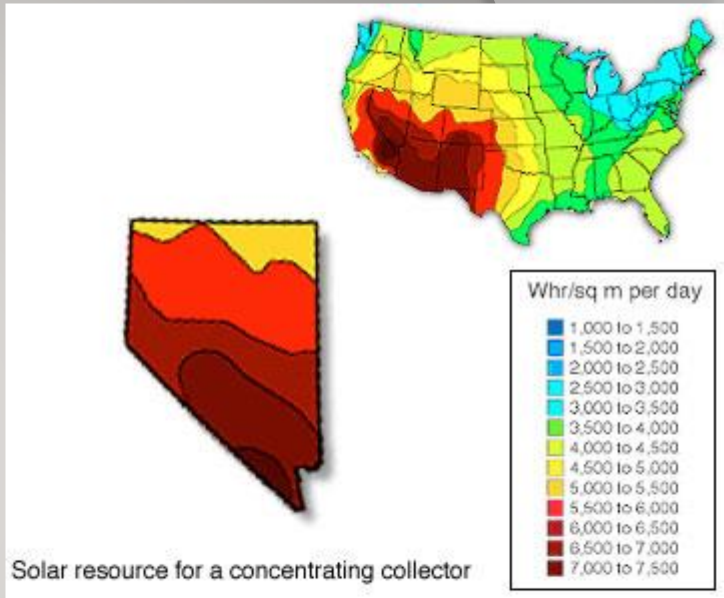
Organic Photovoltaics

Kitran Colwell – Fall 2009 – Physics 211A

Solar Energy

- Why solar?
  - No pollution (aside from manufacture/disposal)
  - Abundant supply (during clear weather/daytime)
  - (Somewhat) Easy to collect/use
  - Can be used to create electricity or H_2 or heat
  - Most other renewables are indirectly solar power anyway (wind, hydroelectric, tidal, biofuel, etc.)
- At 15% efficiency, $(150\ km)^2$ (about 8,700 mi^2) of Nevada would provide electricity for the whole US, assuming 2 m^2 supports 1 m^2 PV (for structure, angle, etc.)
- At 10% efficiency, 17,000 mi^2 across the US would be enough



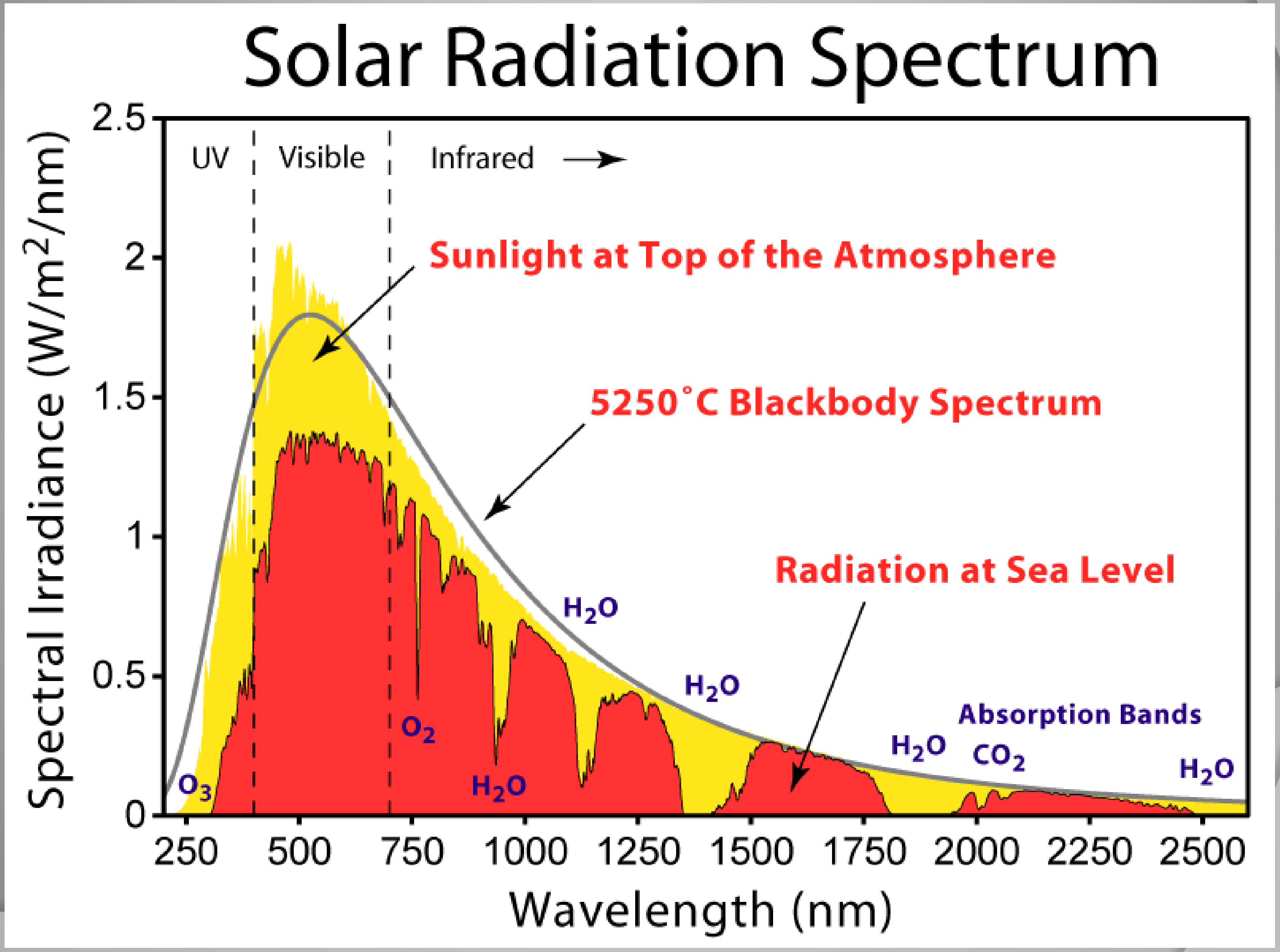
Solar resource for a concentrating collector

