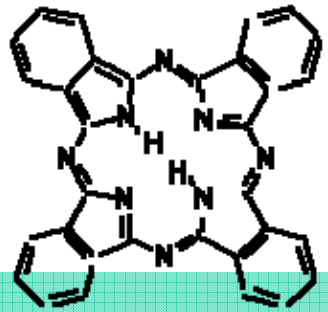
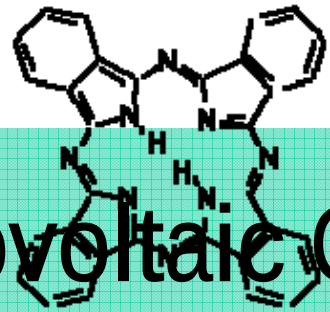
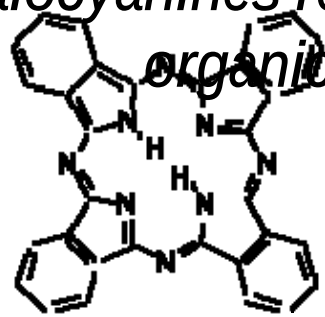




Improving Organic Photovoltaic Cells

Spectral properties of several metal phthalocyanines related to their role in increasing organic solar cell efficiency

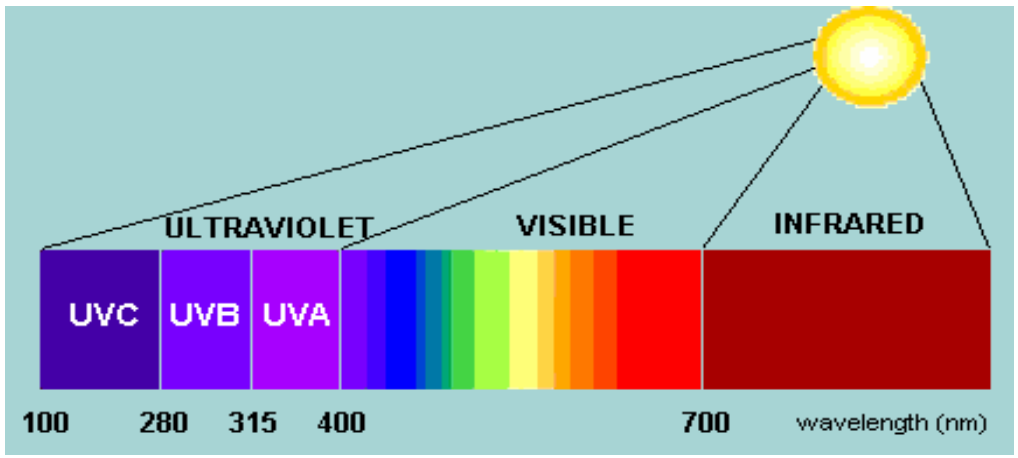


Helen Gerardi

August 1, 2005

Solar Energy to Meet Earth's Power Needs

- Earth uses 13 trillion watts of power a year -13 Terawatts (TW)
- Sun deposits 120,000 TW of energy a year



- Inorganic Solar Cells More Costly Because of Materials
- Organic Solar Cells
  - Low cost
  - Lightweight
  - Flexible
  - Large-Area
  - Efficient

