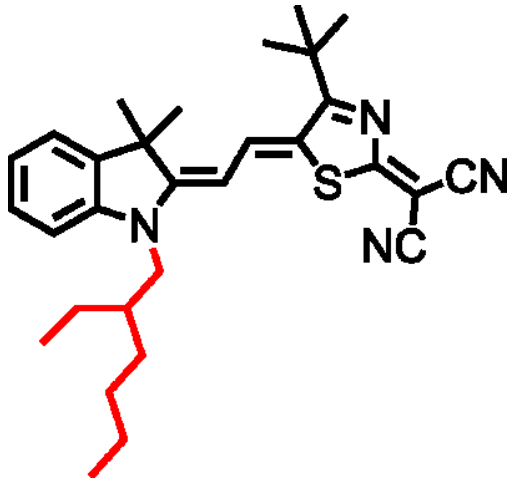
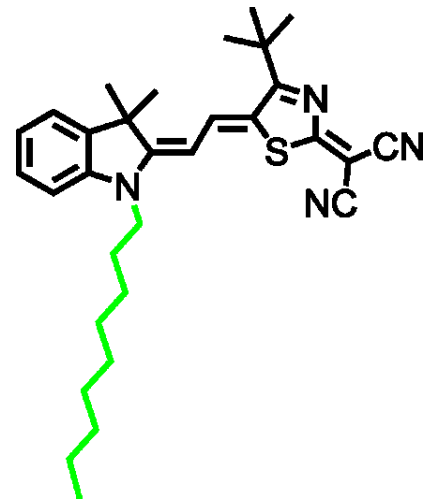
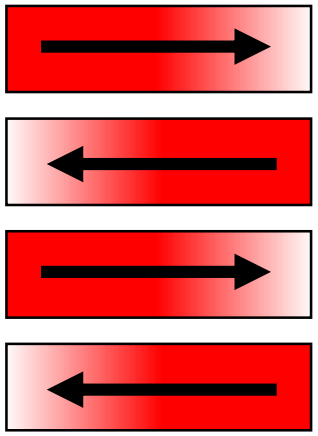
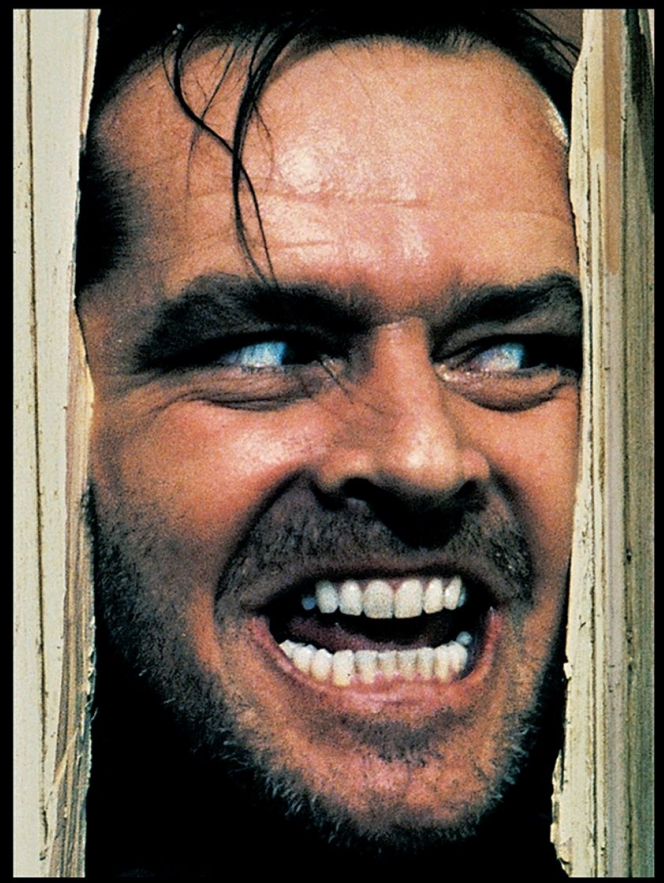