Relevant Data	
Average US annual electricity consumption (2008)	3.96 trillion kWh (450 GW)
Average annual surface irradiance (NV)	2300 kWh/m^2
Average annual surface irradiance (US)	1800 kWh/m^2

Solar Energy

- The Spectrum
  - About 1.3 kW/m^2 of solar energy reaches upper atmosphere – about 1 kW/m^2 reaches surface
  - Peak arrival of energy at 504 nm (2.48 eV), peak arrival of photons at 879 nm (1.41 eV)
- Photosynthesizing organisms and terrestrial eyesight have evolved to take advantage of ~500 nm light

Solar Energy

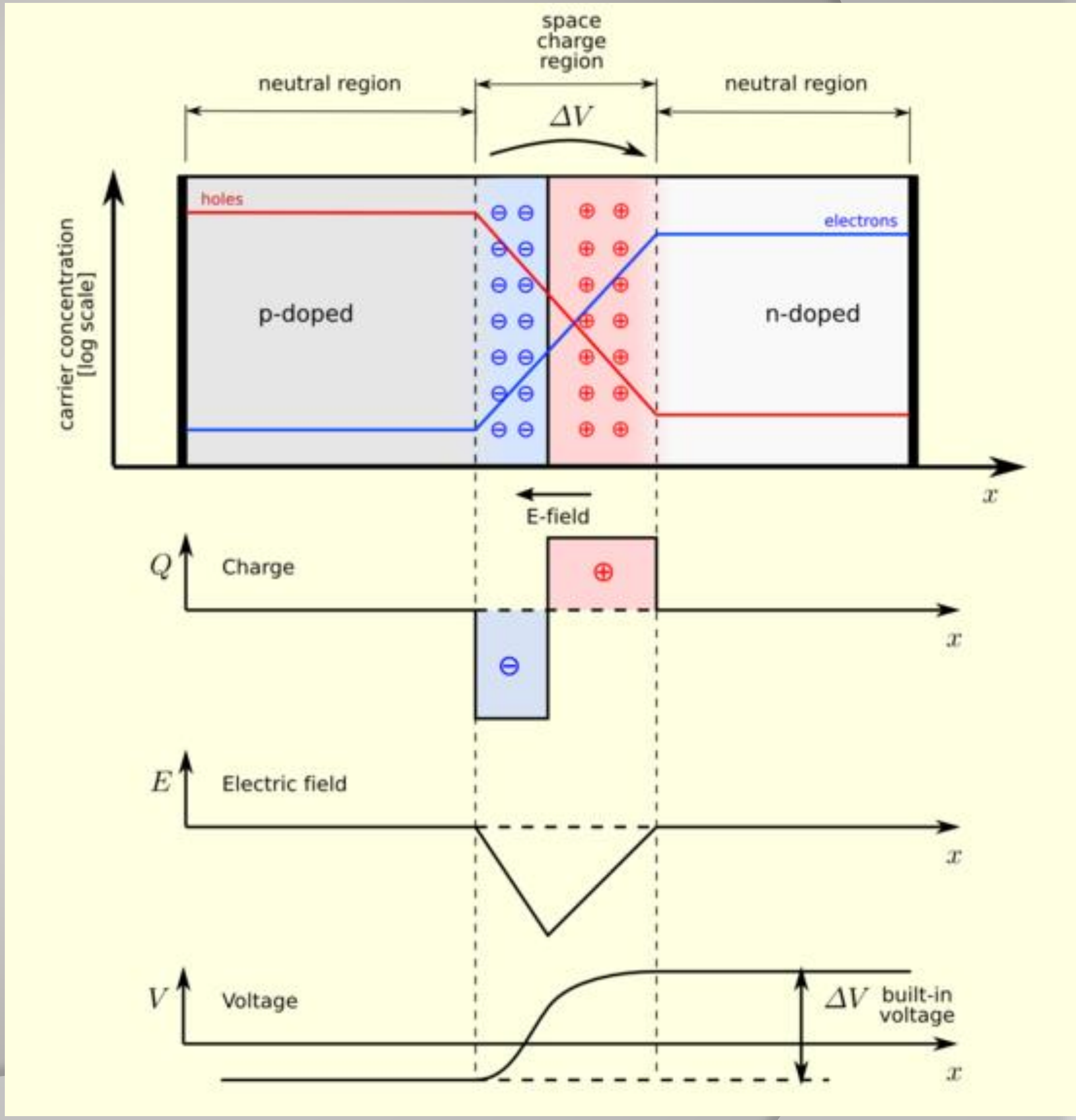


Inorganic Photovoltaics

- Semiconductors
  - Some have band gaps in optical range (Si has 1.1 eV), and can absorb solar photons
  - Absorbed photons generate **excitons**, bound hole-electron pairs (binding energy about 0.4 eV)
  - Dope with donor materials (P, As) to create n-type semiconductor (free electrons); dope with acceptor materials (B, Ga) to create p-type (free holes)