The Organic Heterojunction

Four Processes

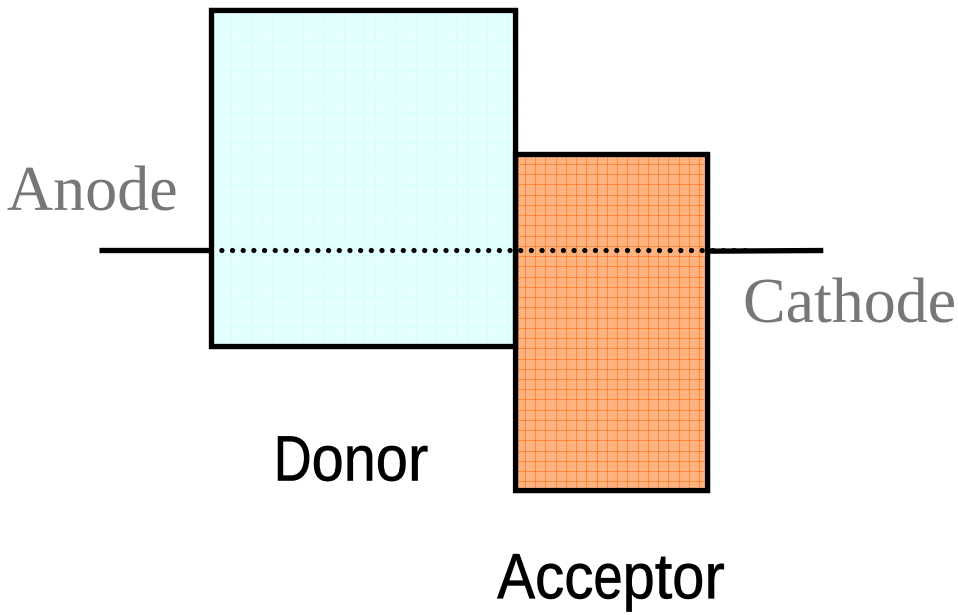
(1) Absorption

(2) Exciton Diffusion

(3) Charge Transfer

(4) Charge Collection

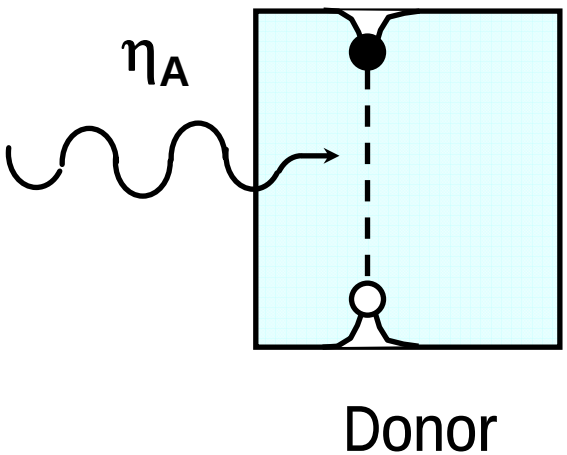
Basic Device Structure



Organic Heterojunction

Absorption

(1) $\eta_A > 50\%$



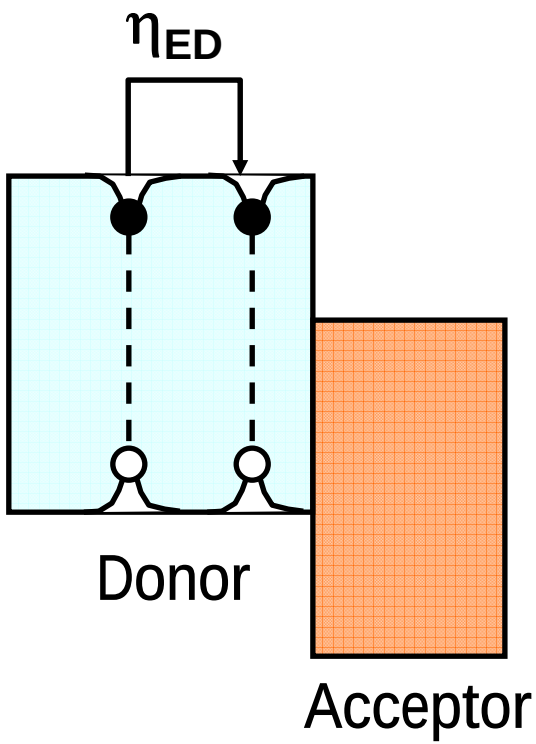
Optical absorption length ~ 1000Å

Organic Heterojunction

Exciton Diffusion

(1) $\eta_A > 50\%$

(2) $\eta_{ED} \sim 10\%$



Exciton diffusion length ~ 50Å

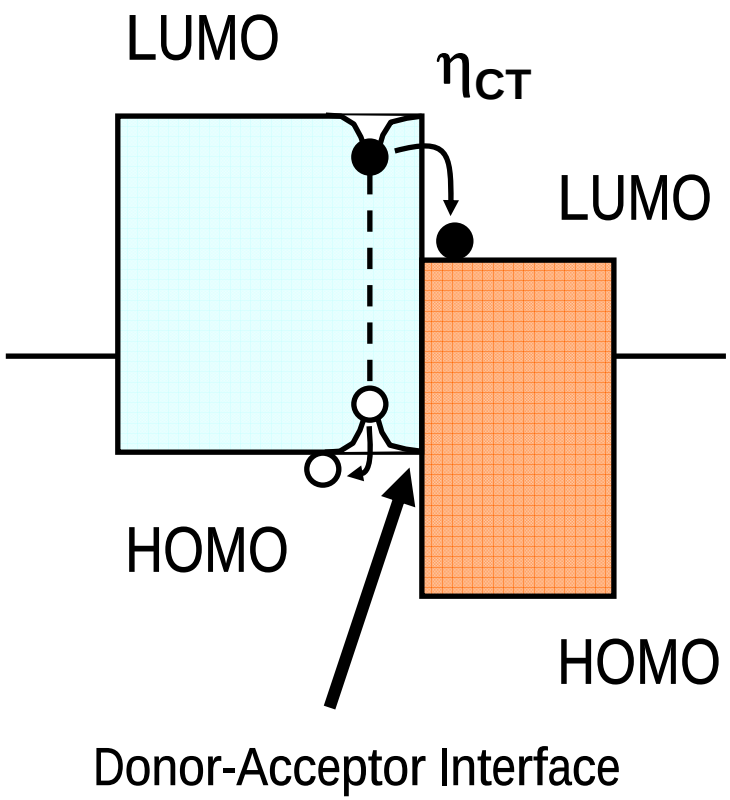
Organic Heterojunction

Exciton Dissociation by Charge Transfer (CT)

