

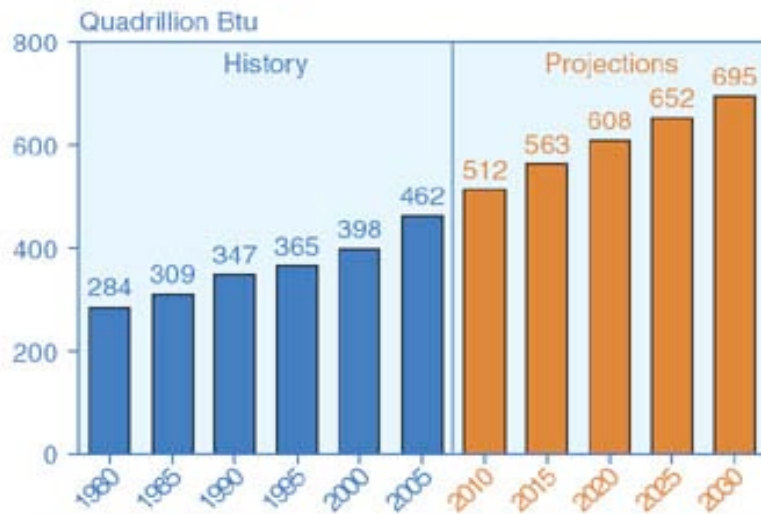
“Air Stable” Organic Photovoltaics from Small Molecules

Alon Gorodetsky
Columbia University

7/9/09

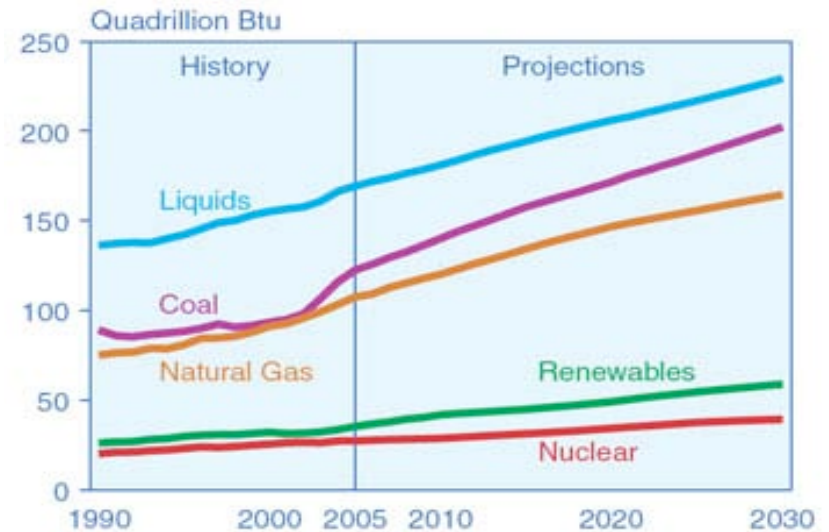
Global Demand for Energy

World Marketed Energy Consumption, 1980-2030



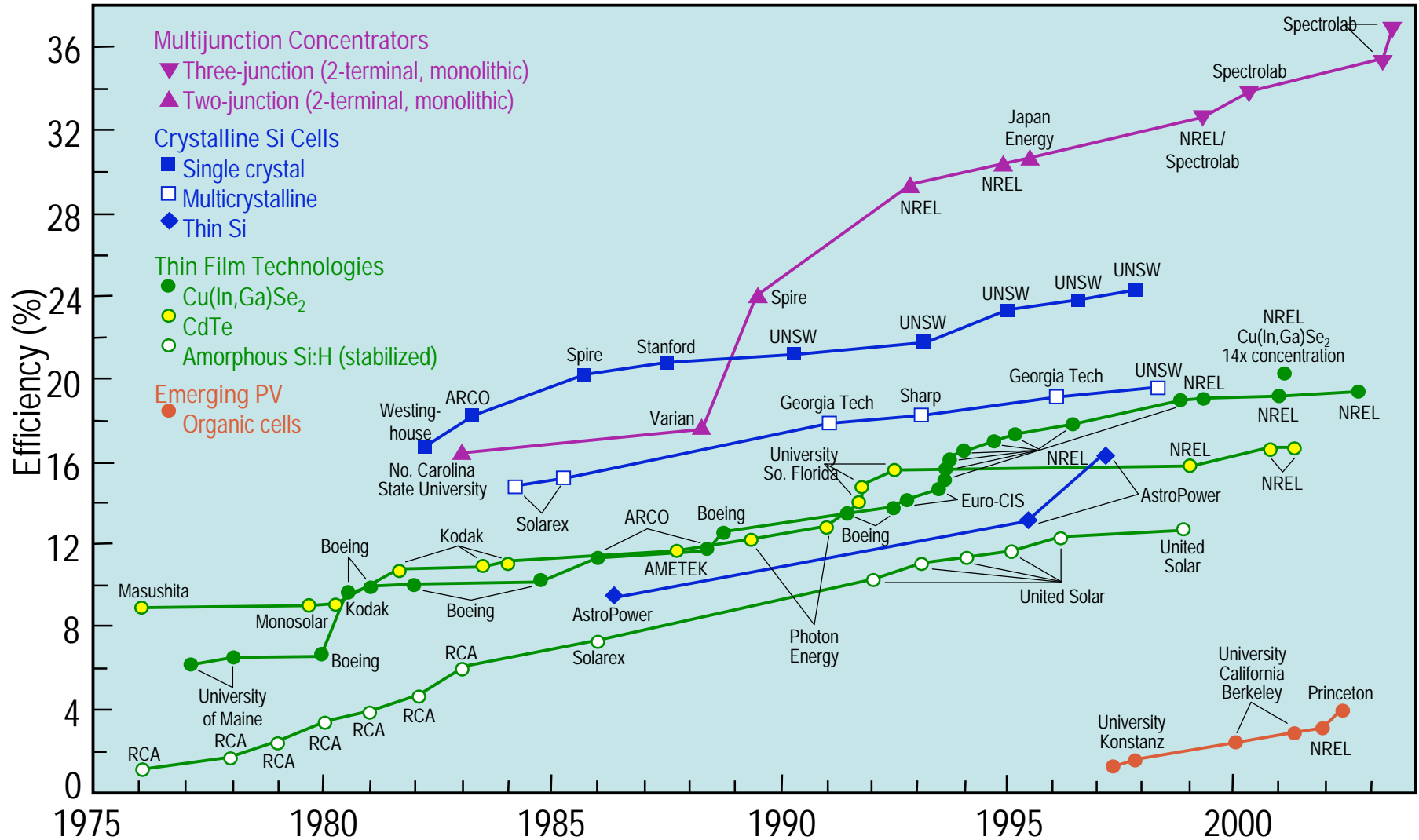
Sources: **History:** Energy Information Administration (EIA), *International Energy Annual 2005* (June-October 2007), web site www.eia.doe.gov/iea. **Projections:** EIA, *World Energy Projections Plus* (2008).

World Marketed Energy Use by Fuel Type, 1990-2030

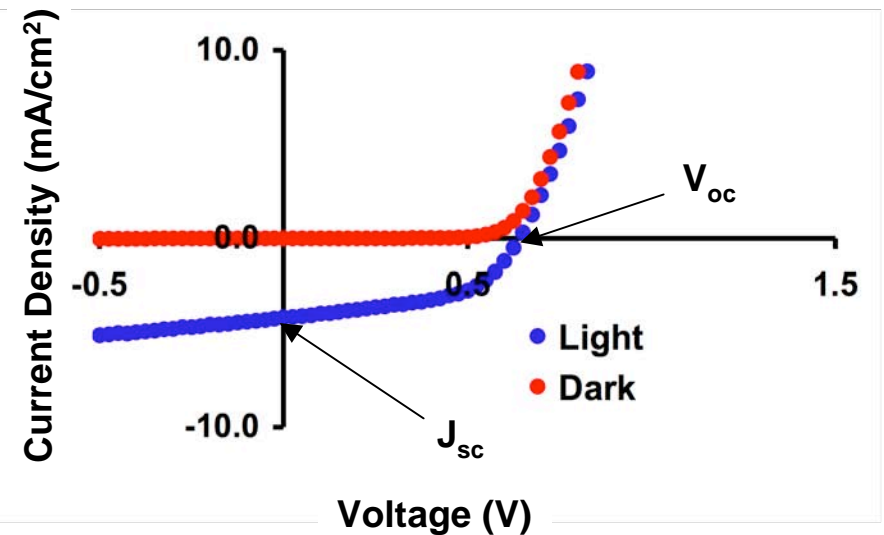
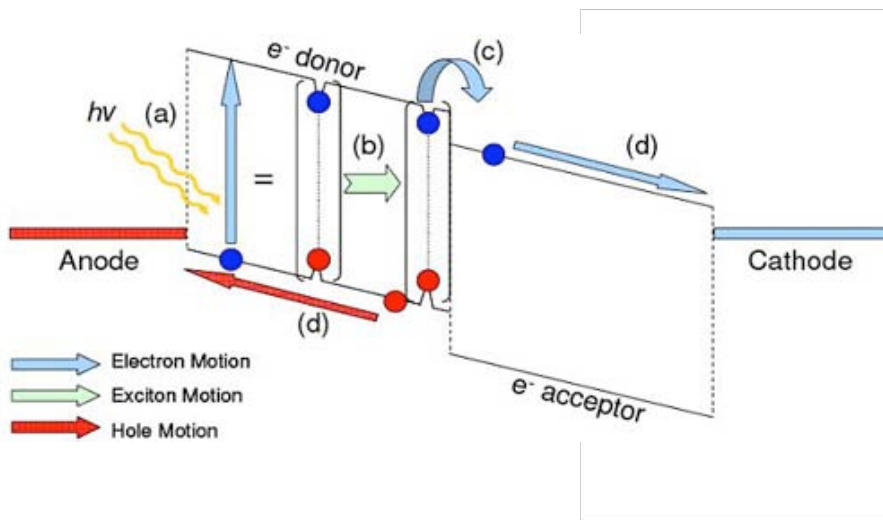