Inorganic Photovoltaics

- PV Diode
  - When an n- and p-type semiconductor are placed together, electrons flow from p-type to n-type, but not the other way
  - The holes and electrons drift towards electrode contacts, where they are extracted to do work

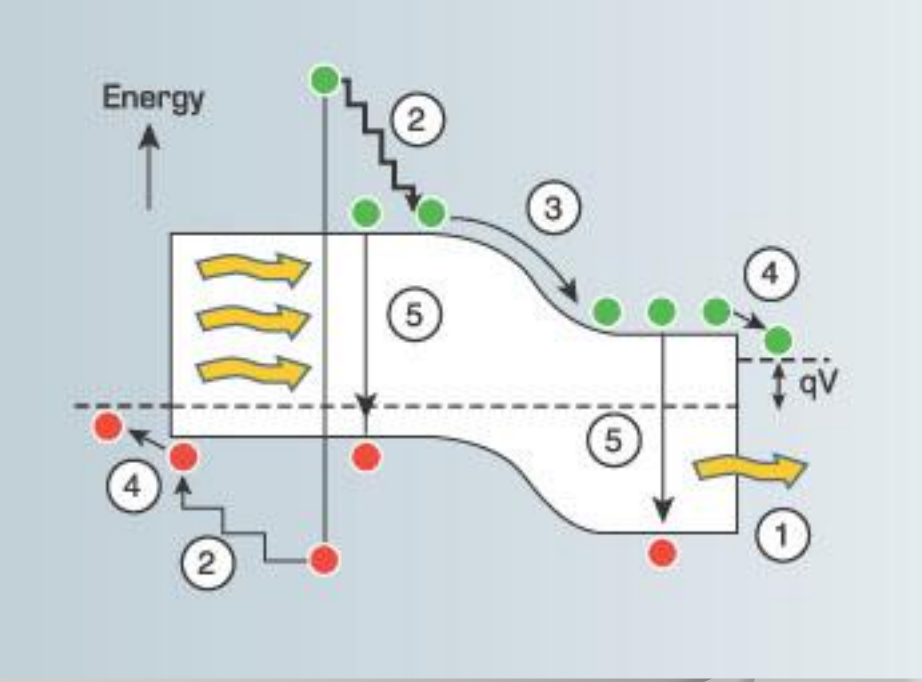


Inorganic Photovoltaics

- The Cell
  - We coat the Si with an antireflective coating to reduce reflection loss to <5%
  - Place a transparent (ITO=$In_{2-x}Sn_xO_3$ or something IR transparent) electrode or small-area contact grid (don't block light) across top and bottom to collect carriers
  - Cover with glass for protection from elements
- Voila! Generic 1st generation solar cell, up to 15% efficient

Inorganic Photovoltaics

- Losses
  - Several ways in which energy is lost:
    1. Low energy photons pass through cell without creating exciton
    2. High energy photons lose excess energy to phonons (heat)
    3. Losses at junction
    4. Losses at contact
    5. Electron-hole recombination (and exciton decay)
- First 2 account for 70% of loss alone
  - If we try to make bandgap smaller to use more photons (higher current), strength of electric field decreases, lowering power (P=I*V)
  - Maximum power at band gap of 1.4 eV
  - Multi-junction devices have several back-to-back cells of different gaps (up to 43% efficient)



Inorganic Photovoltaics

- Problems
  - Often requires growth of large single crystal Si – clean room, microfab…expensive (>$2.50/W)
  - Fragile and unable to accommodate curved surfaces
  - Can’t alter properties (band gap, mobility, etc.) very much
- Maybe there’s another way…

