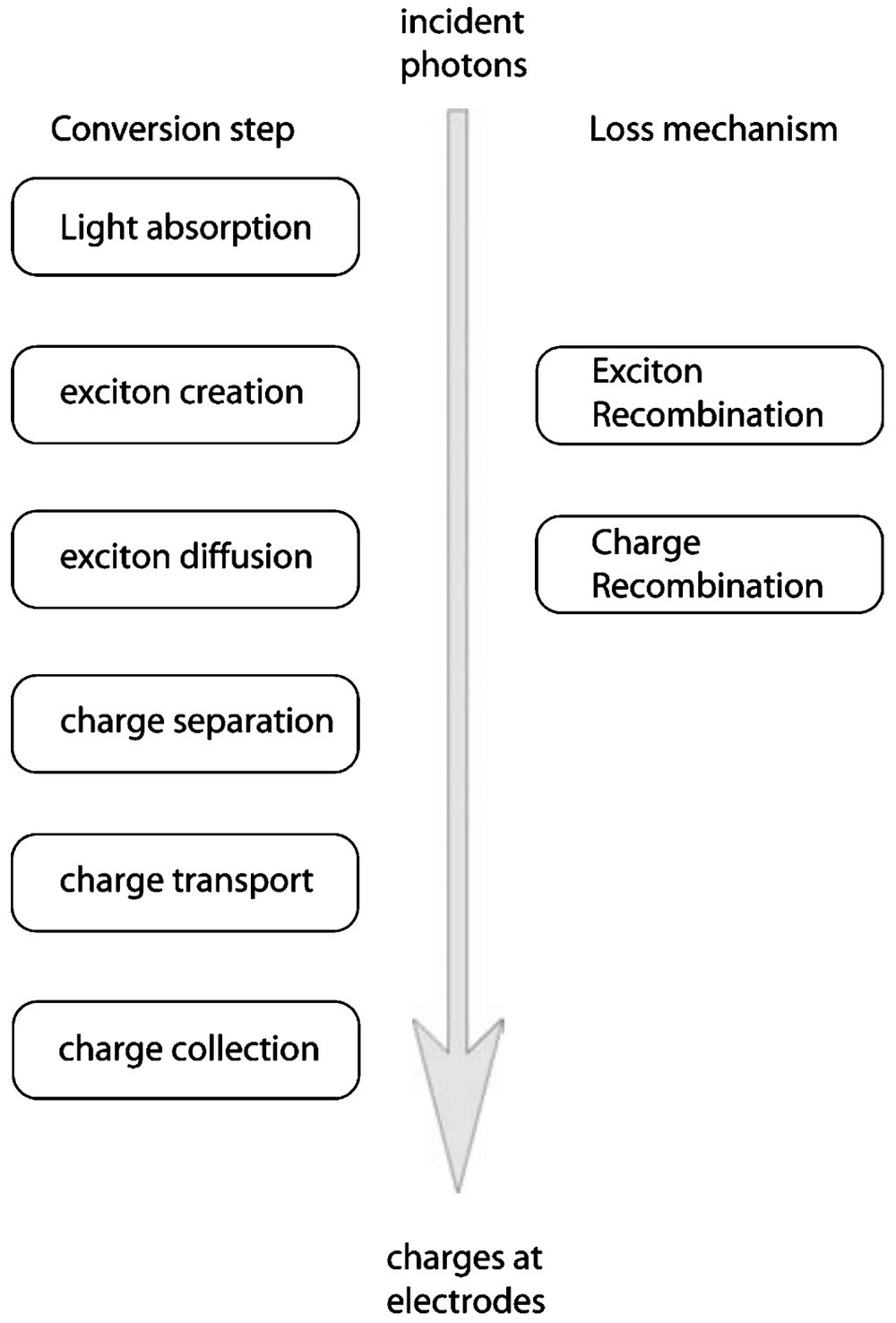
It's possible to get good efficiency from a homopolymer...

Only if you don't have to synthesize it!

Wait... What About Everything Else?