Self Assembly polar molecules: a way to control CT state formation



MEROCYANINES



Cyanine dyes - building blocks for complex matter

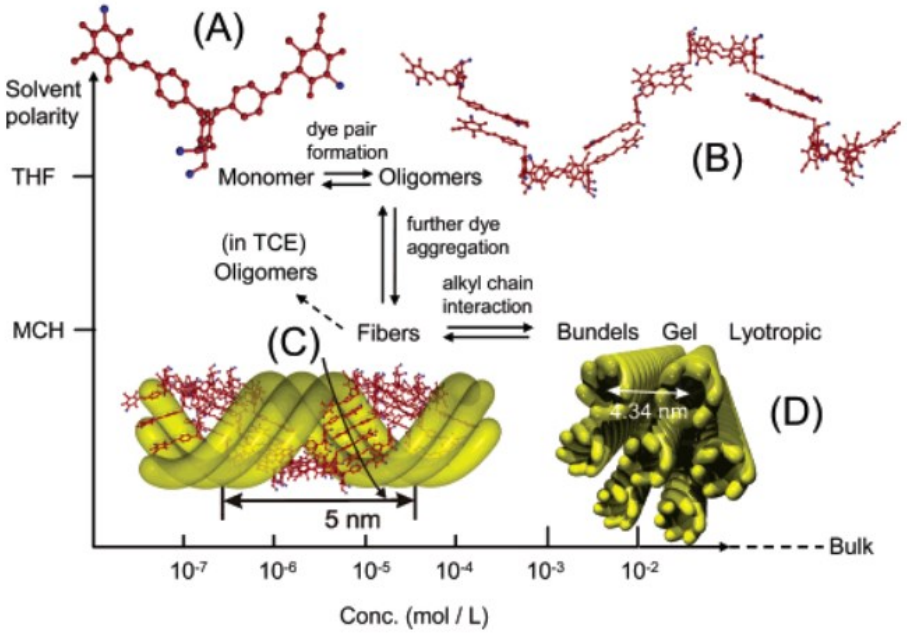
Cyanine type dyes are known from 1947

Why interesting: simple electronic structure

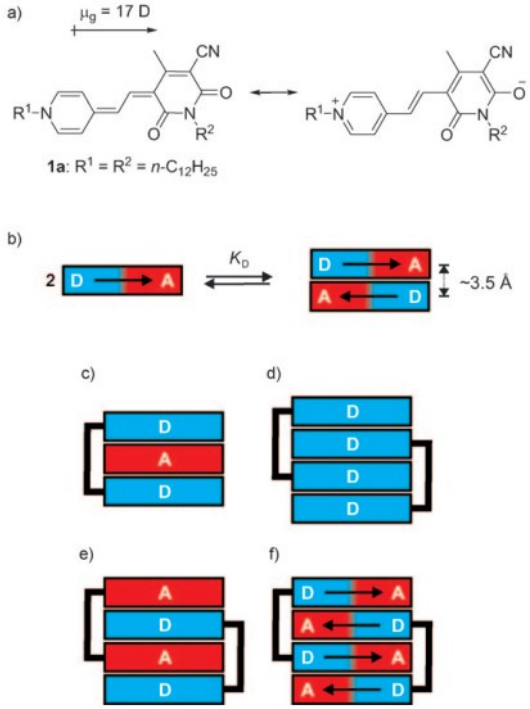
Easy to model and to synthesize

Large dipole moment – complex formation

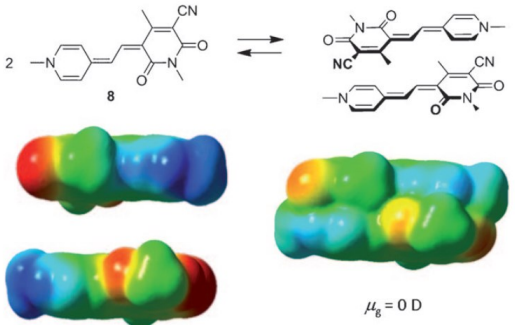
Dipole-dipole interaction



Fibers and bundles



Molecular tweezers



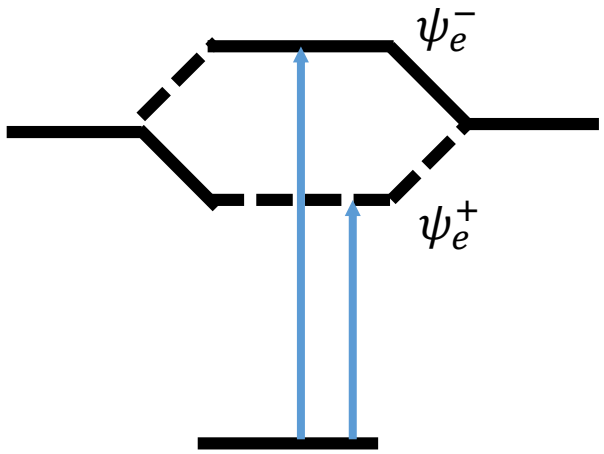
Centrosymmetric dimers

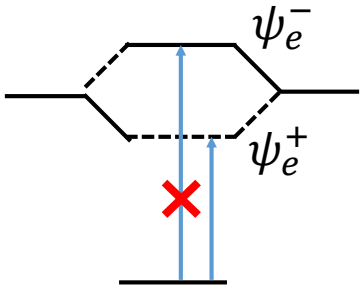
H and J aggregates

Resonance interaction of excited states

$$\psi_e^- = \frac{1}{\sqrt{2}}(\psi_1^*\psi_2 - \psi_1\psi_2^*)$$

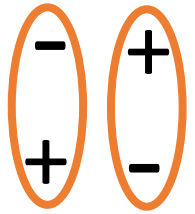
$$\psi_e^+ = \frac{1}{\sqrt{2}}(\psi_1^*\psi_2 + \psi_1\psi_2^*)$$