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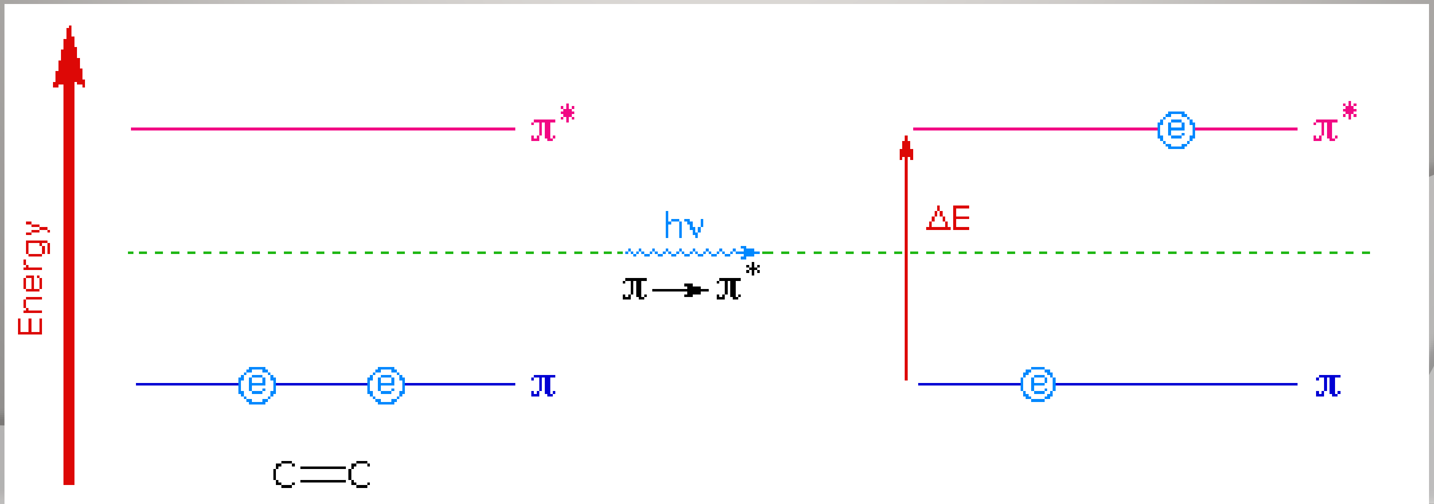
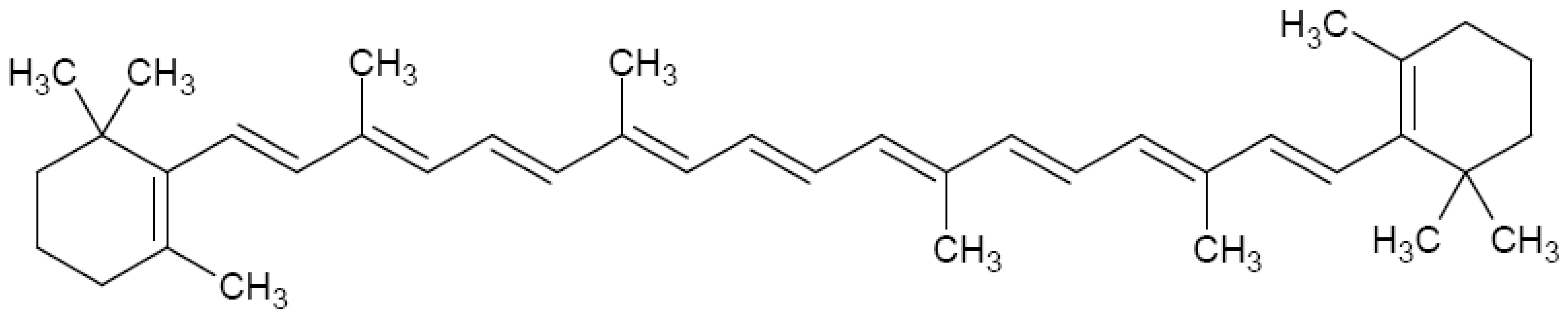
- Molecules
  - Certain classes of organic molecules have excitable energy levels in the optical range
  - “Band gap” is now the HOMO-LUMO gap: highest occupied molecular orbital to lowest unoccupied molecular orbital
  - Generally require **conjugation**, an extended network of delocalized π-bonds, for optical excitations



ORGANIC PHOTOVOLTAICS

- Molecules
  - Extensive conjugation also enhances the absorption coefficient
  - Need not be linear – rings, alkyl groups, and polar additions enrich the spectra
  - This conjugation gives many familiar biochemicals their color
- Example: β-carotene
  - Absorption peak at 455 nm (HOMO-LUMO gap of 2.7 eV) implies absorption in cyan, compliment is orange, the color of carrots



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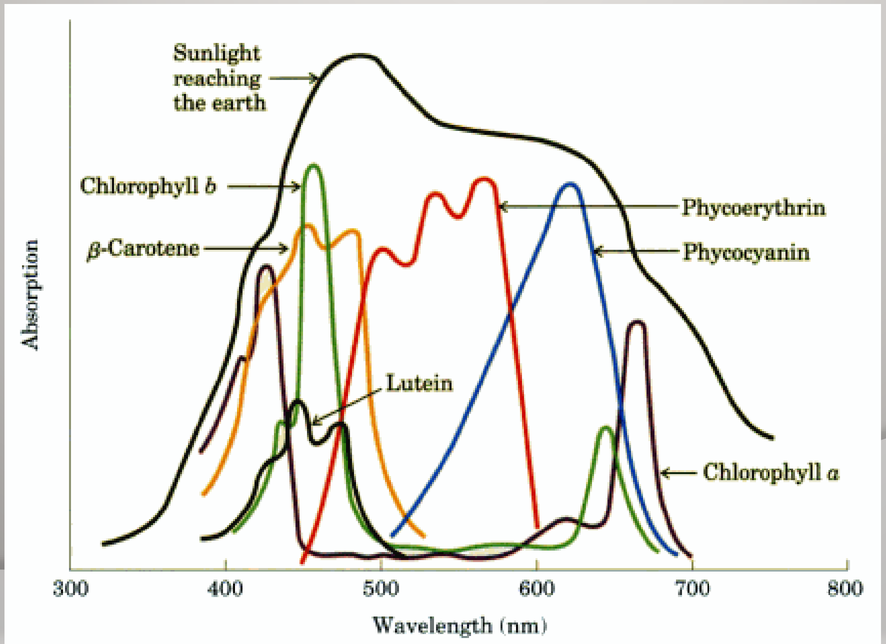
- Natural Occurrences
  - Conjugated organic molecules provide basis for energy entrance into biosphere: cyclic tetrapyrroles, like chlorophyll
  - Plants and other photosynthesizing organisms also use accessory pigments (like carotenoids) to capture other wavelengths
- How does the excitation move, and how does this do work?