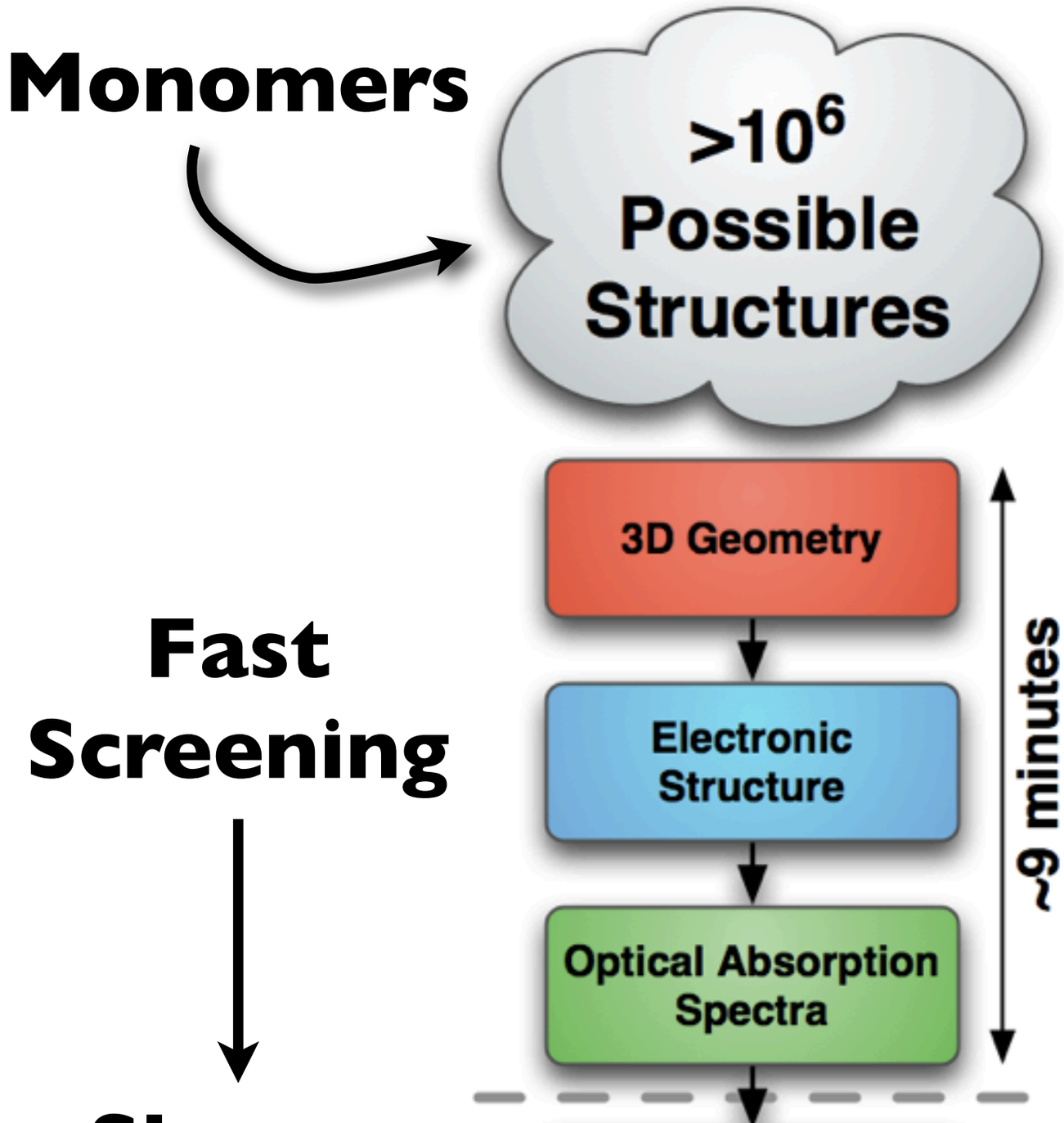
- Criteria address ***two steps***
- Still need to understand
  - exciton diffusion
  - charge recombination
  - charge separation
  - charge transport

    ...
- Not to mention:
  - **Absorption Intensity**
  - **Disorder, Defects**
  - **Charge Transport**
  - **Stability, Solubility**
  - **Synthetic Accesibility**