(1) η_A > **50%**

(2) η_{ED} ~ 10%

(3) η_{CT} ~ 100%



Organic Heterojunction

Charge Collection At Anode and Cathode

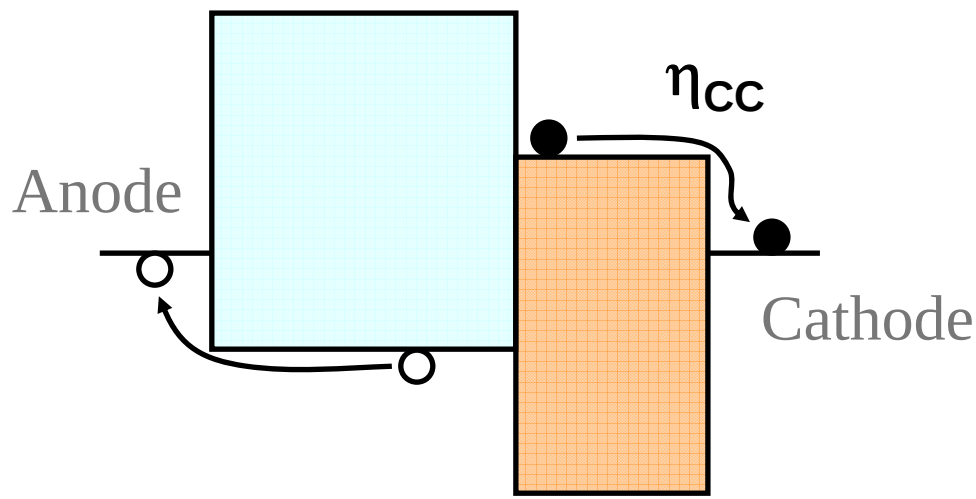
(1) $\eta_A > 50\%$

(2) $\eta_{ED} \sim 10\%$

(3) $\eta_{CT} \sim 100\%$

(4) $\eta_{CC} \sim 100\%$

Limiting Steps



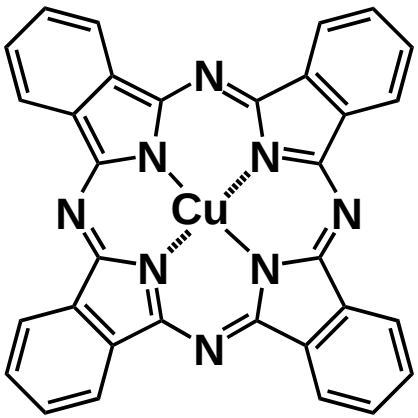
$$\eta_{EQE} = \eta_A \cdot \eta_{ED} \cdot \eta_{CT} \cdot \eta_{CC} \sim 10\%$$

What I looked at this summer…

- Types of Phthalocyanines
  - Characteristics of Metal Ligand
- Properties of These PCs
  - UV-Visible Absorption Spectra
  - Which materials absorbed more of solar spectrum (increase η_A)
- Mixed Layer Absorption
  - Donor-Acceptor Mixture to increase exciton diffusion efficiency (η_{ED})
  - CuPc:C_{60} and SnPc:C_{60}
- Aggregation Effects
  - Dimer
  - Crystalline Structure

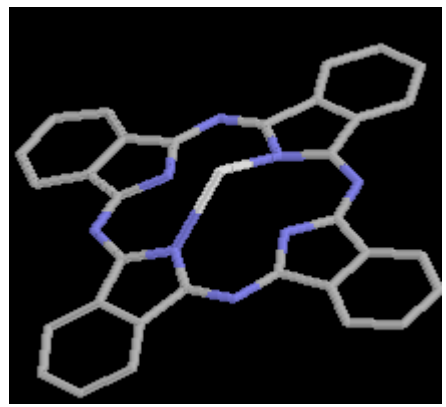
What are Phthalocyanines?