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- Excitons
  - Once the electron is excited to the LUMO, it and the hole left behind are free to diffuse throughout the delocalized π-network as a bound pair, or exciton
  - Without subsequent charge separation, the exciton decays quickly as the hole and electron recombine
- Charge Separation
  - If both a donor and acceptor-type molecule are present, an exciton at the interface may separate into an electron (free to drift and diffuse in the acceptor [A] and a hole in the donor [D])
  - Provided they don’t meet and recombine, the electron and hole are mobile in the A and D respectively, and can be extracted as current at electrodes, just like the inorganic case

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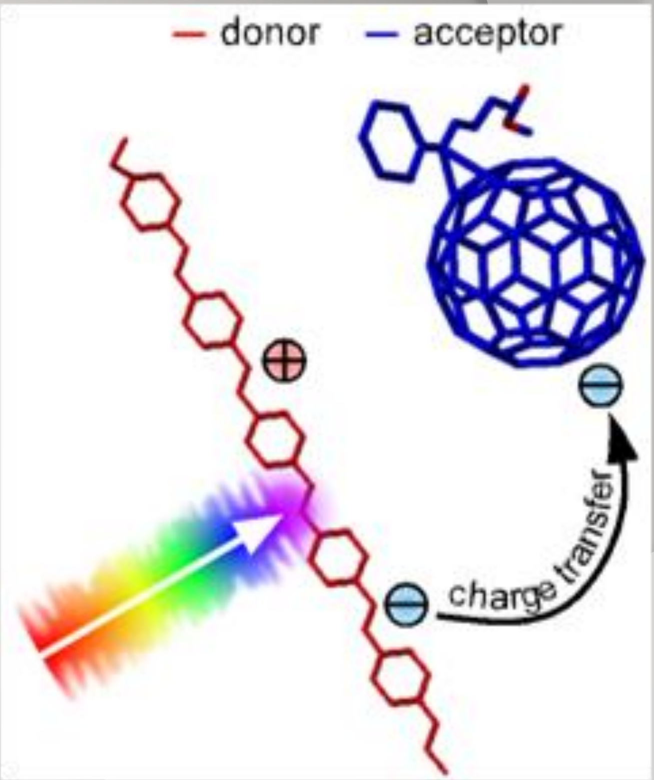
- Donor Molecule
  - The donor is usually the species that absorbs the light, and so is an extensively conjugated system
  - Often used are polymers, such as P3HT (poly-3-hexylthiophene)
- Acceptor Molecule
  - Needs to conduct electrons well, so often PCBM (“buckyballs”) are used
  - Sometimes both species can absorb light and generate excitons



Organic Photovoltaics

- Bulk Heterojunction
  - Roughly 100 nm thick
  - The D and A can be mixed uniformly, heated, and allowed to cool to form domains (annealing)
  - Our question was: What does the heterojunction morphology do to efficiency?
- Balancing Factors
  - If the domains of D and A are too large, excitons will decay before they reach an interface
  - If there is too much interface, the separated carriers will meet and recombine
  - If there is not a pathway to reach the electrodes, the carriers get trapped, and do no work
  - There must be an optimal structure (or class of structures)!