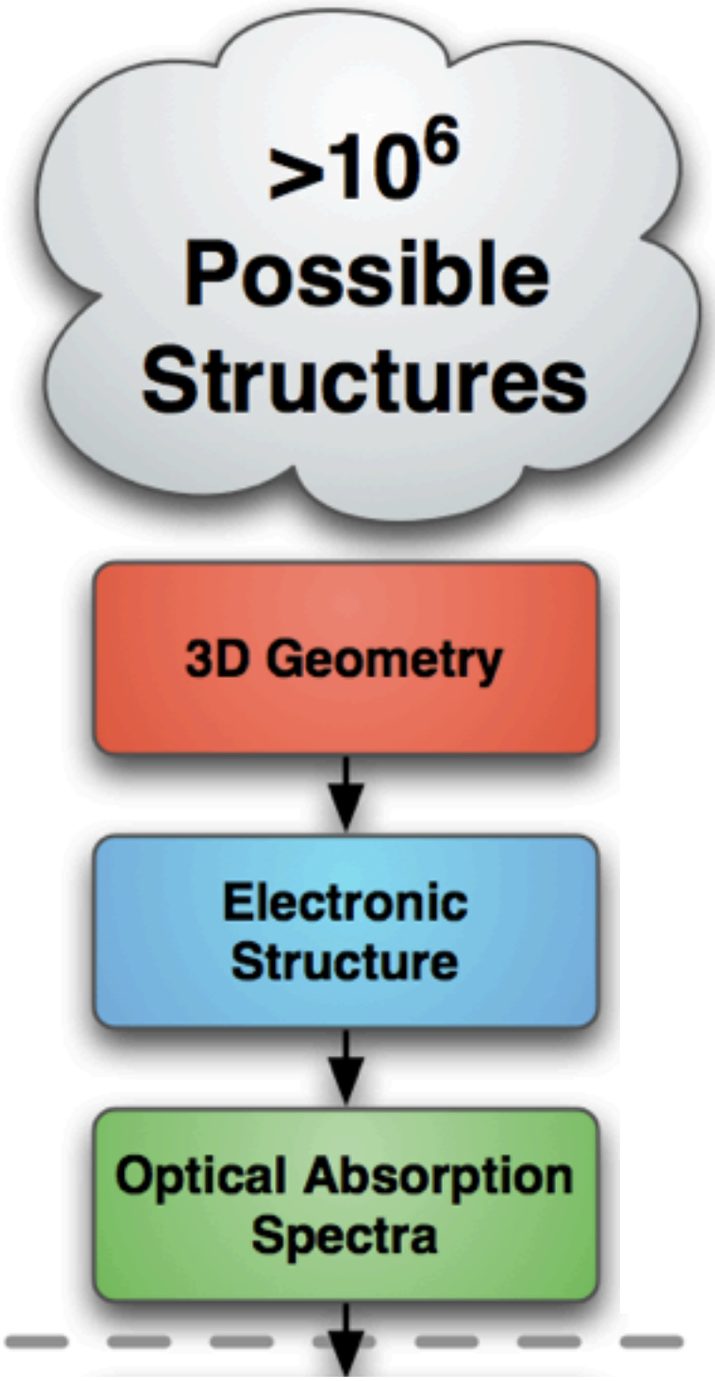


Cheminformatics Pipeline for Organic PV

- Combinatorial problem:
  - 150+ monomers
  - 1-3 in each co-polymer
  - Symmetry & sequence
- Generate a LARGE database
  - Filter for electronics
  - Filter for photonics
  - Filter for chemistry
- Compute & analyze



Implementation Details



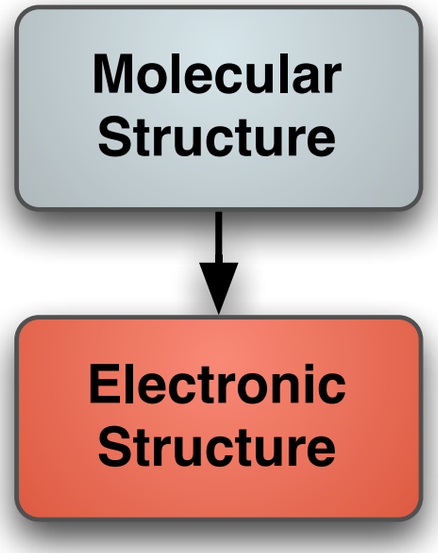
- Monomers as SMILES
- Pick a dimer (catenate strings)
- Enumerate possible oligomers

- **Open Babel**: Generate 3D coords
- **Open Babel**: Conformer Search
- **Gaussian**: Geometry Optimization