Sources: **History:** Energy Information Administration (EIA), *International Energy Annual 2005* (June-October 2007), web site www.eia.doe.gov/iea. **Projections:** EIA, *World Energy Projections Plus* (2008).

Progress in Photovoltaic Technologies



The Simplified Organic Photovoltaic Mechanism of Operation



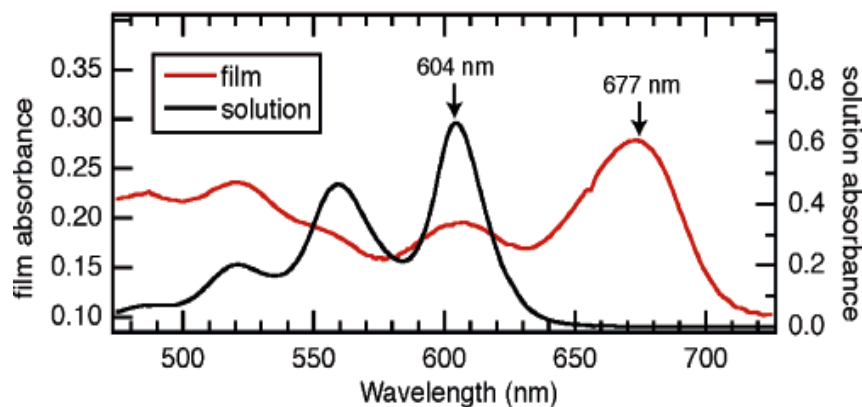
- a) Absorption of a photon and formation of an exciton
- b) Diffusion of the exciton to an interface
- c) Separation of the exciton at the interface
- d) Collection of hole and electrons at the electrodes

$$\text{Efficiency} = \frac{FF * J_{sc} * V_{oc}}{P_{inc}}$$

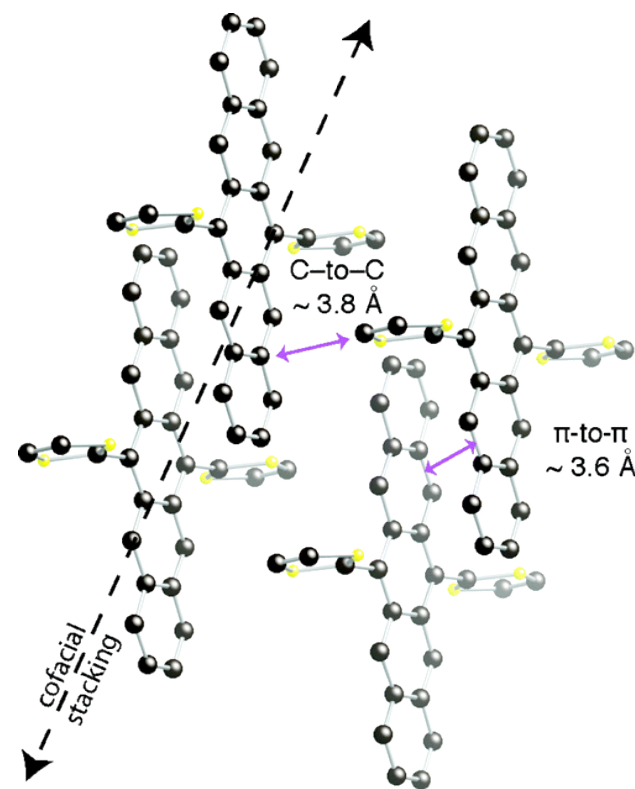
What Do I Mean by “Air Stable?”

- All devices tested in ambient atmosphere without encapsulation
- Little to no efficiency degradation over hours of testing (with or without constant illumination)
- Some degradation (~25 %) after 24 hours of air exposure
- Aluminum cathode is main source of decay

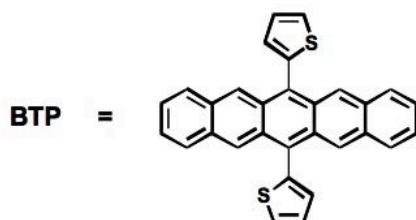
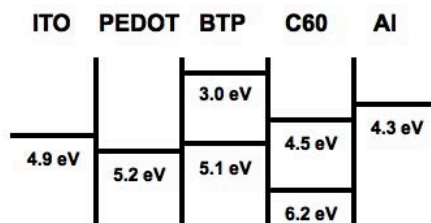
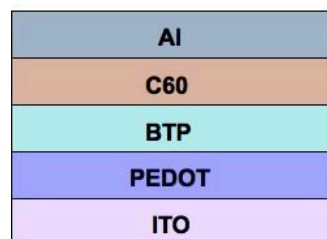
Starting Point: 6,13-bis(2'-thienyl)pentacene



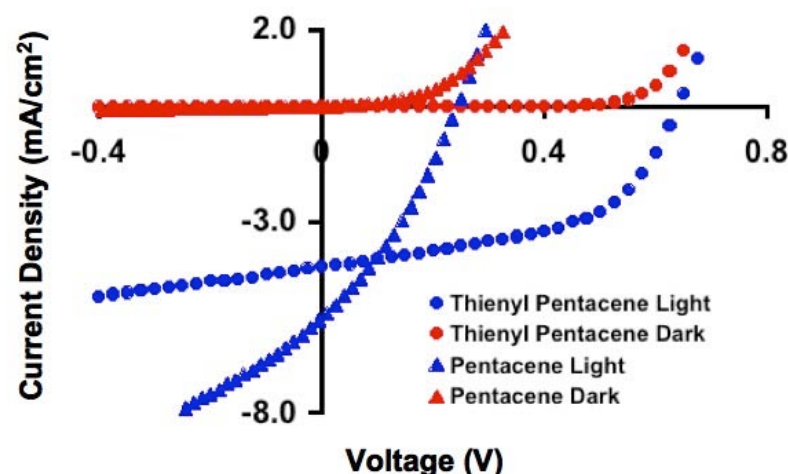
- Properties of thienyl pentacene:
 - Simple synthesis
 - Structurally well characterized
 - Red shifted absorbance in films
 - Carrier mobilities of $0.1 \text{ cm}^2/\text{V}\cdot\text{s}$
 - Solution processable