- Structure



Copper Phthalocyanine

Zinc Phthalocyanine



Lead Phthalocyanine

Phthalocyanines Observed in this Experiment

- Copper PC (CuPC)
- Zinc PC (ZnPC)
- Lead PC (PbPC)
- Tin PC (SnPC)
- Nickel PC (NiPC)

Cavity Diameter and Planarity

Influence of atom size and configuration on absorption

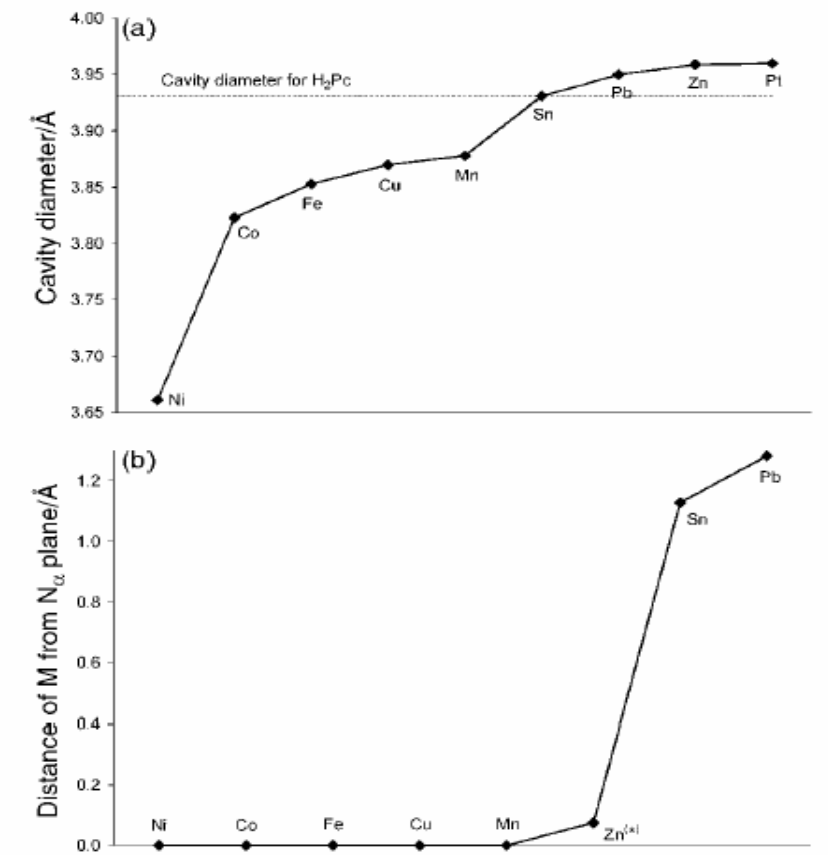
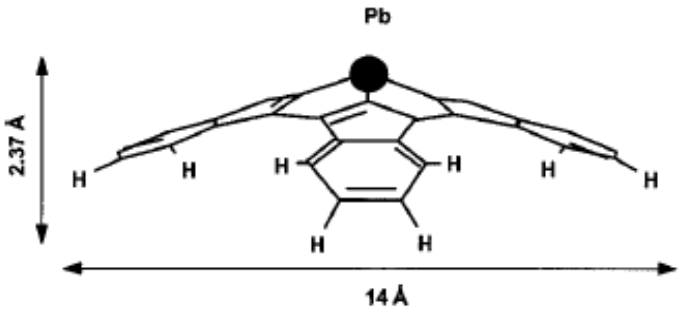


Fig. 6 The variation in phthalocyanine cavity size (a) and an illustration of the non-planarity of large metal ions in simple metal phthalocyanines (b) from data obtained from the CSD. (* The 0.075 Å value for ZnPc is taken from our previous DFT calculation.[2])