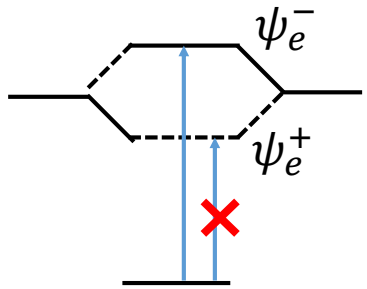




J-aggregate

ψ_e^+ is allowed

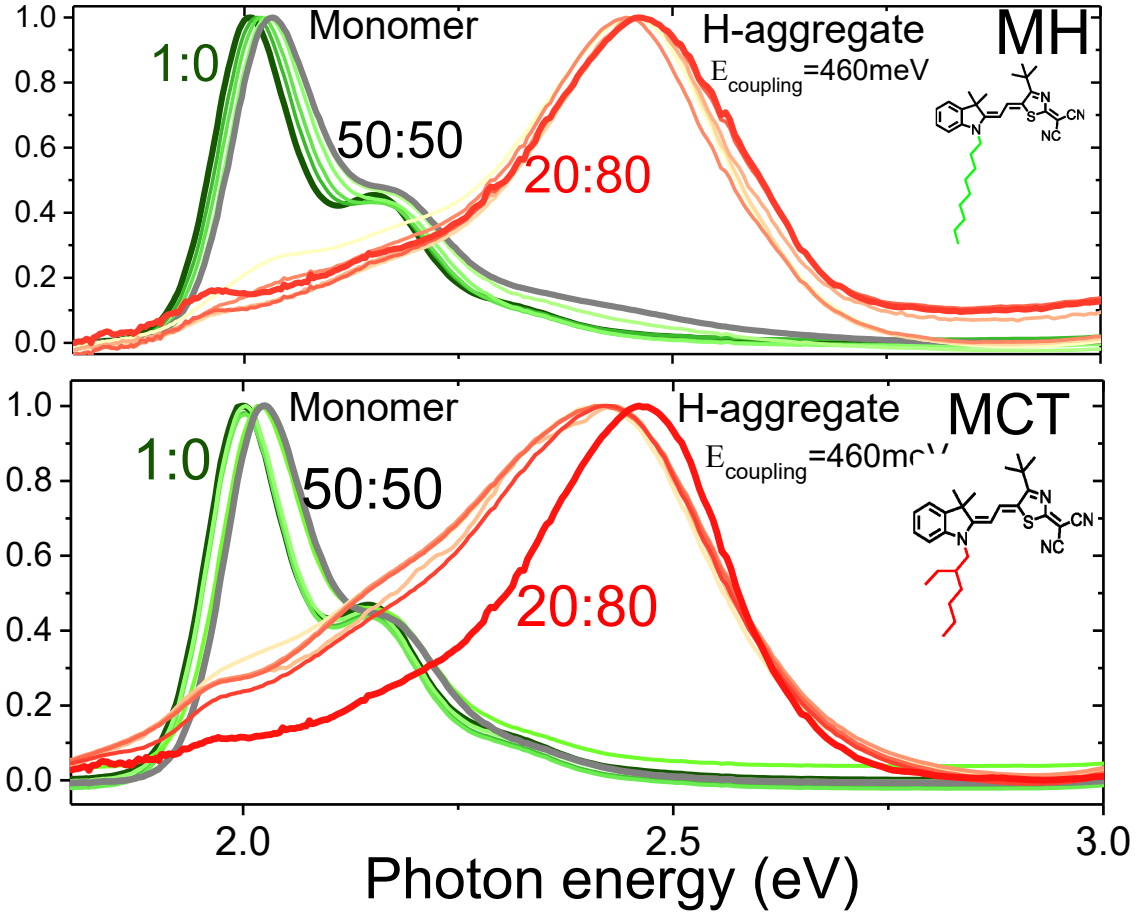




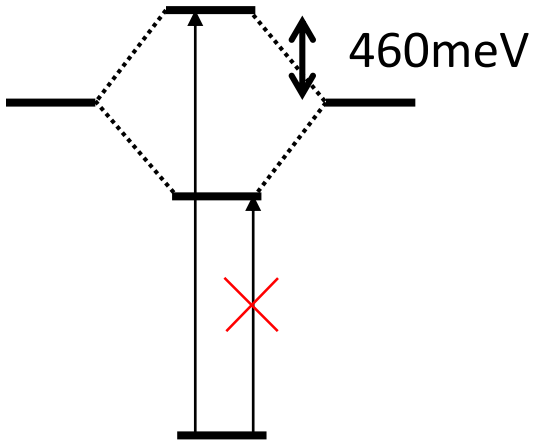
H-aggregate

ψ_e^- is allowed

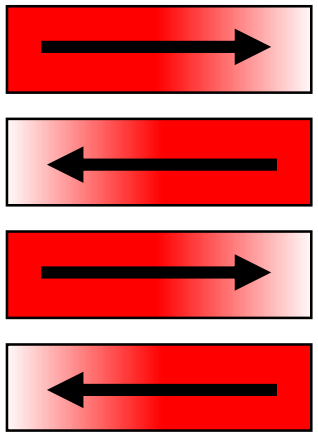