Photovoltaics from Thienyl Pentacene

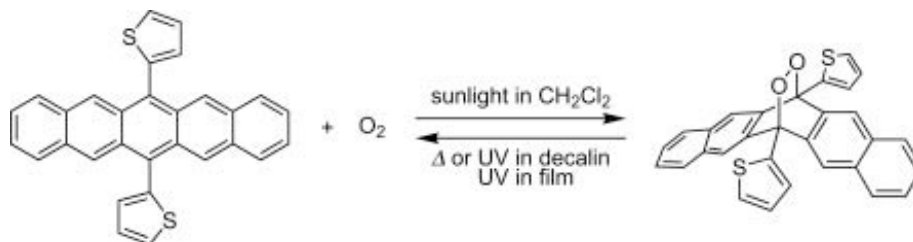
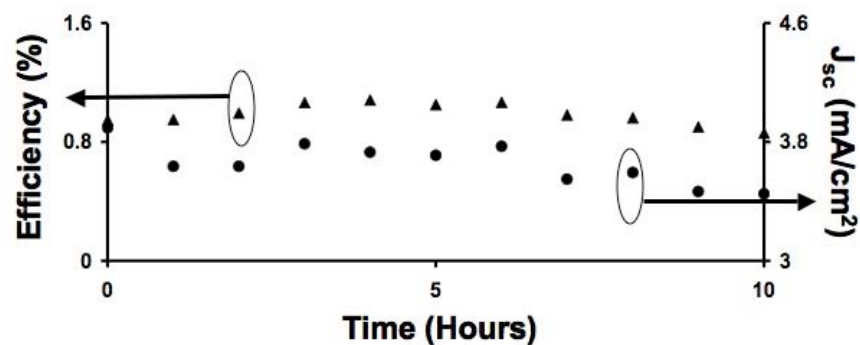
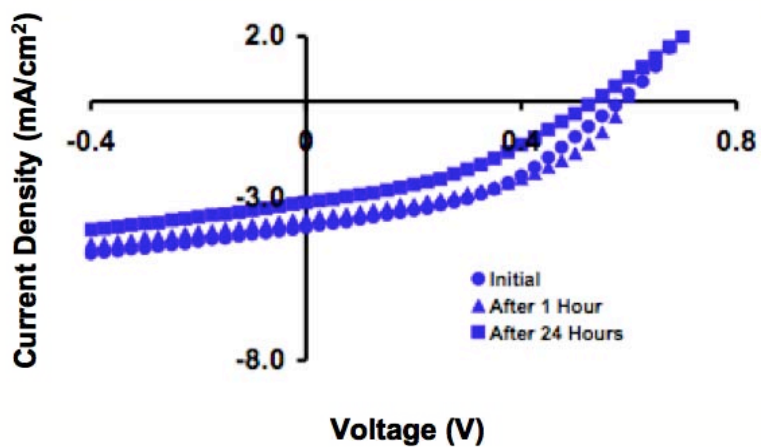


$\eta = 1.4 \%$, $J_{sc} = 4.2 \text{ mA/cm}^2$, $V_{oc} = 0.63$, $FF = 0.53$

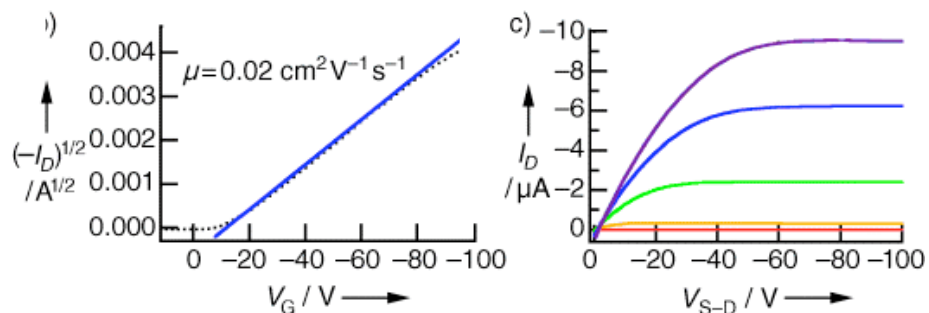
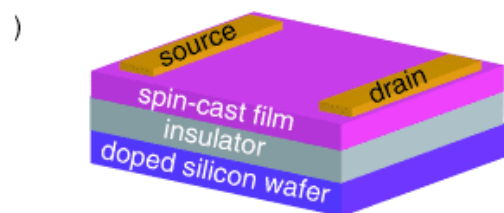
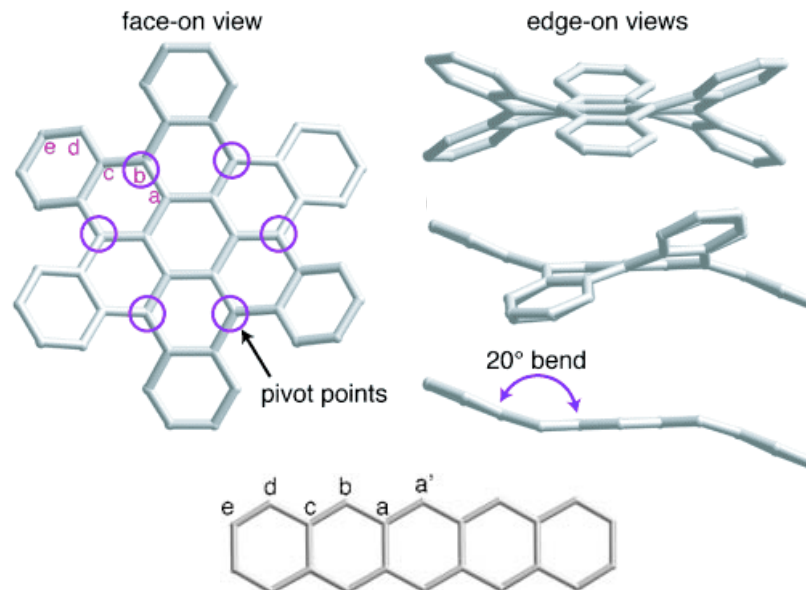
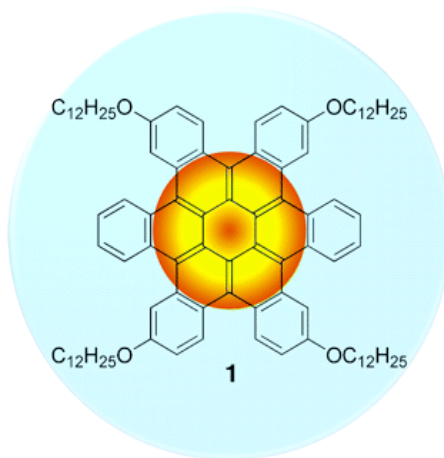


Journal	Year	Material	Structure	Efficiency	Authors
APL	2004	Deposited Pentacene	ITO/PEDOT/Pentacene/C60/BCP/Al	Estimated at 1.5	Kippelen Group
APL	2004	Deposited Pentacene	ITO/PEDOT/Pentacene/C60/CsFI/Al	1.07	Malliaras Group
	2006	Deposited Pentacene	ITO/PEDOT/Pentacene/C60/BCP/Ag	1.6	Nunzi Group
APL	2007	Deposited Pentacene	ITO/PEDOT/Pentacene/C60/Al	0.52	Dissanayake
Org Elec	2008	Deposited Pentacene	ITO/PEDOT/Pentacene/C60/BCP/Mg:Ag	0.82	Anthony Group
APL	2007	Deposited Pentacene	ITO/PEDOT/Pentacene/C60/BCP/Al	Estimated at 1.5	Kippelen Group
Org Elec	2008	Deposited Pentacene	ITO/PEDOT/Pentacene/C60/BCP/Al	1.5	Jones Group
Org Elec	2006	Spun TIPS Pentacene	ITO/PEDOT/TIPS Pentacene/C60/CsFI/Al	0.52	Malliaras/Anthony Groups
Org Elec	2008	Deposited TIPS Pentacene	ITO/PEDOT/TIPS Pentacene/C60/BCP/Mg:Ag	0.74	Anthony Group