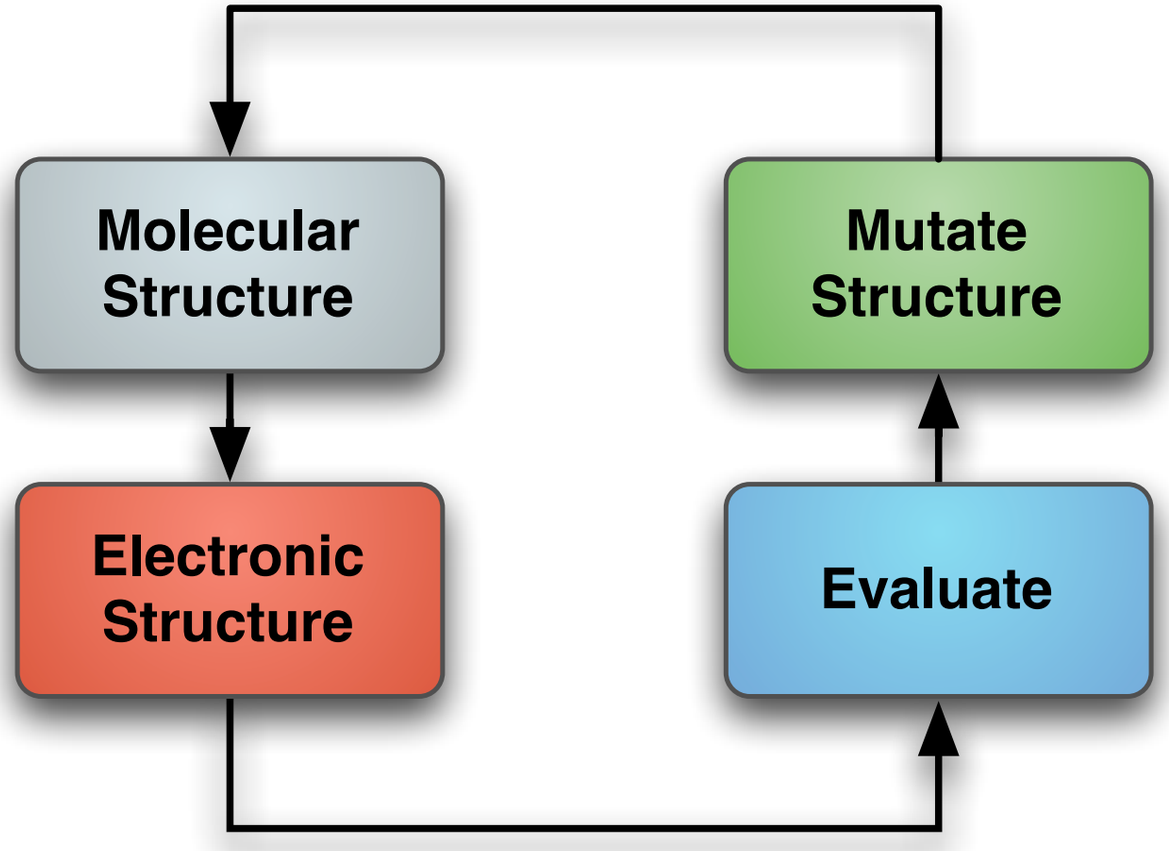
- **Gaussian**: Excitation Energies
- **cclib**: Extract Data