ORGANIC PHOTOVOLTAICS

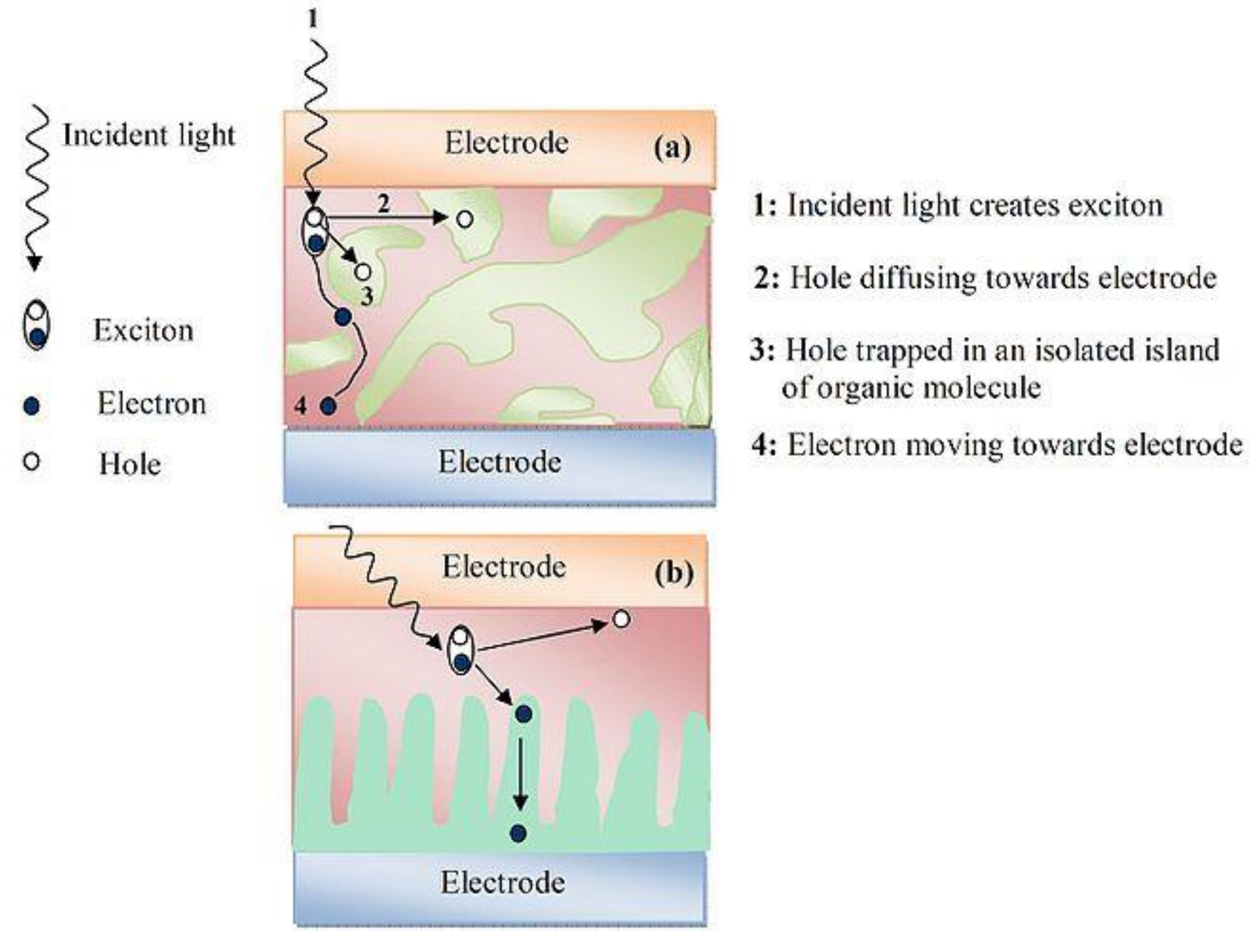
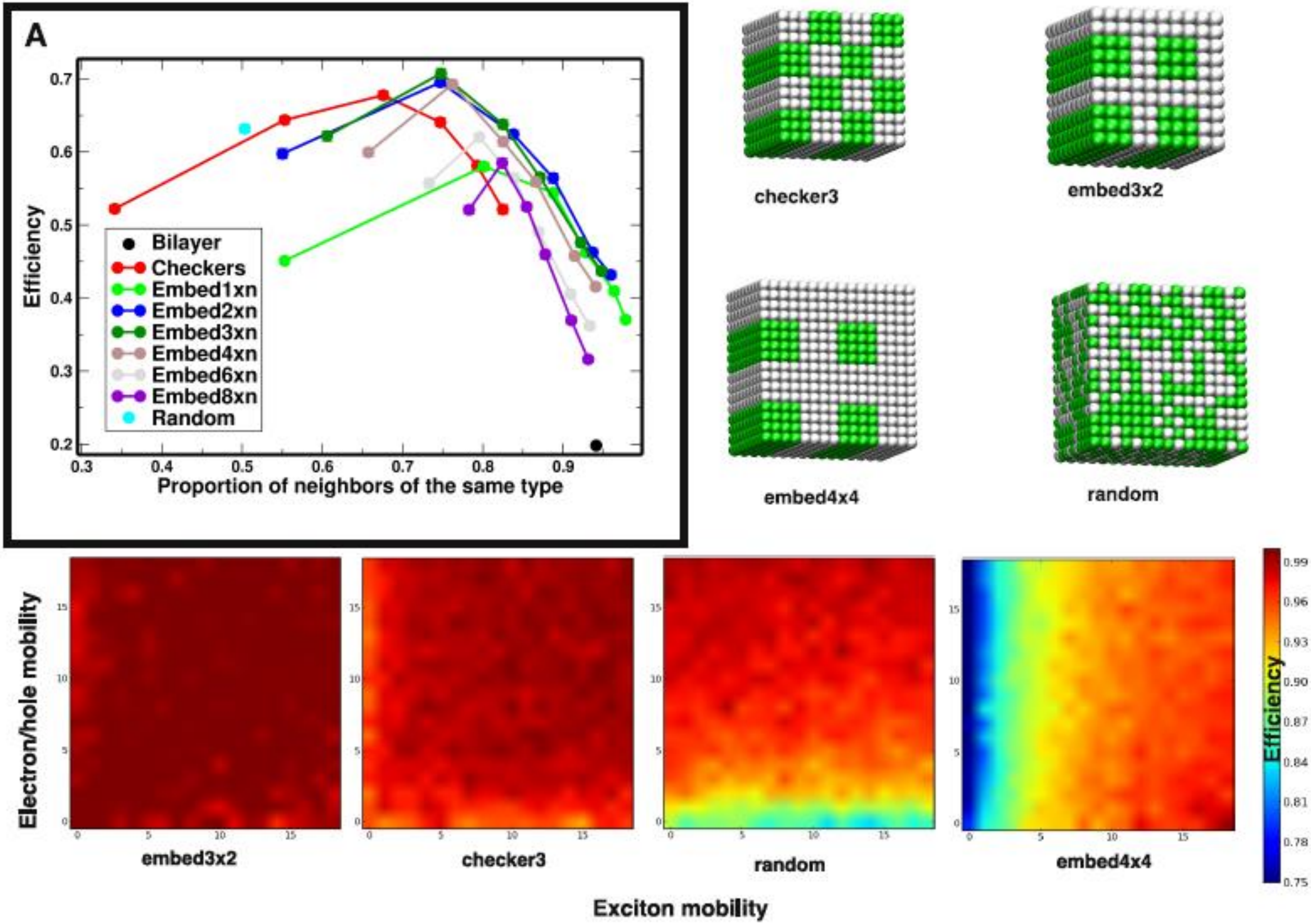