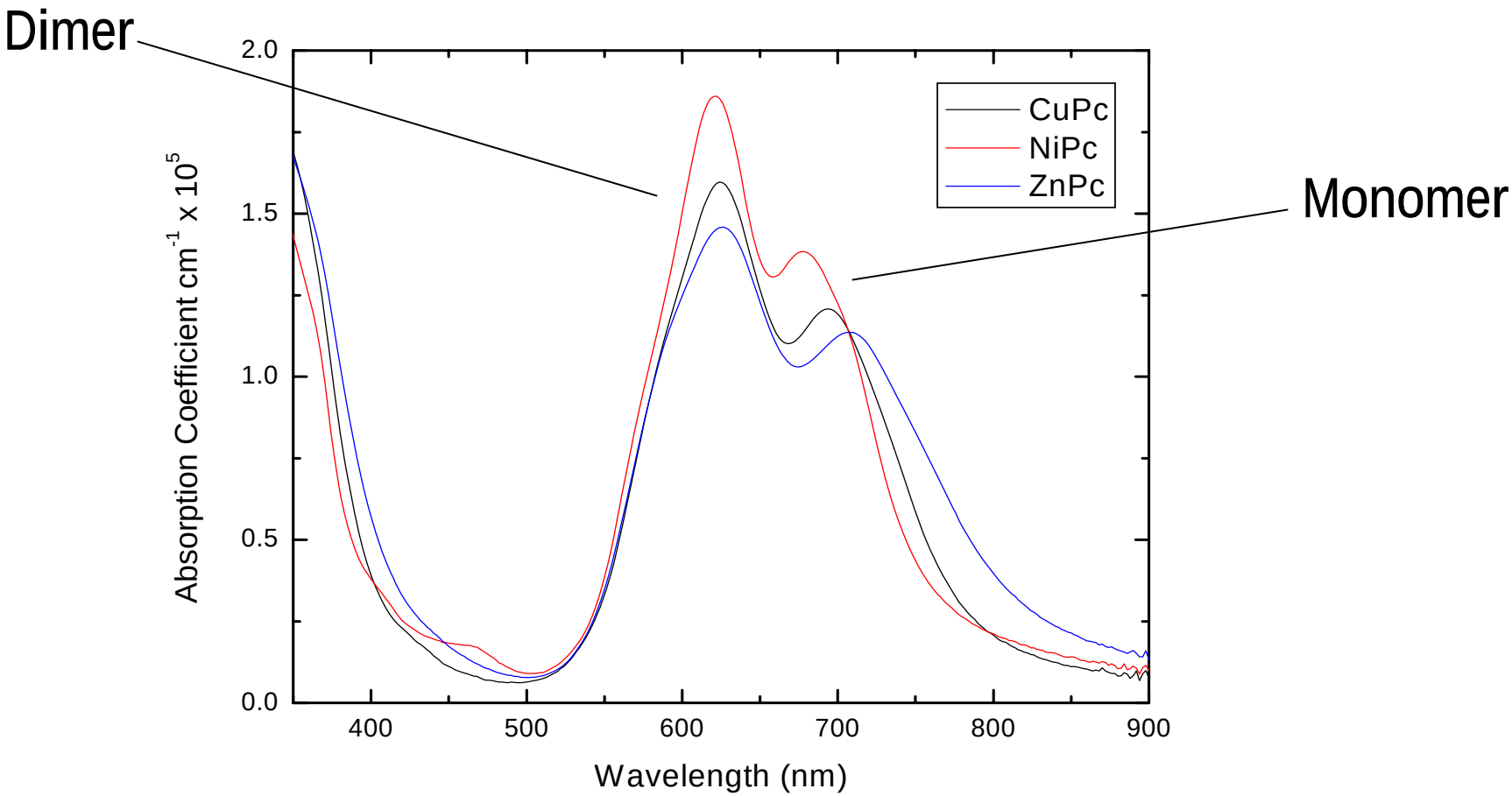


Lead Phthalocyanine

Phys. Chem. Chem. Phys., 2001, **3**, 1419–1426

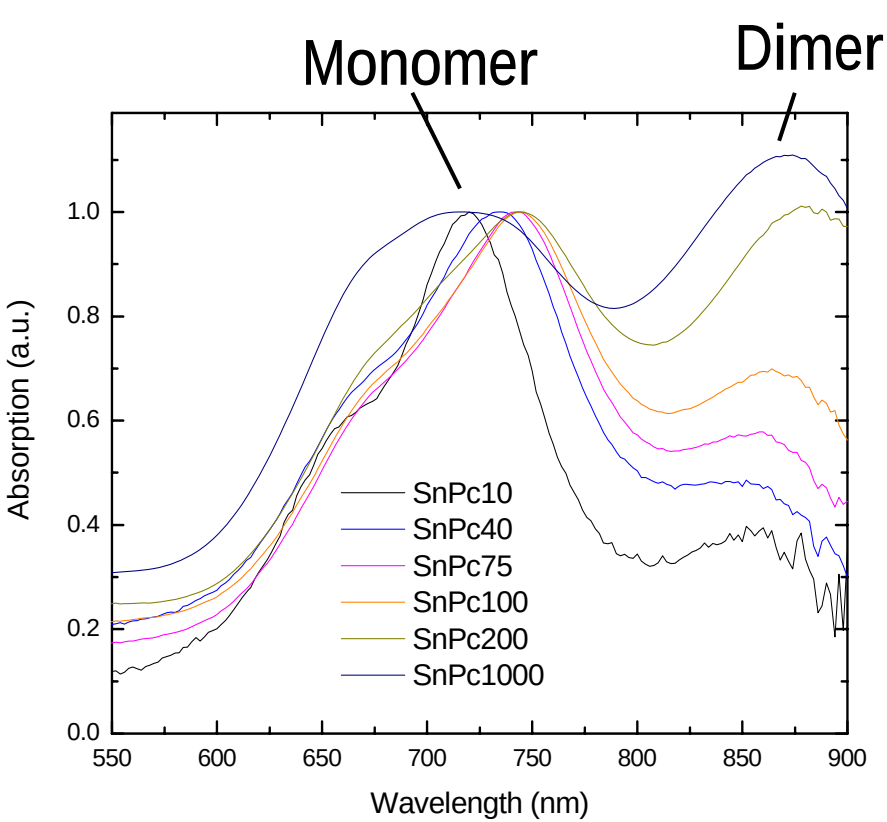
UV-Visible Absorption of These Metal PCs