Closing the Loop

Standard Computational Chemistry

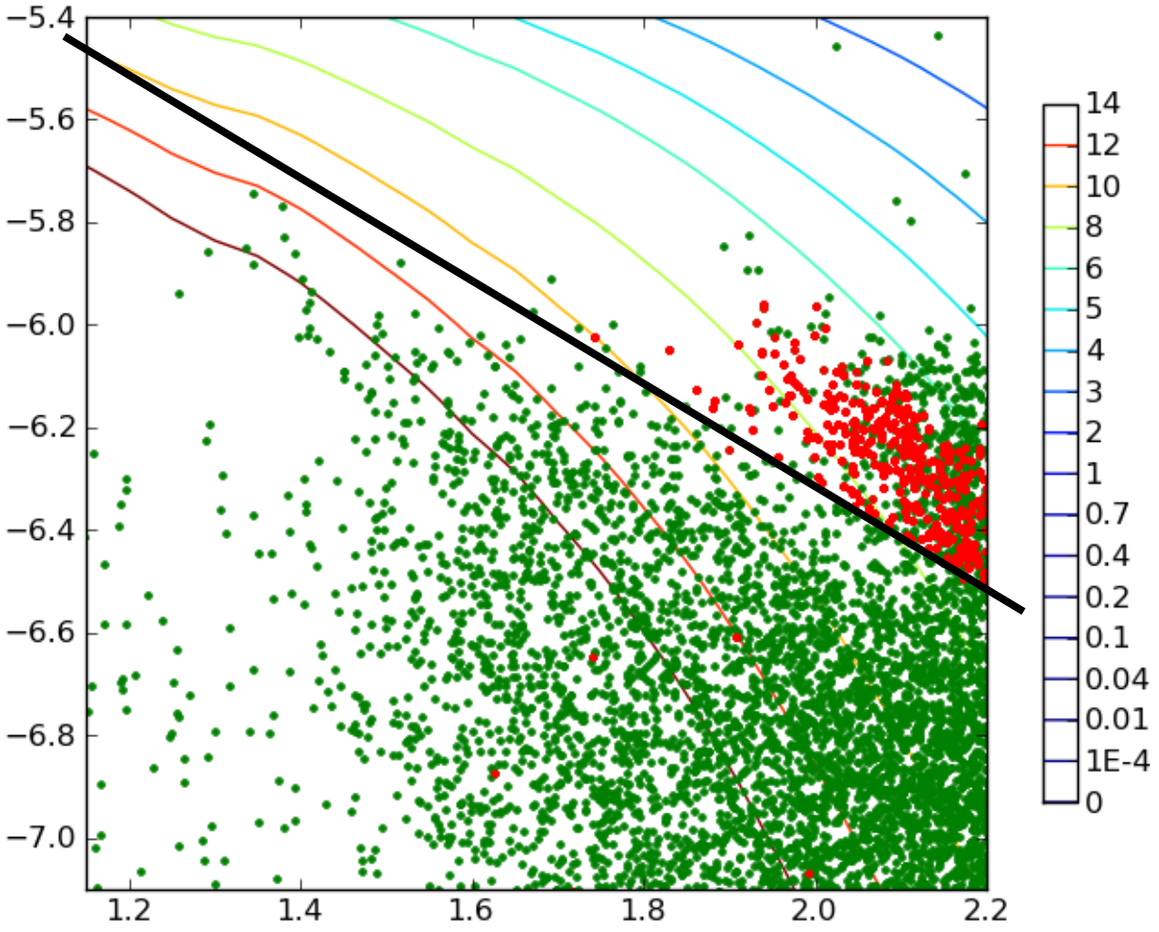


Genetic Algorithm "Needle-Finding"

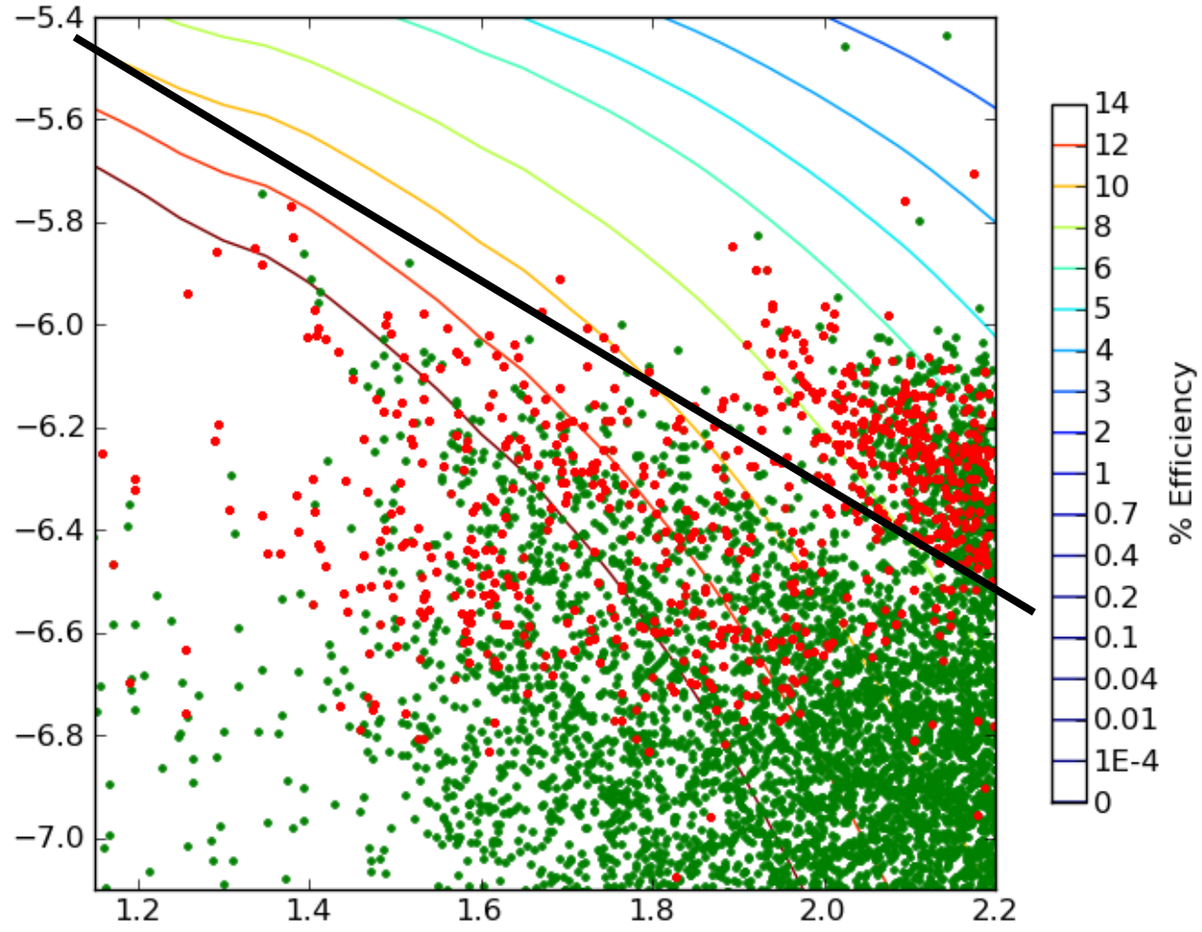


Target Function for Genetic Algorithm?