H-aggregate formation in liquid phase



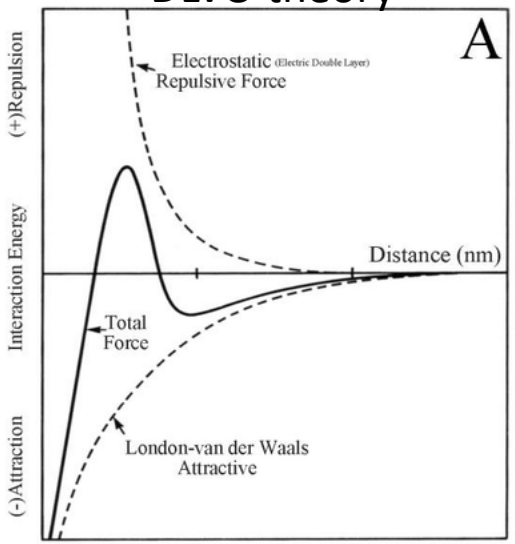
Blue shift: H-aggregate



Dipole assisted stacking

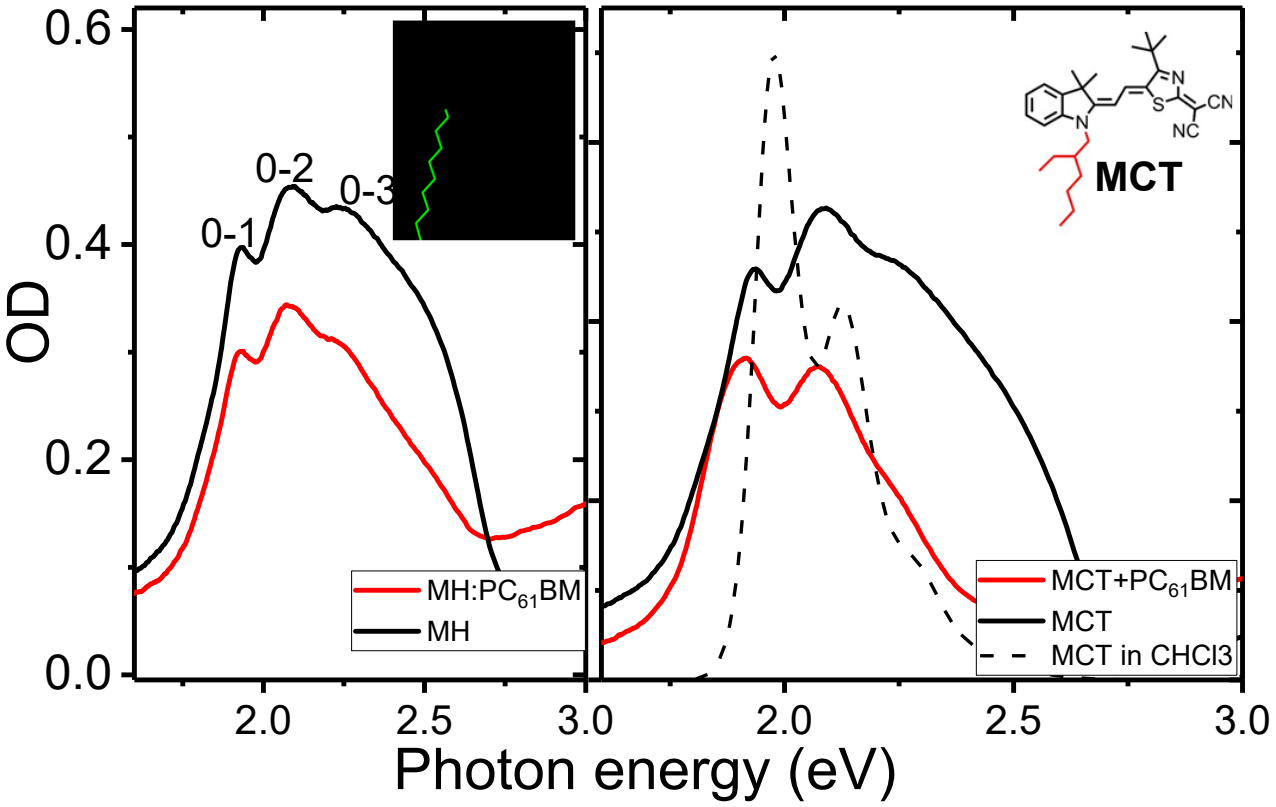


DLVO theory