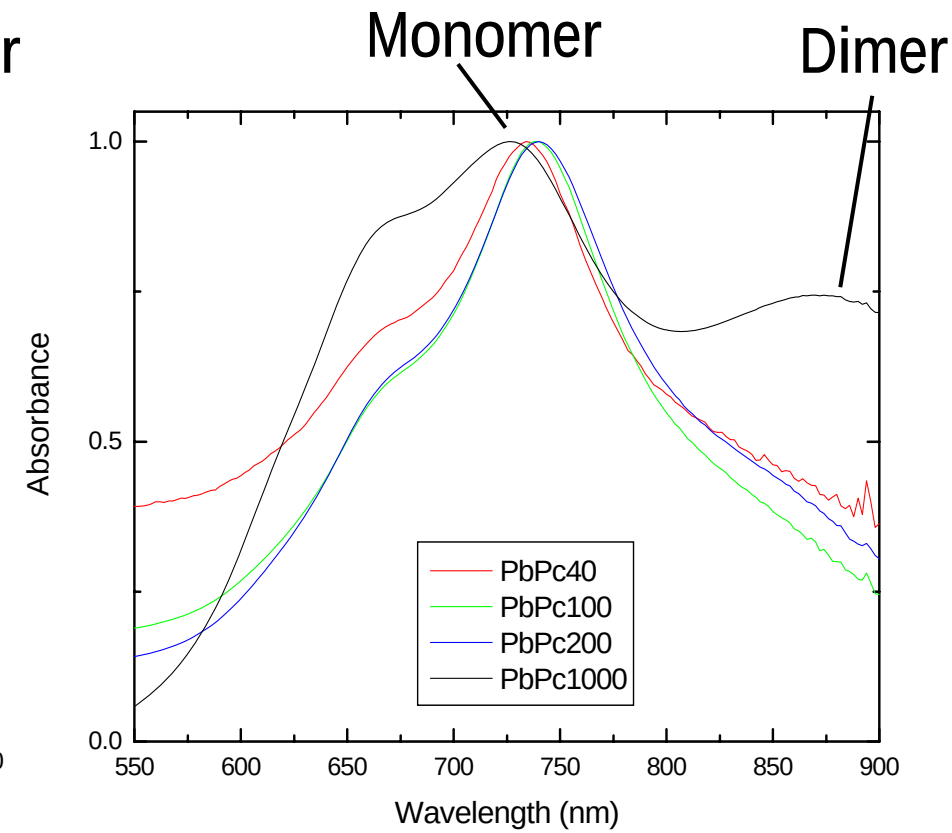
- Absorption Spectrum of CuPC, ZnPC, and NiPC