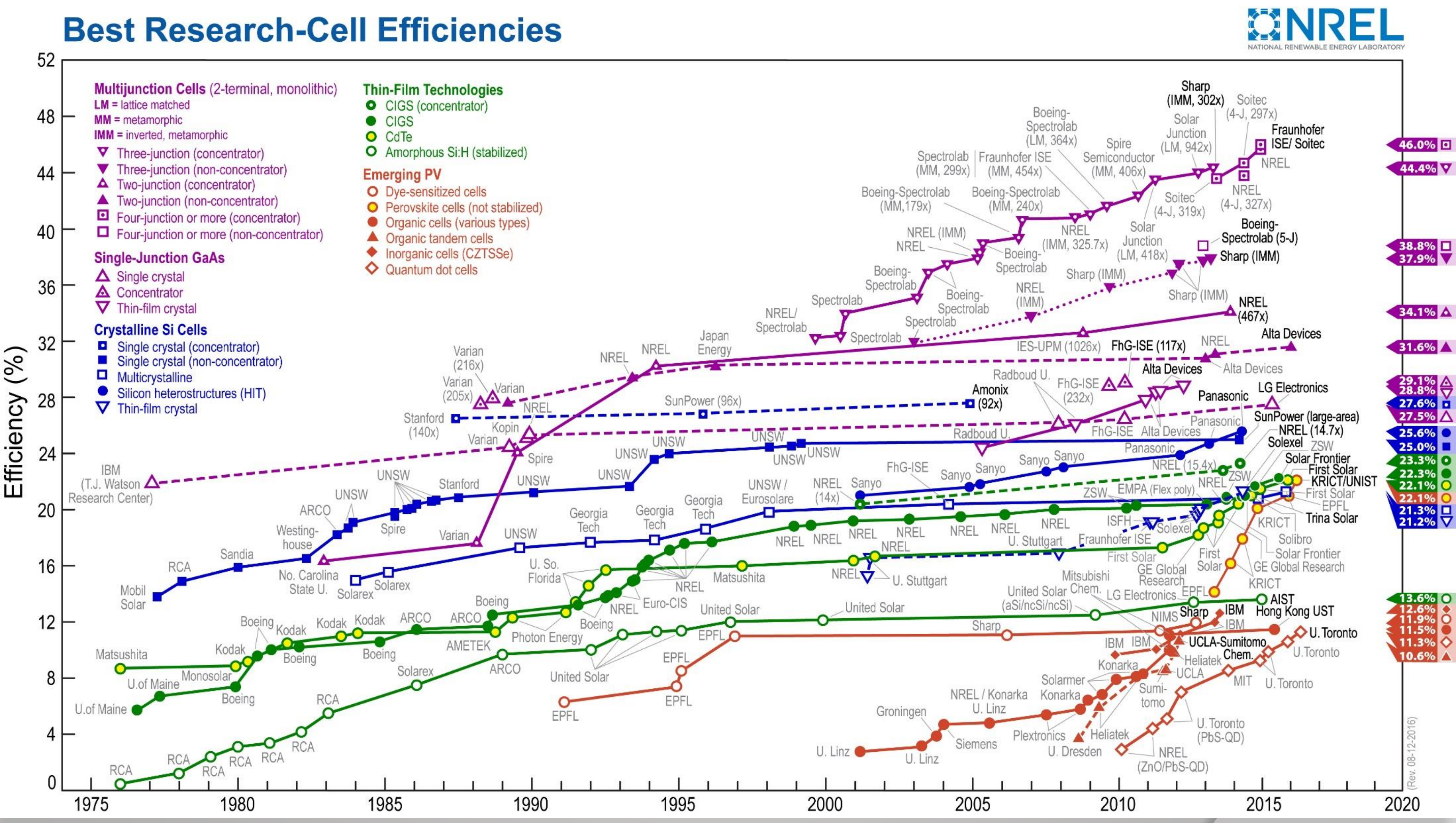
Fig 5 (a): Highly folded Hetero-junction,
(b): Hetero-junction with controlled growth


A
Efficiency
Proportion of neighbors of the same type
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
Bilayer
Checkers
Embed1xn
Embed2xn
Embed3xn
Embed4xn
Embed6xn
Embed8xn
Random
checker3
embed3x2
embed4x4
random
Electron/hole mobility
embed3x2
checker3
random
embed4x4
Exciton mobility
Efficiency
0.99
0.96
0.93
0.90
0.87
0.84
0.81
0.78
0.75

ORGANIC PHOTOVOLTAICS

- The Benefits
  - Organic chemicals are cheap ($0.10-0.50/W)
  - Flexible design (someday “paint” might work)
  - Very customizable gaps, mobility, spectra, etc.
  - Multi-junction design possible
- The Challenges
  - Poor efficiency (6.8% so far…Multi-junction?)
  - Can degrade over time (A good thing?)
  - Don’t produce as much current