Efficiency



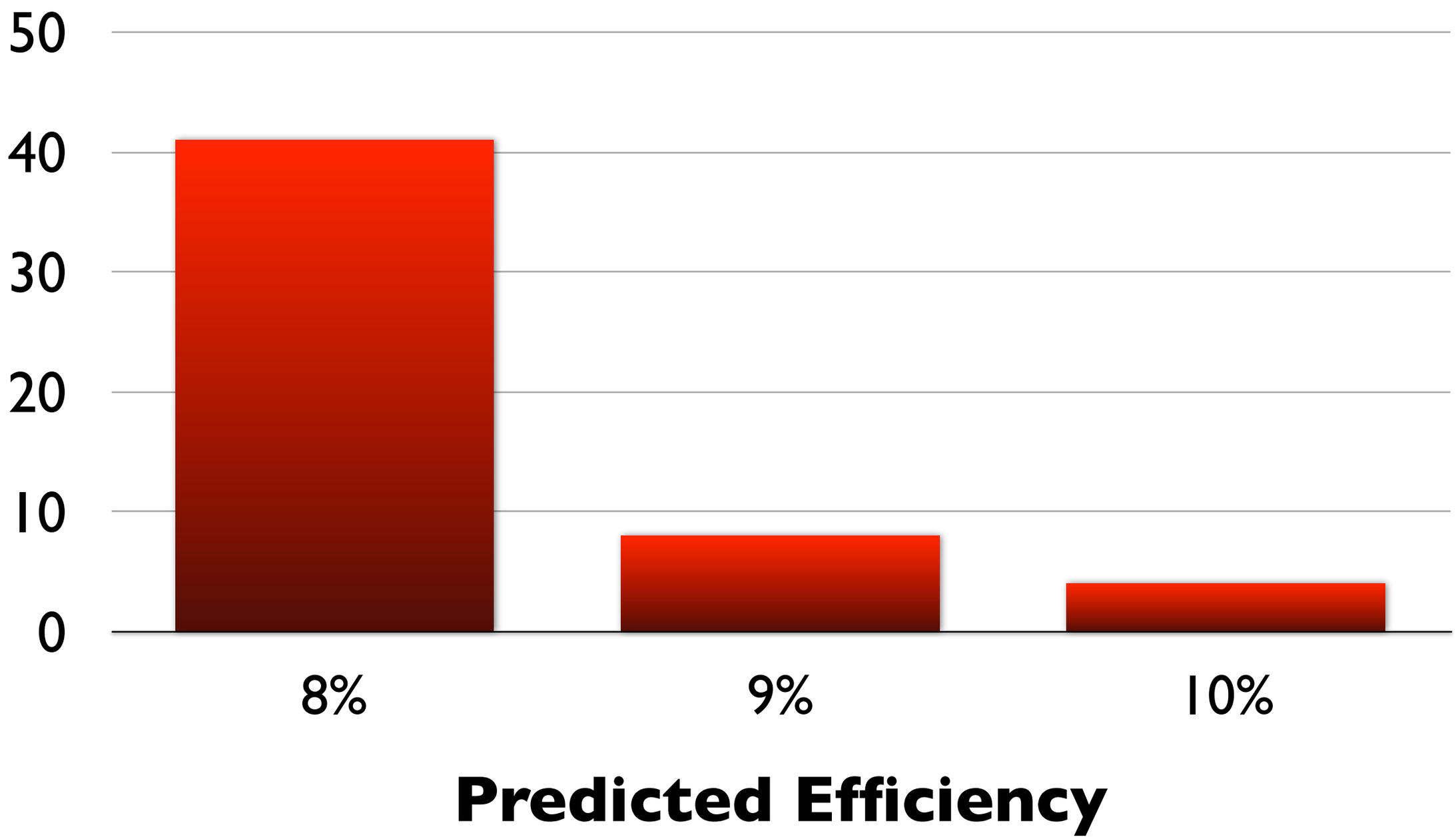
Distance to Maximum



Green: Exhaustive Search

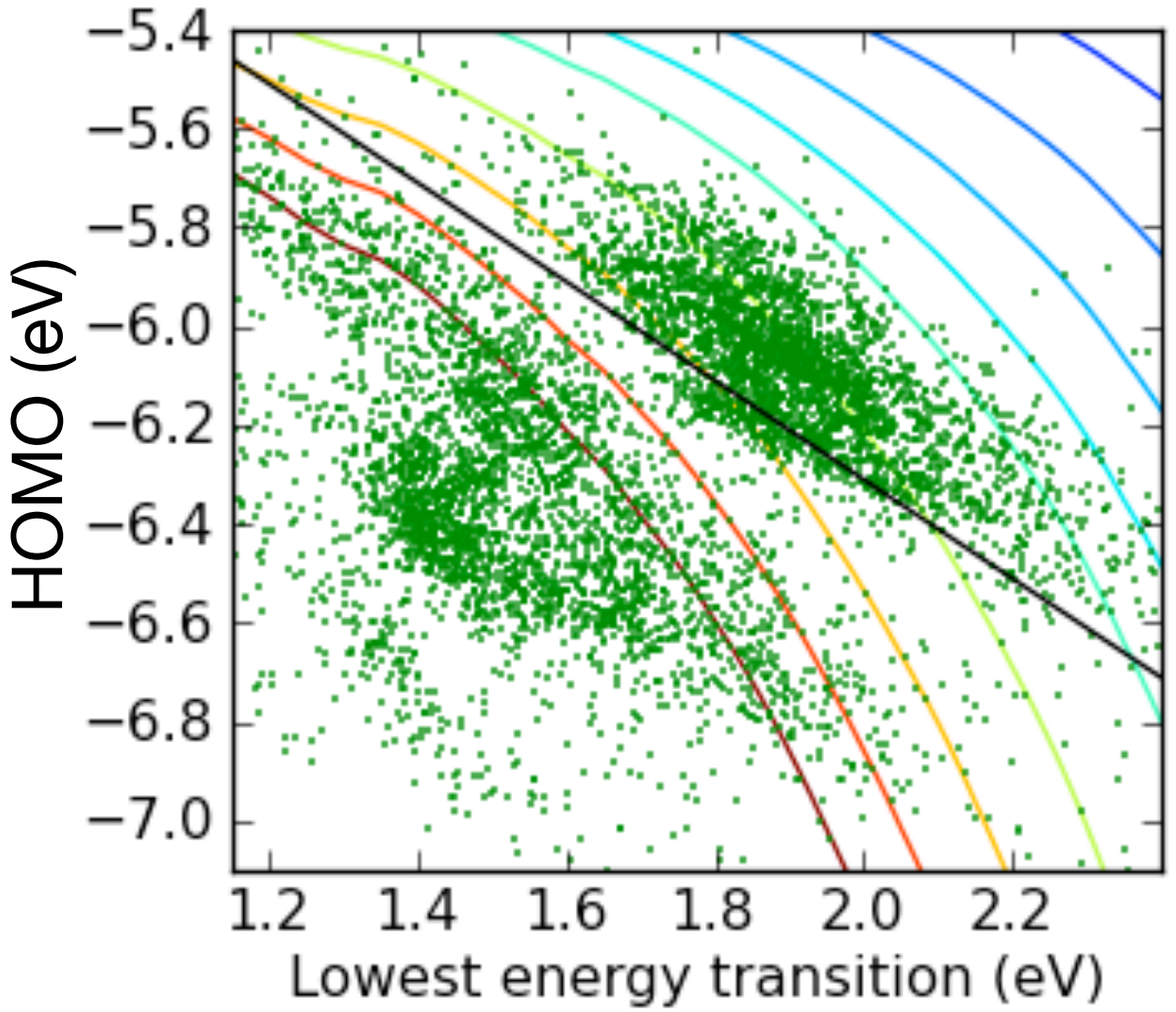
Red: Genetic Algorithm

Statistics for Tetramers



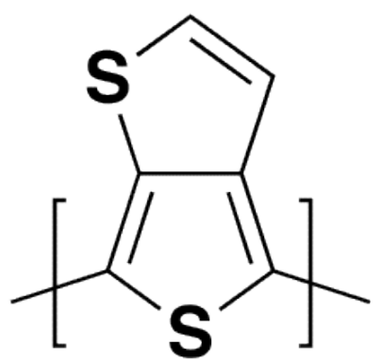
Performance of GA

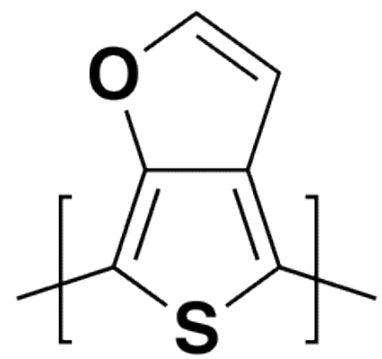
- Test on tetramers vs. exhaustive search
- Explored ~4% of total space
- Found on average:
  - 7.2 of top 10 candidates
  - 58.7 of top 109 candidates
- New strategy for hexamers & octamers
  - GA followed by local search
  - Pick top monomers