UV-Visible Absorption of These Metal PCs

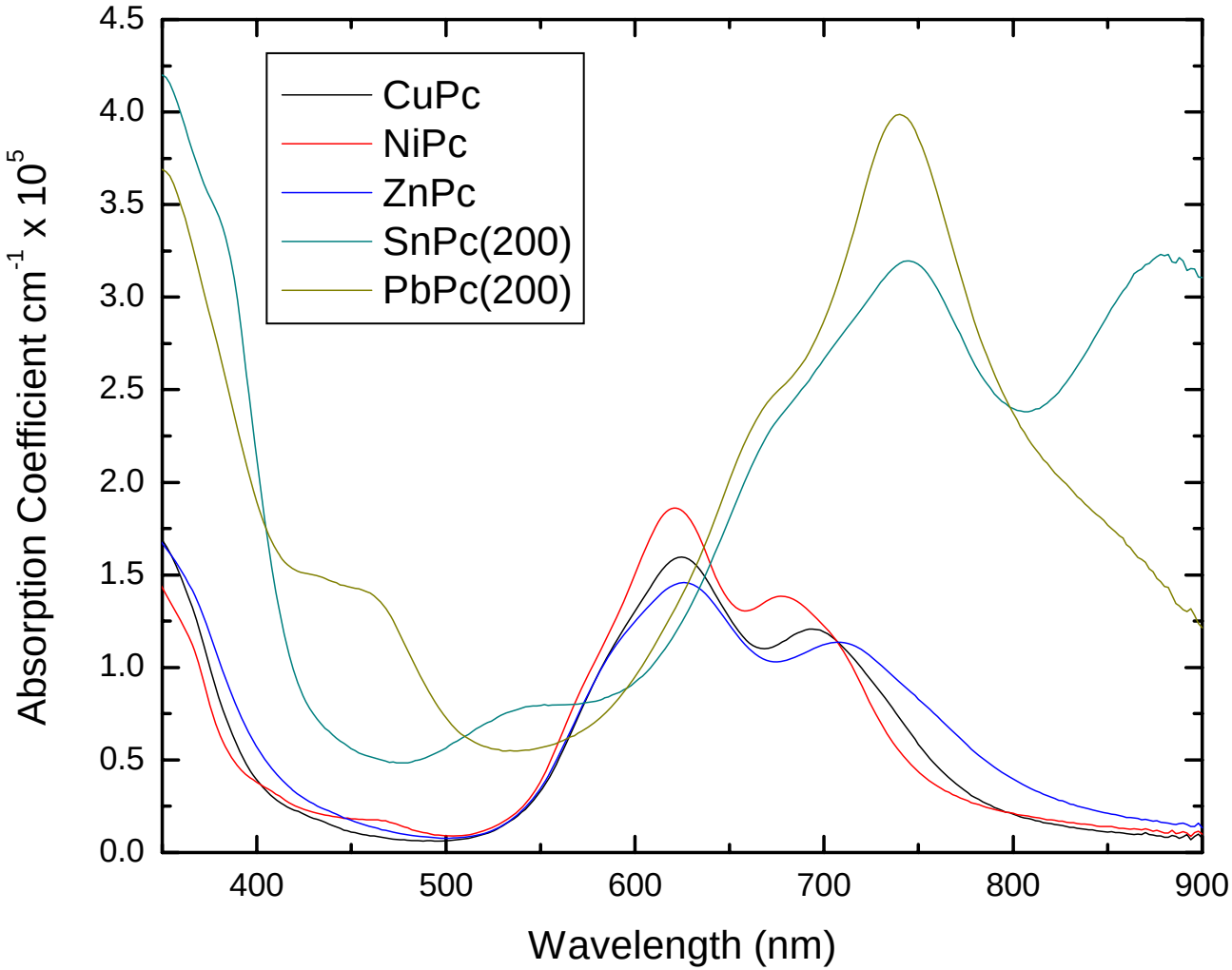
- Absorption Spectrum of SnPC and PbPC





UV-Visible Absorption of These Metal PCs

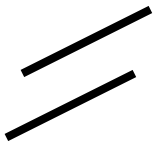
- Plotted Together



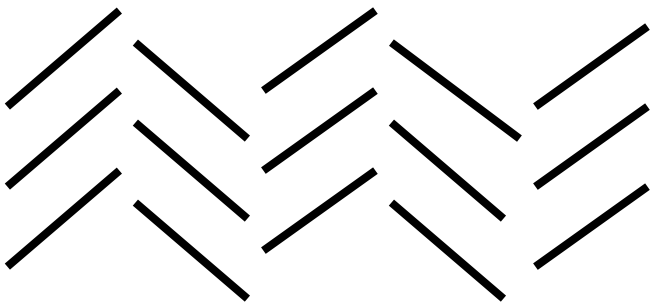
Differences in Absorption

Planar Phthalocyanines

- Dimer Configuration



- Crystalline Structure
  - Herringbone

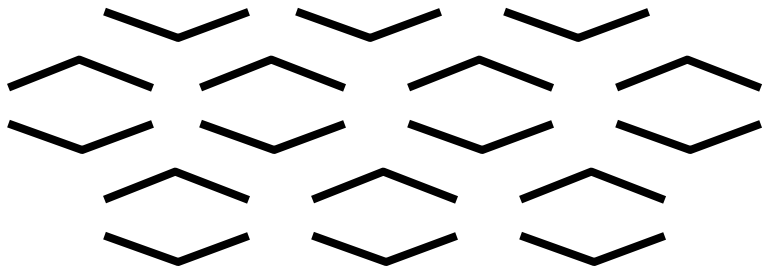


Non-Planar Phthalocyanines

- Concave/Convex Configurations

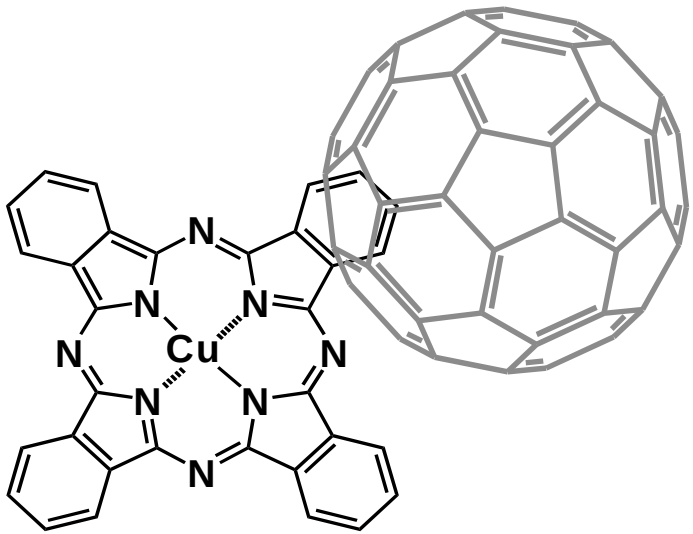
Concave Convex

- Crystalline Structure



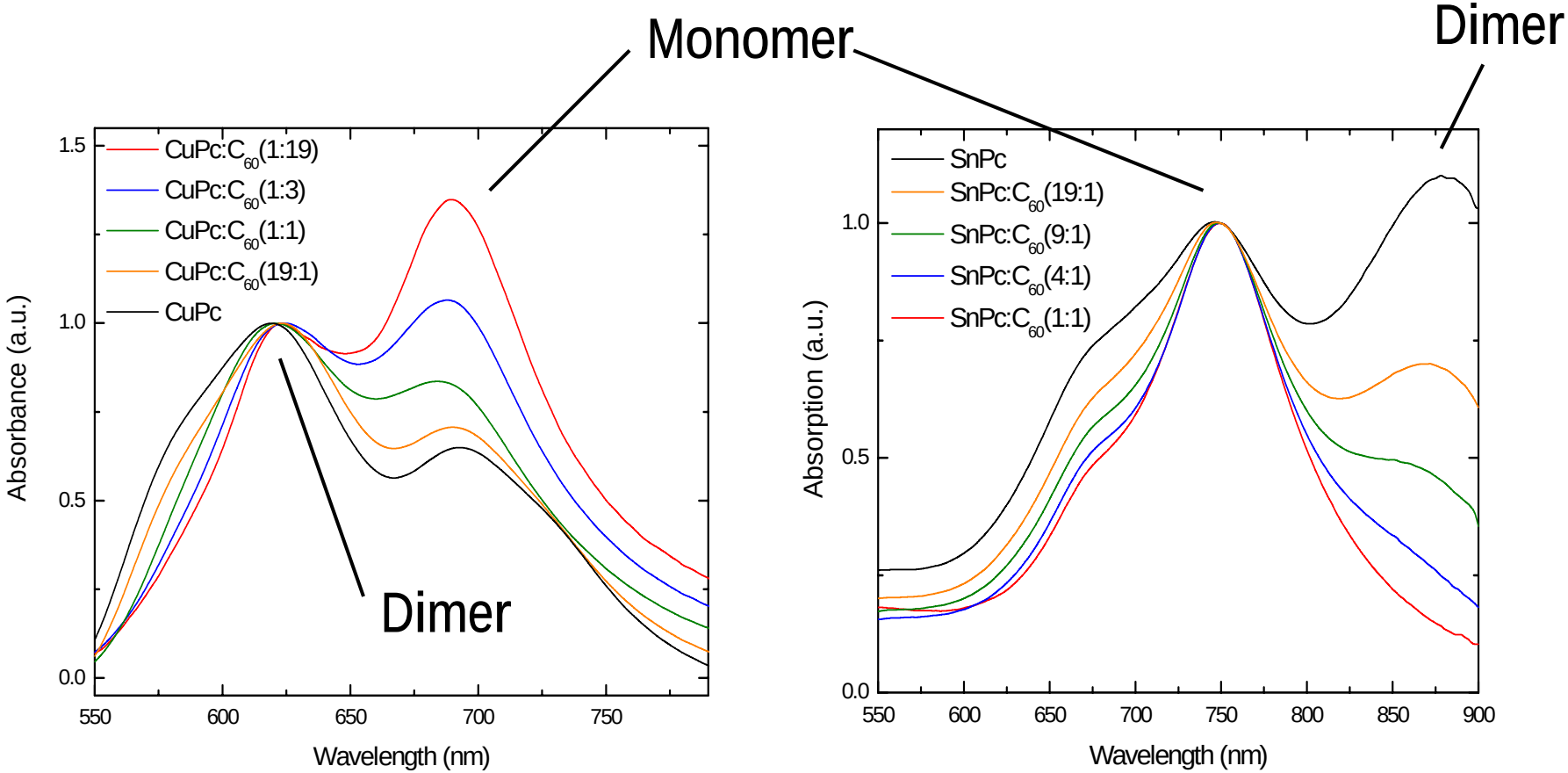
Mixed Layers

Bulk Heterojunction to *Increase* Donor-Acceptor Interface Area



- Effects on Planar (CuPc) Crystalline Structure
- Effects on Non-Planar (SnPc) Crystalline Structure

Mixed Layer Absorption Spectra



Conclusions

- A relation between the type of metal Pc, its geometry, and how it absorbs in the UV-Visible
  - New metal Pc layers used that pick up solar energy in a broader range of wavelengths
- A relationship between crystalline structure, the formation of dimers and the effect of a mixed layer on dimer absorption
  - A mixed layer of a metal Pc and an acceptor material increases exciton diffusion efficiency (η_{ED})
- An organic photovoltaic device with enough advantages to compete with inorganic solar cells

Acknowledgements

- Barry Rand
- Professor Stephen Forrest