ORGANIC PHOTOVOLTAICS



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- Images courtesy of Wikipedia

BNNI
Berkeley Nanosciences and Nanoengineering Institute

Computational Nanoscience Group

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- Notes
  - PCBM = [6,6]-phenyl-C_{61}-butyric acid methyl ester

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- Simulations
  - Modeled the system as a lattice of D or A, with hopping probabilities/rates
  - As predicted, large regions with little interface and small regions with too much interface have poor internal quantum efficiency (carrier pairs extracted per photon absorbed)
  - Columns of A embedded in D fared best, but most microstructures were consistent as long as the proportion of same-type neighbors was between 0.65 and 0.8
- Thermal Damage
  - We could also take a suboptimal ordered structure and damage it to create more interface
  - This led to structures of comparable efficiency without the need for nanostructuring

Parameter	Value
Carrier Separation Rate	1000 ps^{-1}
Carrier Recombination Rate	10 ps^{-1}
Exciton Decay Rate	10 ps^{-1} (5 nm)
Exciton Generation Rate	50 nm^{-2} ps^{-1}
Carrier Hopping Rate	~1 nm ps^{-1}
Electric Field Bias	5 V μm^{-1}
Temperature	0.025 eV

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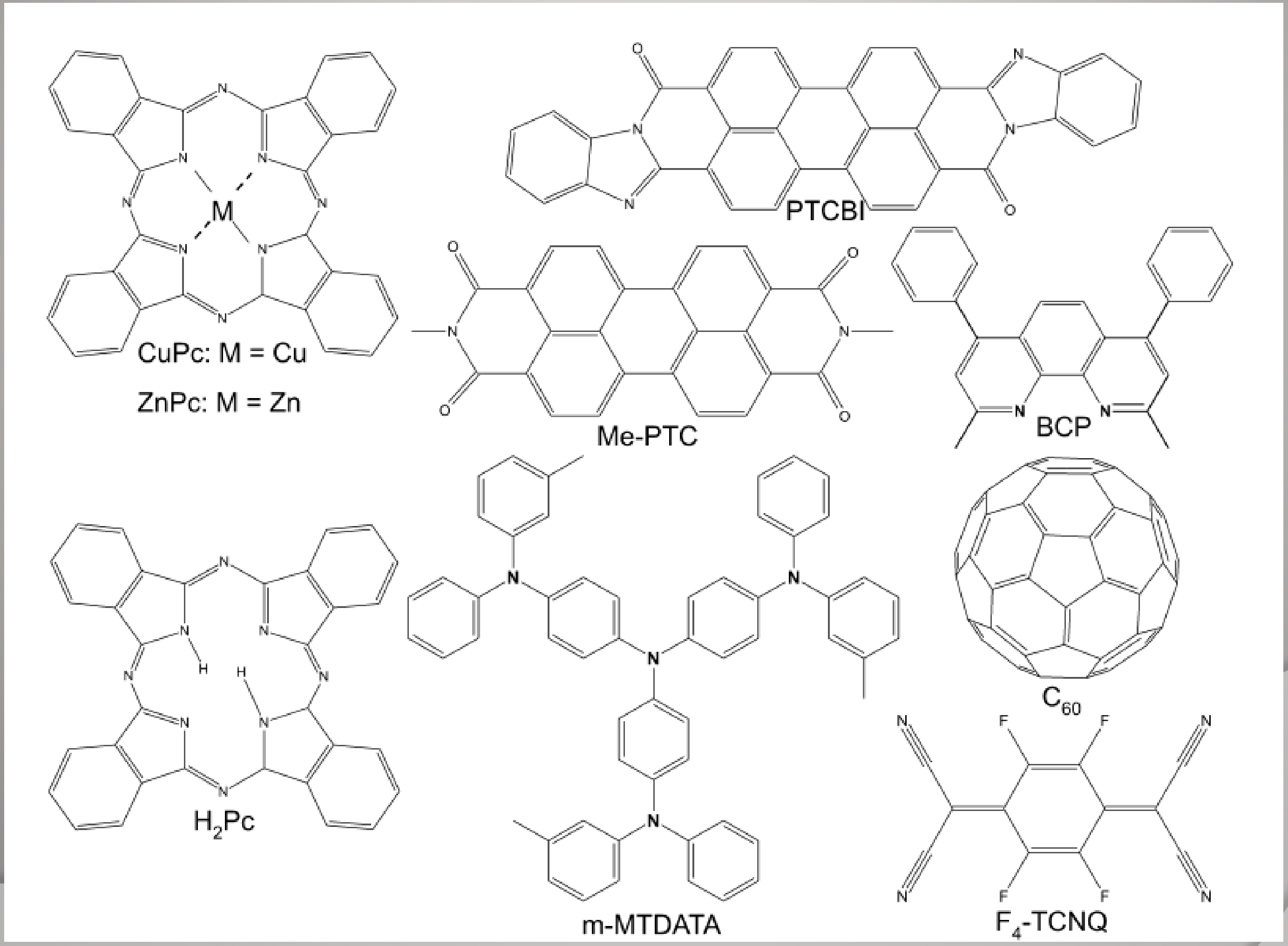
- Molecules often used in MJOPV (vapor deposition)



ORGANIC PHOTOVOLTAICS

- Molecules often used in MJOPV (solution processed)