Advantage: Enhanced Device Stability in Ambient



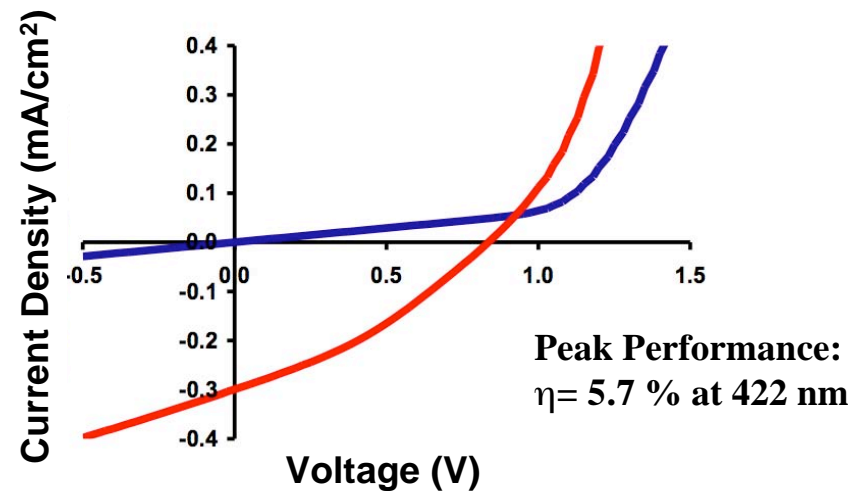
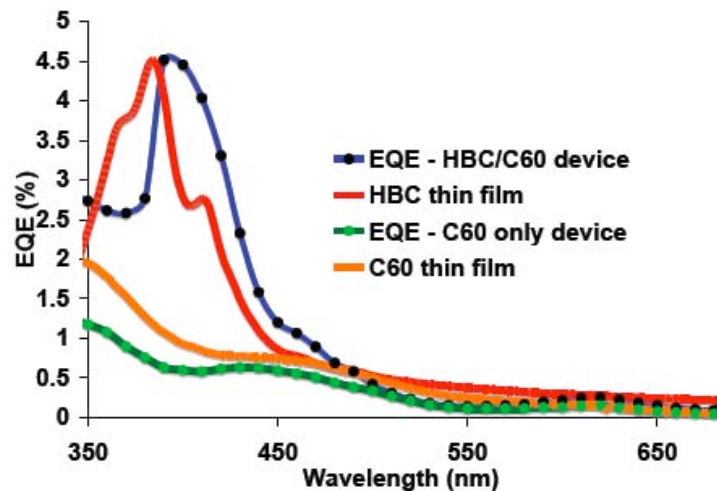
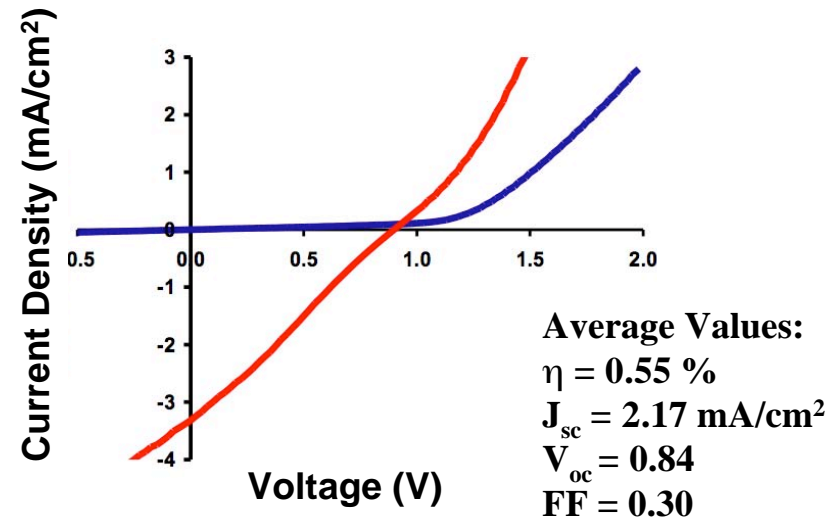
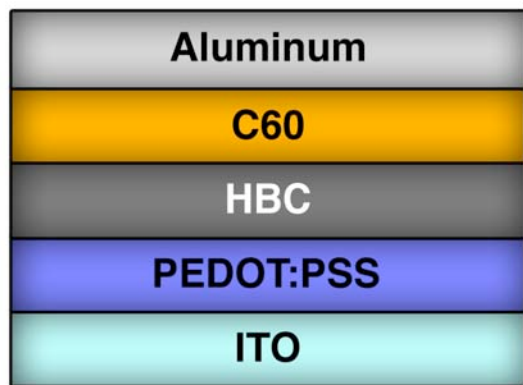
Organic Electronics from Hexabenzocoronene (HBC)



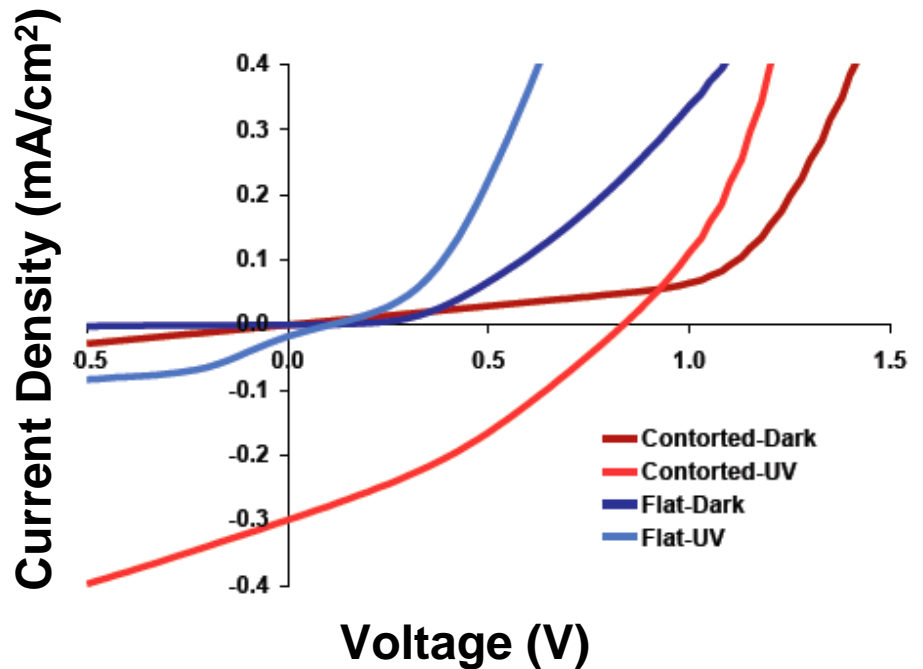
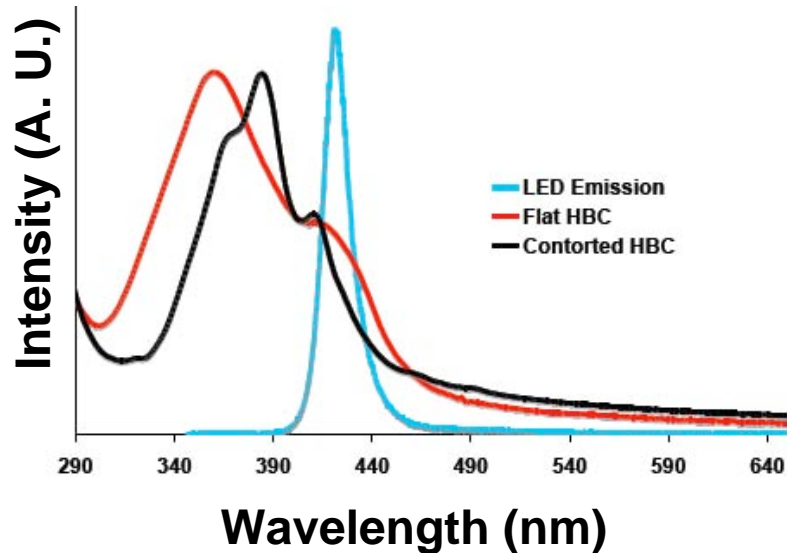
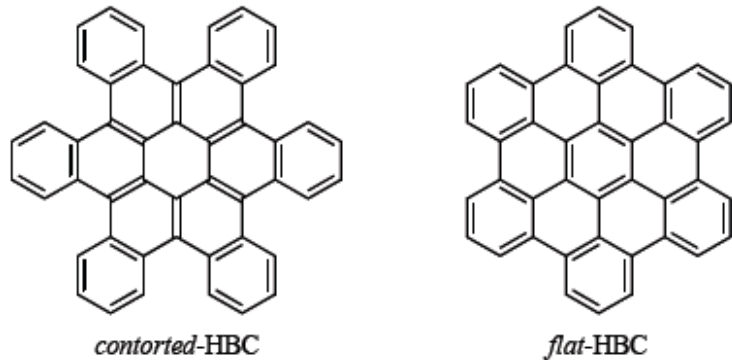
	C-C bond length [Å]	
	1 a ^[a]	Pentacene ^[b]
C _a -C _{a'}	-	1.44
C _a -C _a	1.43	1.46
C _a -C _b	1.40	1.42
C _b -C _c	1.45	1.38
C _c -C _c	1.42	1.45
C _c -C _d	1.42	1.43
C _d -C _e	1.38	1.35
C _e -C _e	1.42	1.43

Xiao, S., et. al. *Angew. Chem. Int. Ed.*, **2005**, 44, 7390.