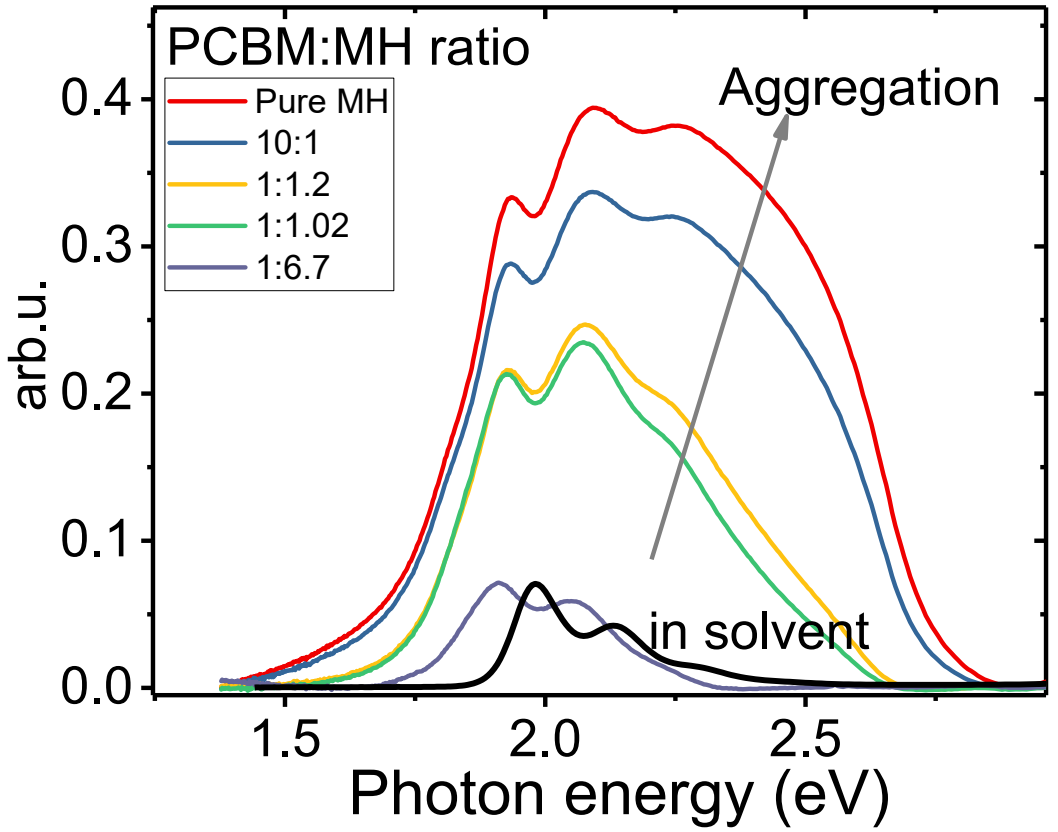


- **Identical electronic structure.**
- Double minimum structure – As expected from DLVO theory
- Different packing behaviour for MCT and MH.
- Sidechain induced difference.