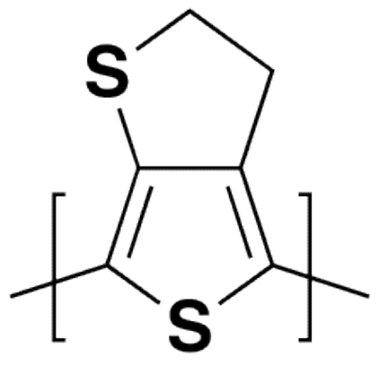


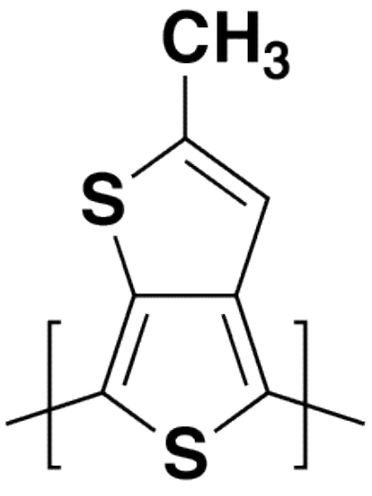
Future Directions

- Allow more elements in monomer database
- Allow GA to mutate monomers
- Add screening steps
  - Solubility
  - Synthetic accessibility
  - Crystal packing
  - Conductivity?



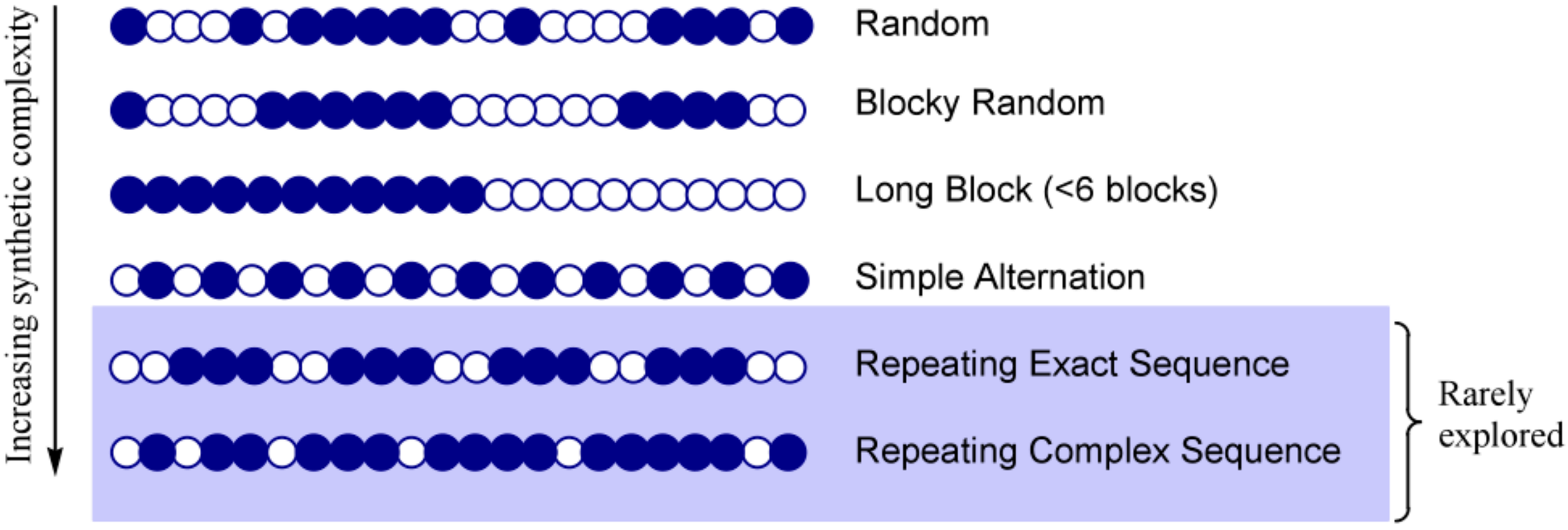






Repeating Sequence Co-Polymers

Sequences exist in synthetic polymers too...



Courtesy Prof. Tara Meyer, U. Pittsburgh

Take-Home Messages

- Use cheminformatics tools!
  - Generate diversity libraries for organic electronics
  - Build workflows for property prediction
    - Genetic algorithms for finding novel targets
- We've developed efficient screening for organic photovoltaics
- Next step: new monomers & sequence

Visual Analysis?
CINF Talk: Tomorrow @4:20 PM