Organic Photovoltaics from Contorted Hexabenzocoronene

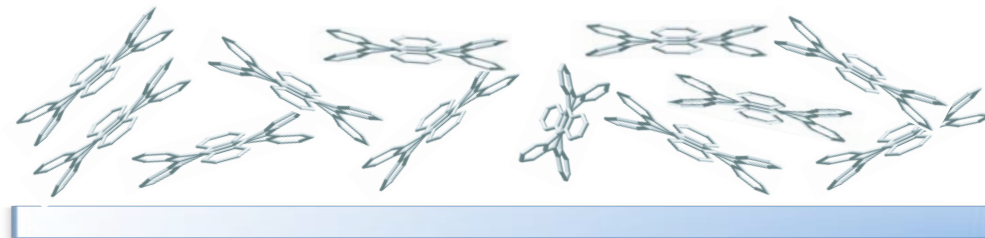
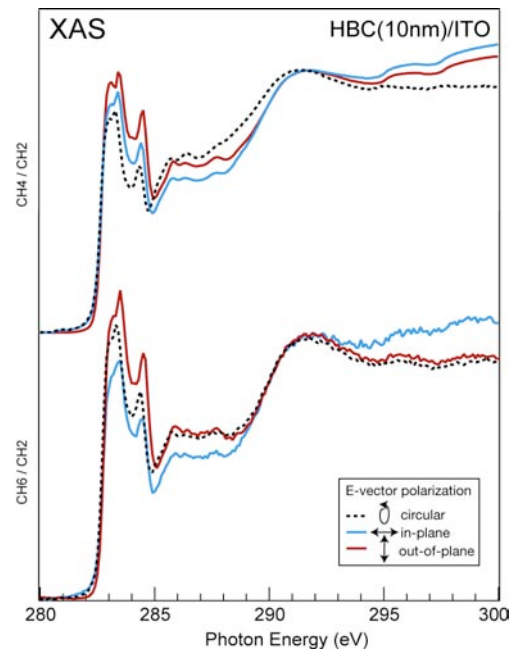
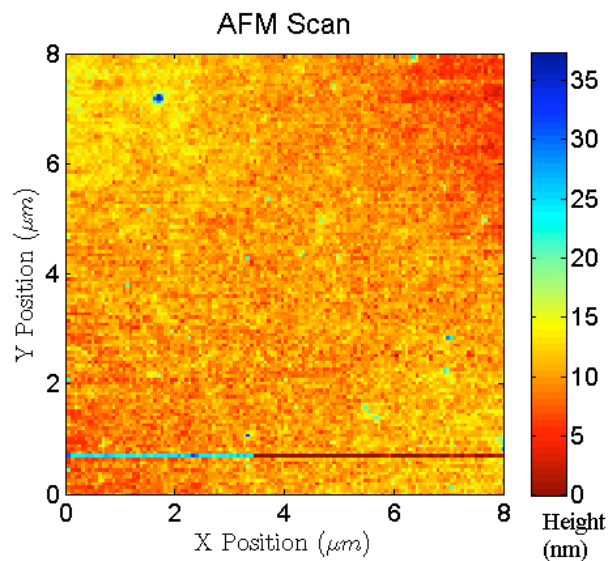


Comparison to Organic Photovoltaics From Flat Hexabenzocoronene

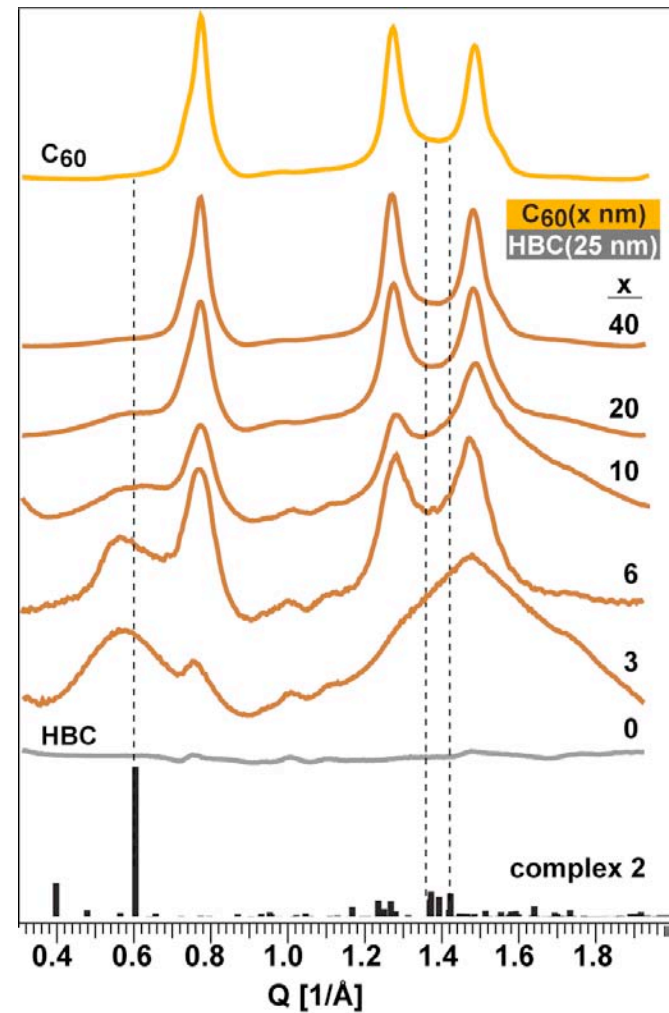
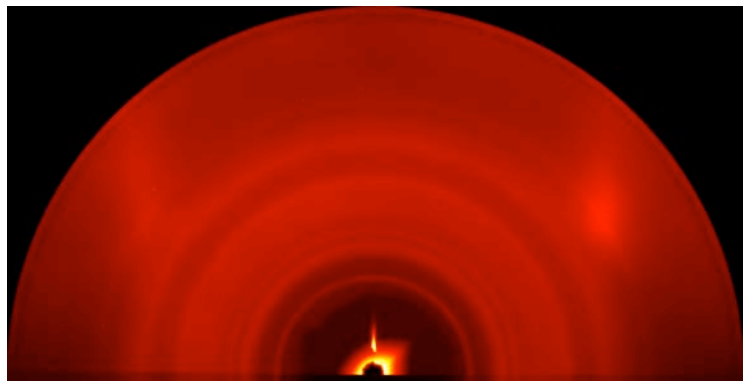
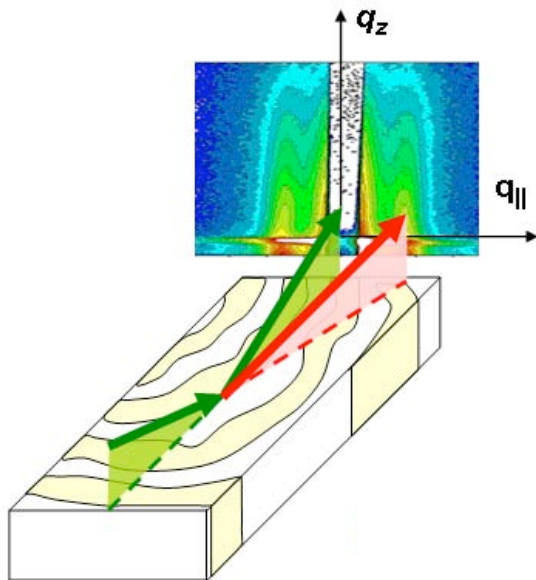


Average Performance:
 $\eta = 3.36\%$ for *contorted*-HBC at 422 nm
 $\eta = 0.03\%$ for *flat*-HBC at 422 nm

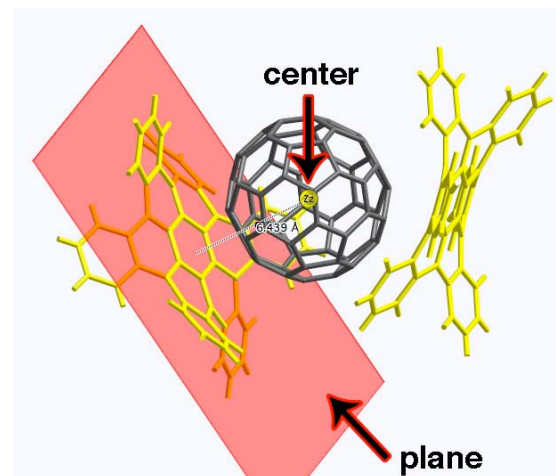
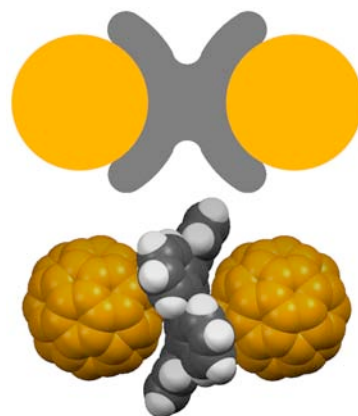
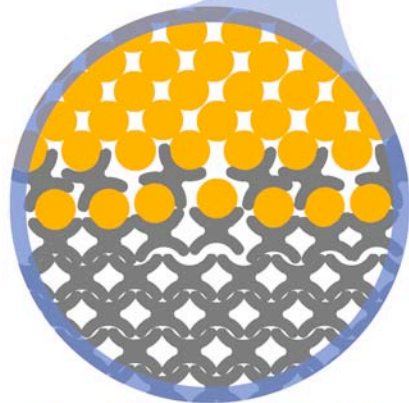
Atomic Force Microscopy and X-Ray Absorption Spectroscopy of HBC Films