Films of MCT and MH



- H-aggregation induced spectral change
- PCBM induced monomer formation

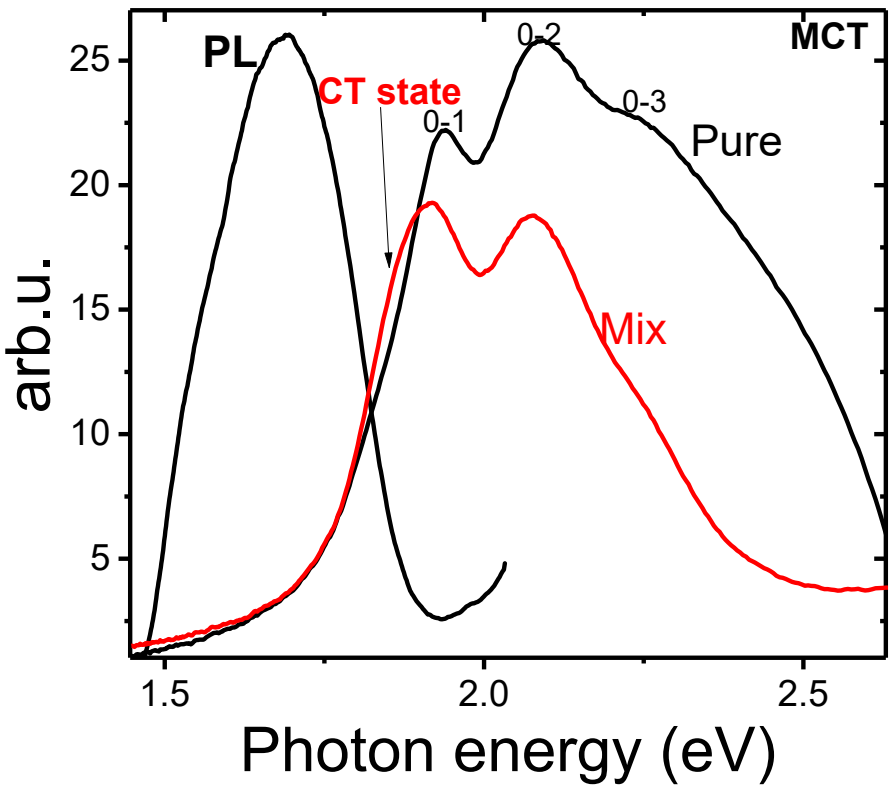


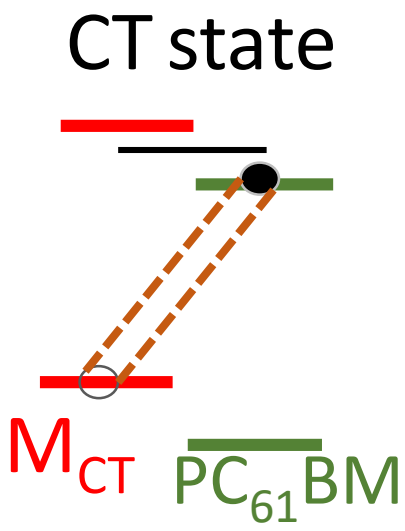
- Aggregation as function of PCBM content