Grazing Incidence X-Ray Diffraction of the HBC/C₆₀ Interface



Ordered Organic/Organic Interfaces Via Molecular Shape Complementarity



LUMO = 2.5 eV

LUMO = 4.5 eV

$V_{oc} \sim 0.90 \text{ V}$

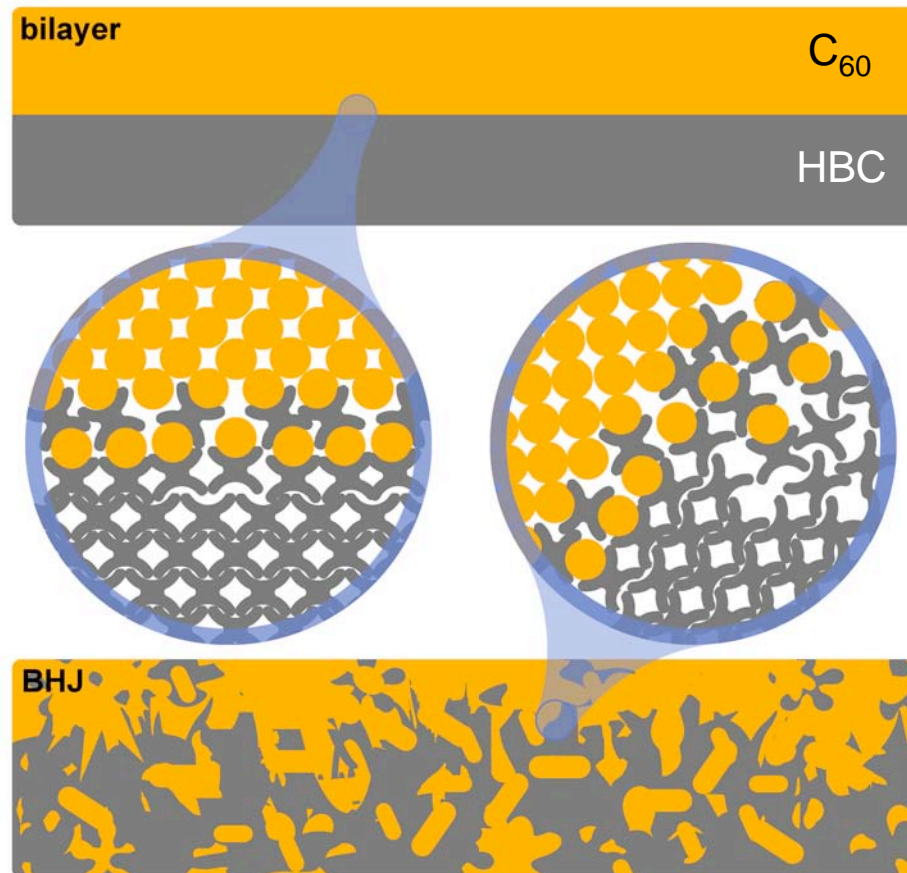
HOMO = 5.5 eV

HOMO = 6.2 eV

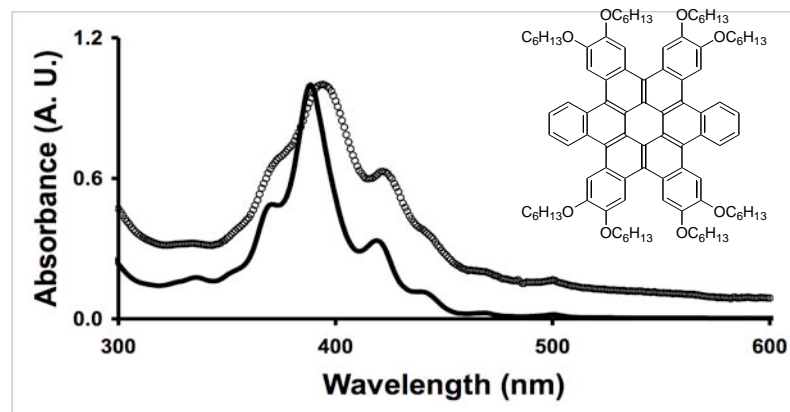
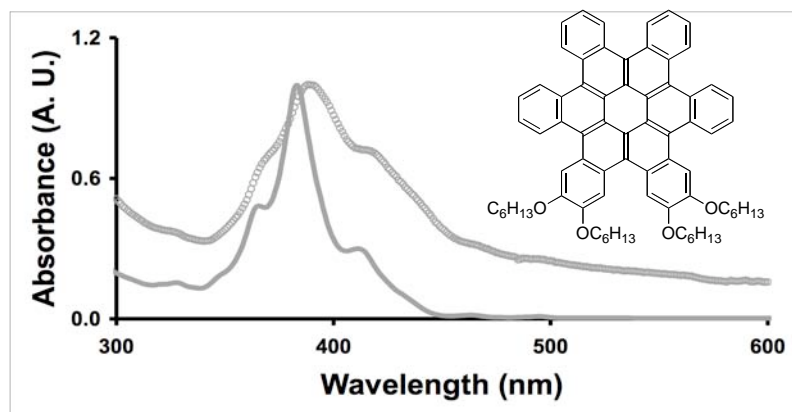
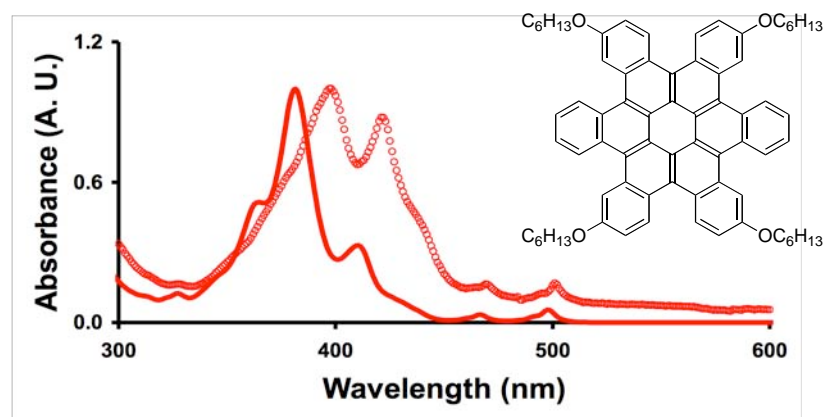
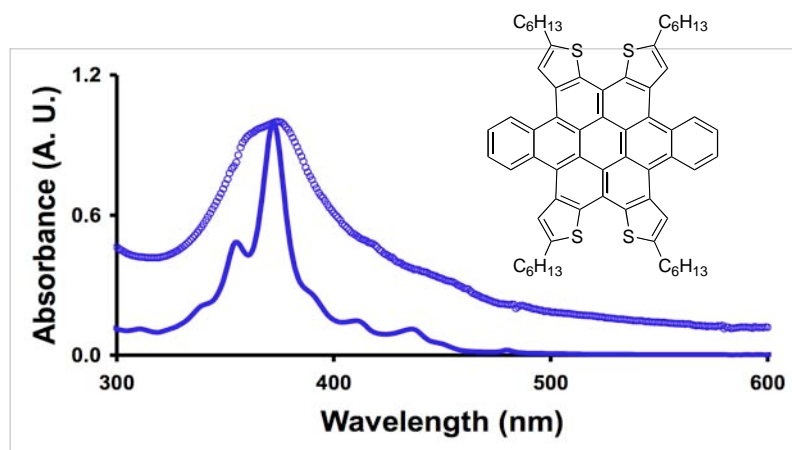
HBC

C₆₀

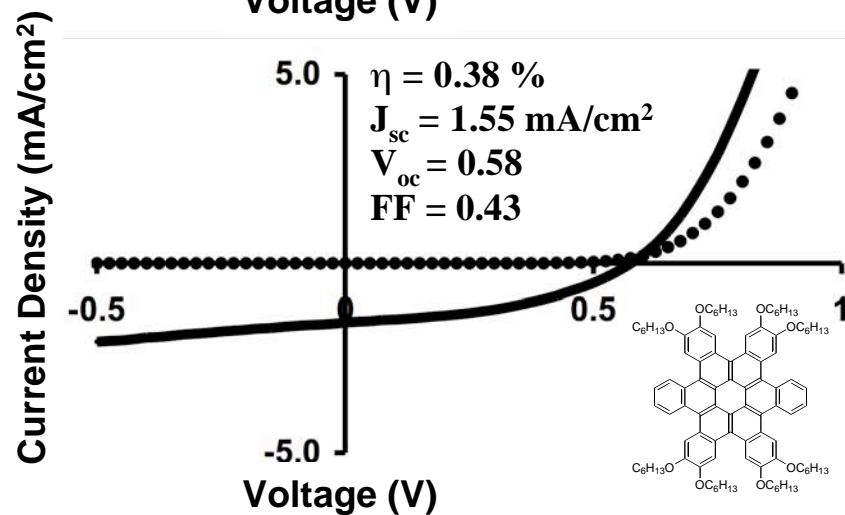
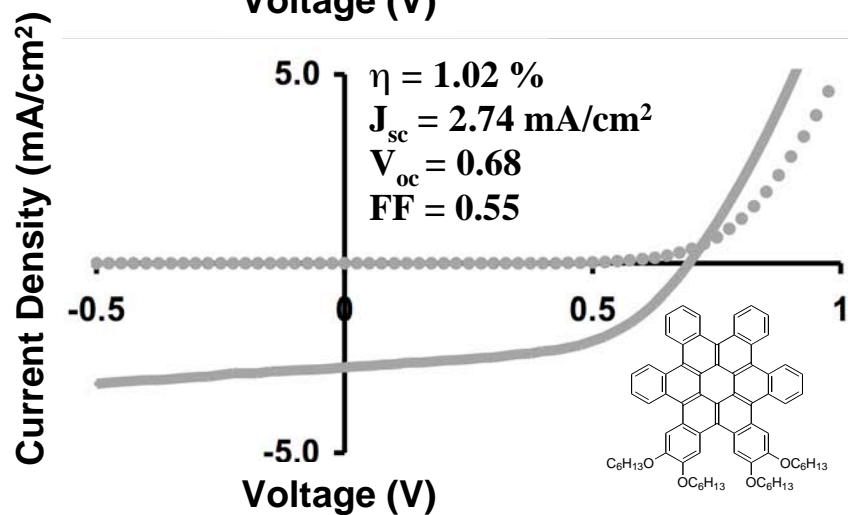
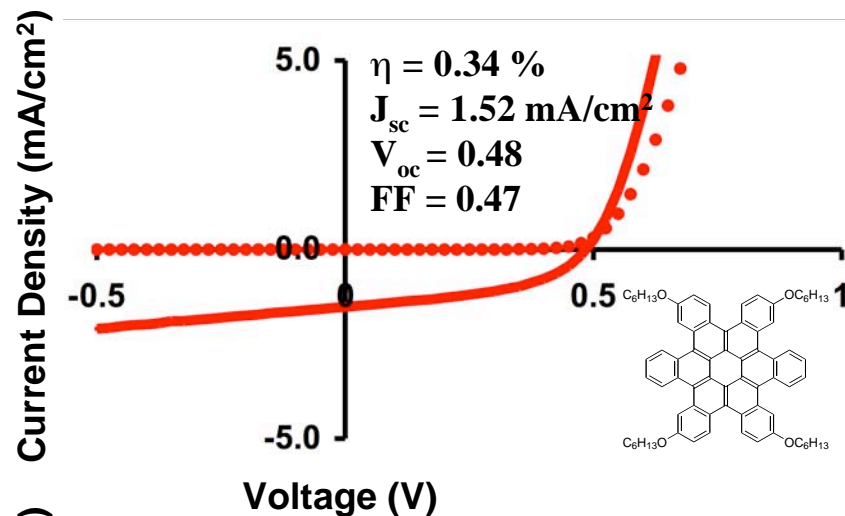
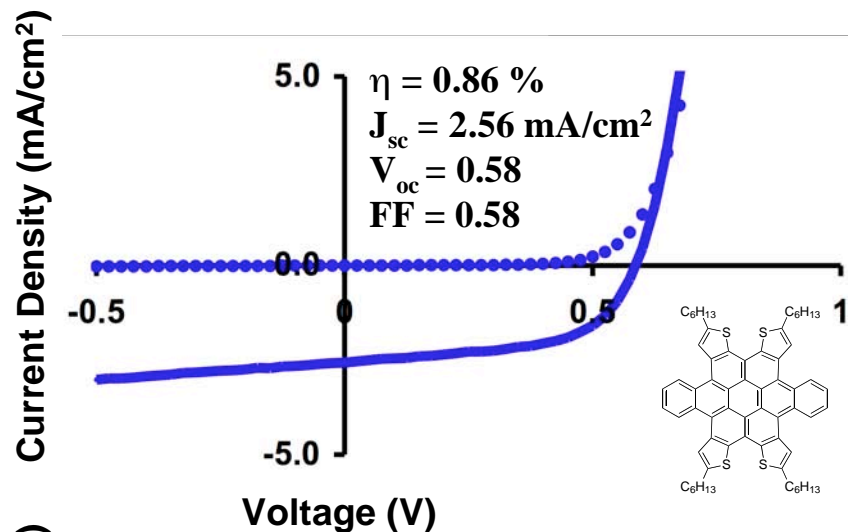
Toward Bulk Heterojunction Device Architectures



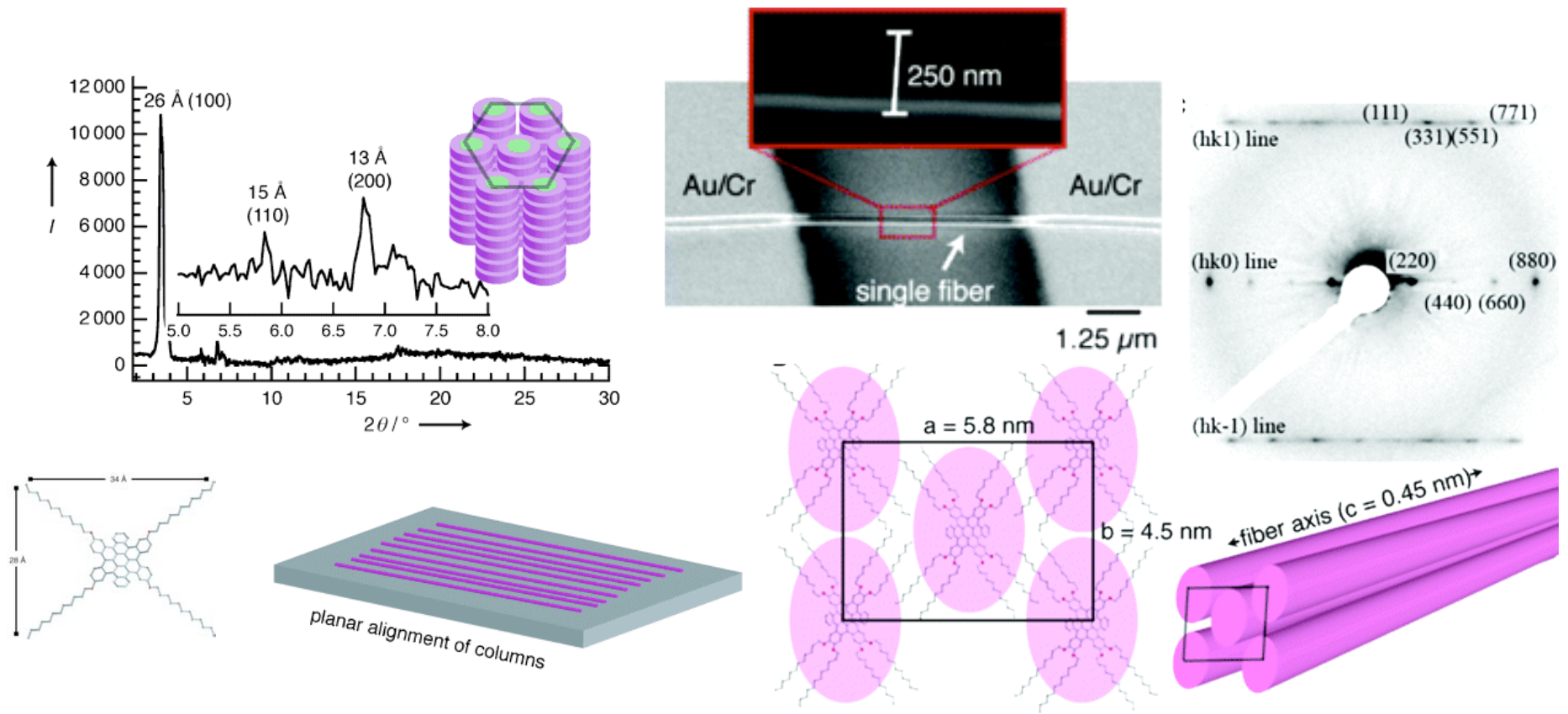
Solution Processable Hexabenzocoronene Derivatives