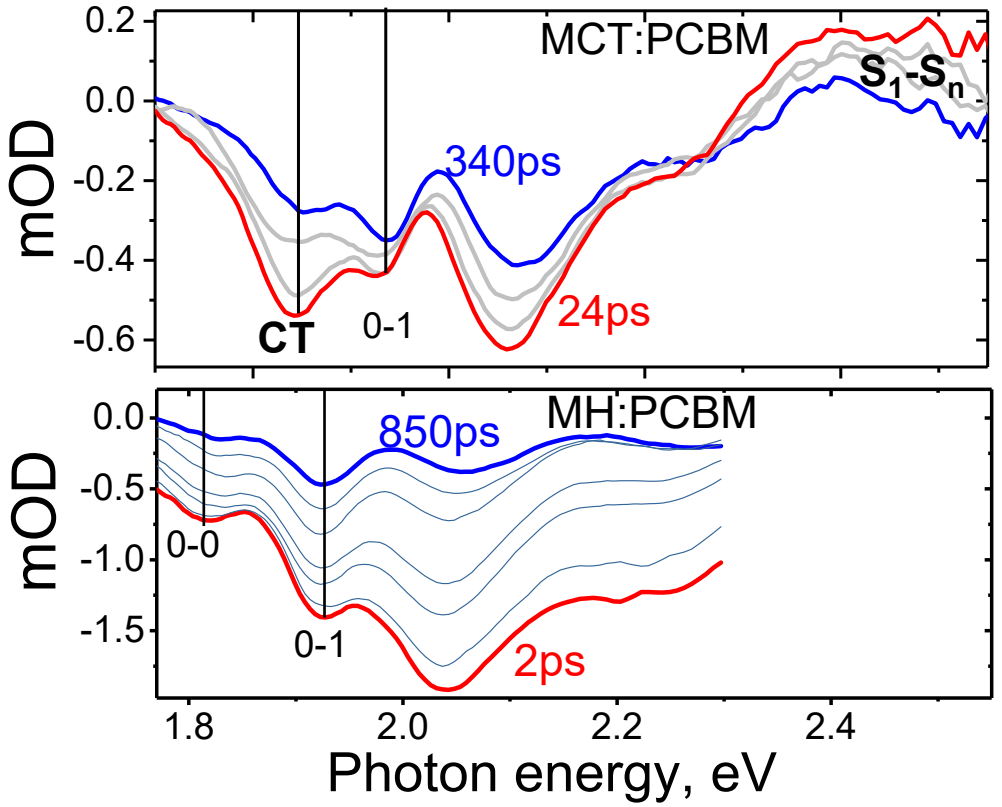
PCBM – MCT interaction is different for MCT and MH

Quantum mechanical theory should reveal the molecular arrangement of MCT:PCBM molecules