Photovoltaics from Hexyl Substituted Hexabenzocoronenes

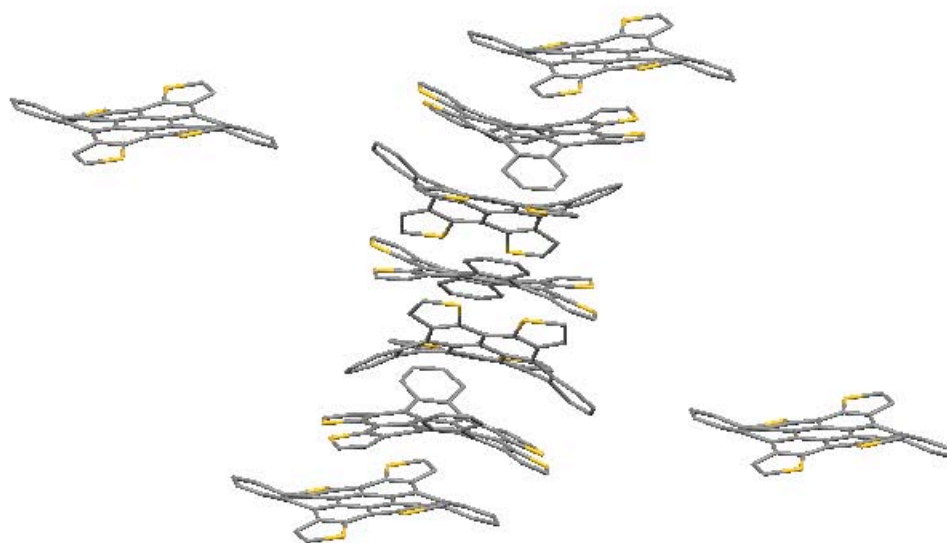
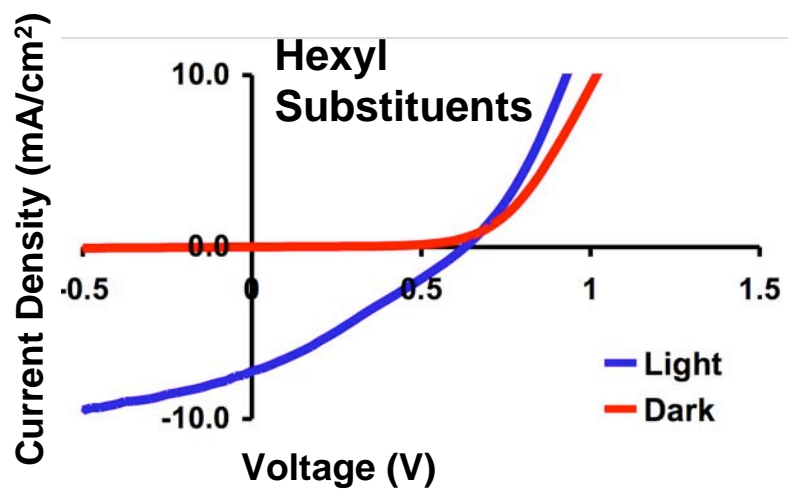
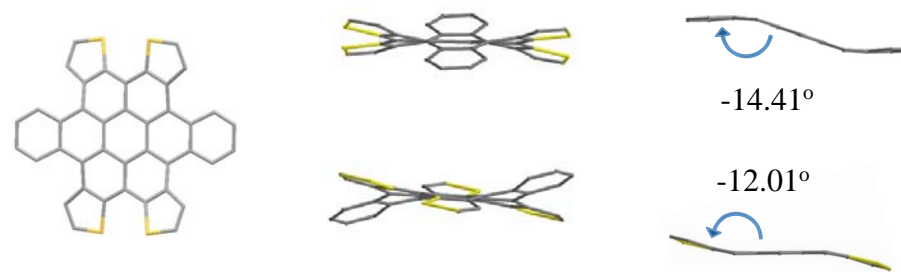
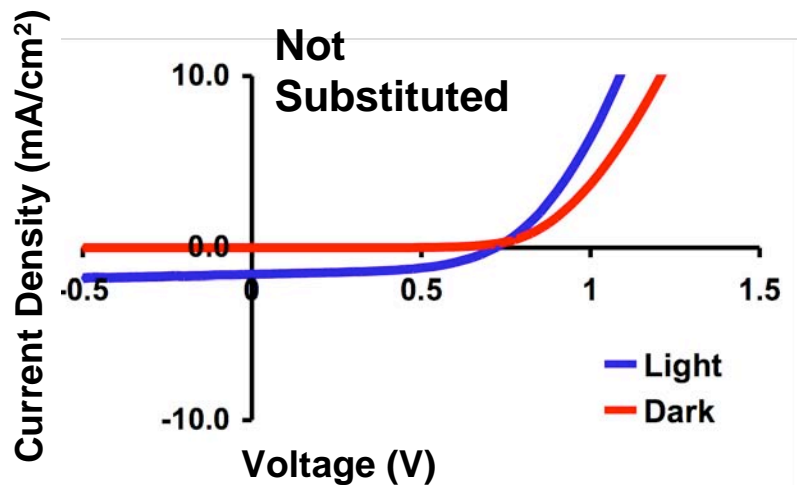


Alkyl Substituents Afford Morphological Control

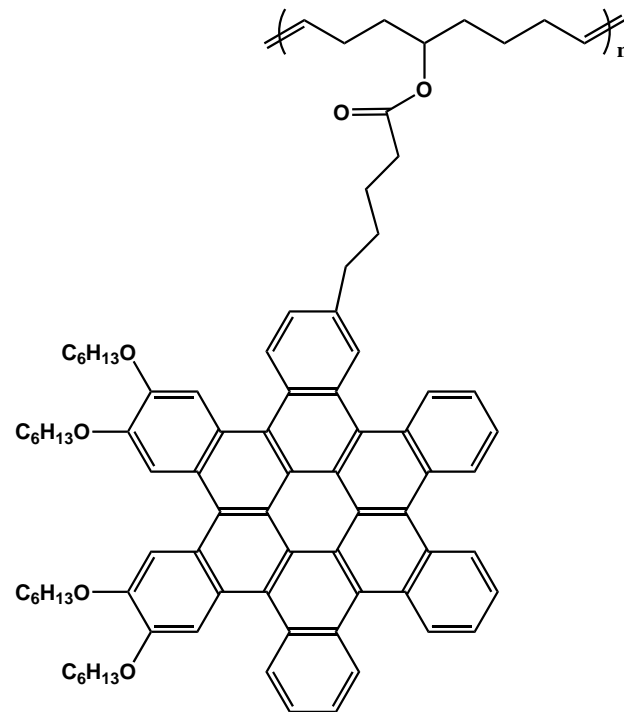
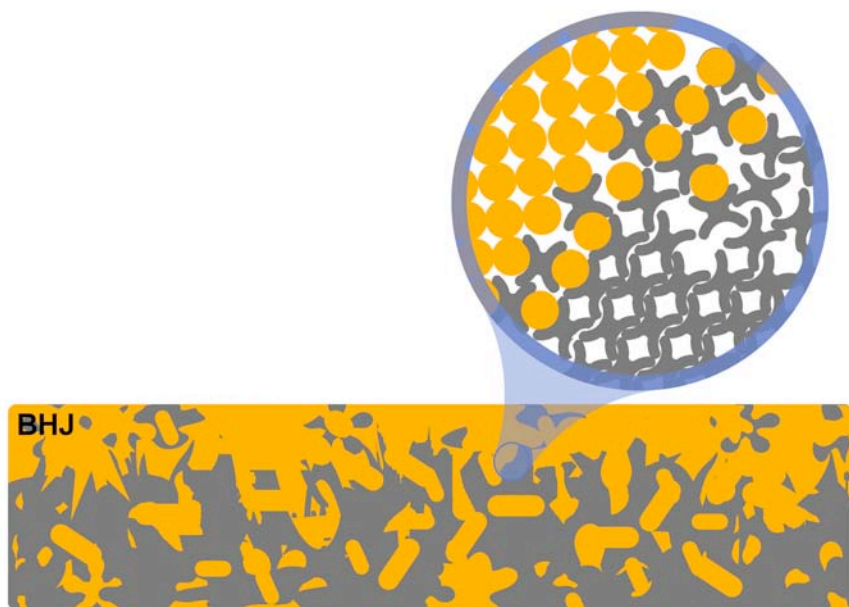


Xiao, S., et. al. *Angew. Chem. Int. Ed.*, **2005**, 44, 7390.
 Xiao, S., et. al. *J. Am. Chem. Soc.* **2006**, 128, 10700.

Focus on Thienyl-Hexabenzocoronene



Next Step: Hexabenzocoronene Polymers



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