PCBM-MCT charge tranfer state

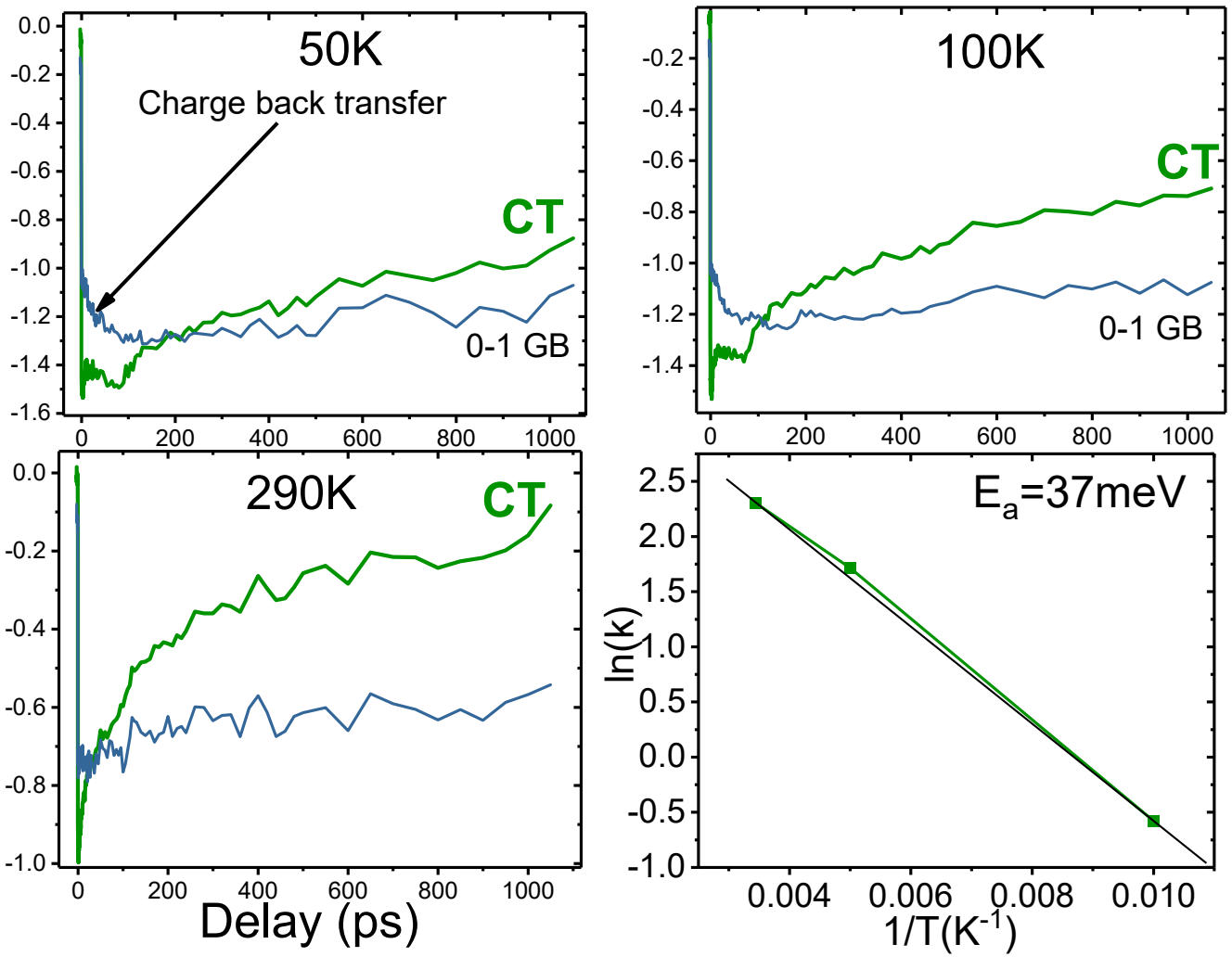




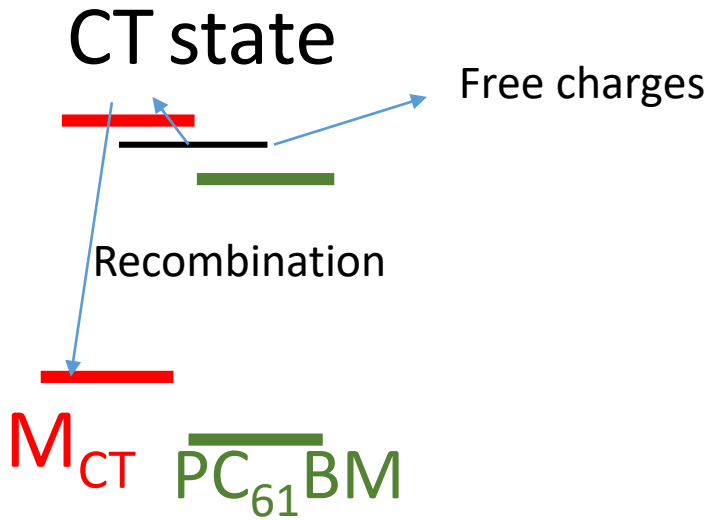


- Indication of a CT state
- CT state decays faster then GB

Activation energy of the CT state in MCT:PCBM



- CT state dissociation has an activation energy of ~37meV



Remaining questions:

- The growth component of the GB signal
- Spike anomaly at 50ps

Conclusions

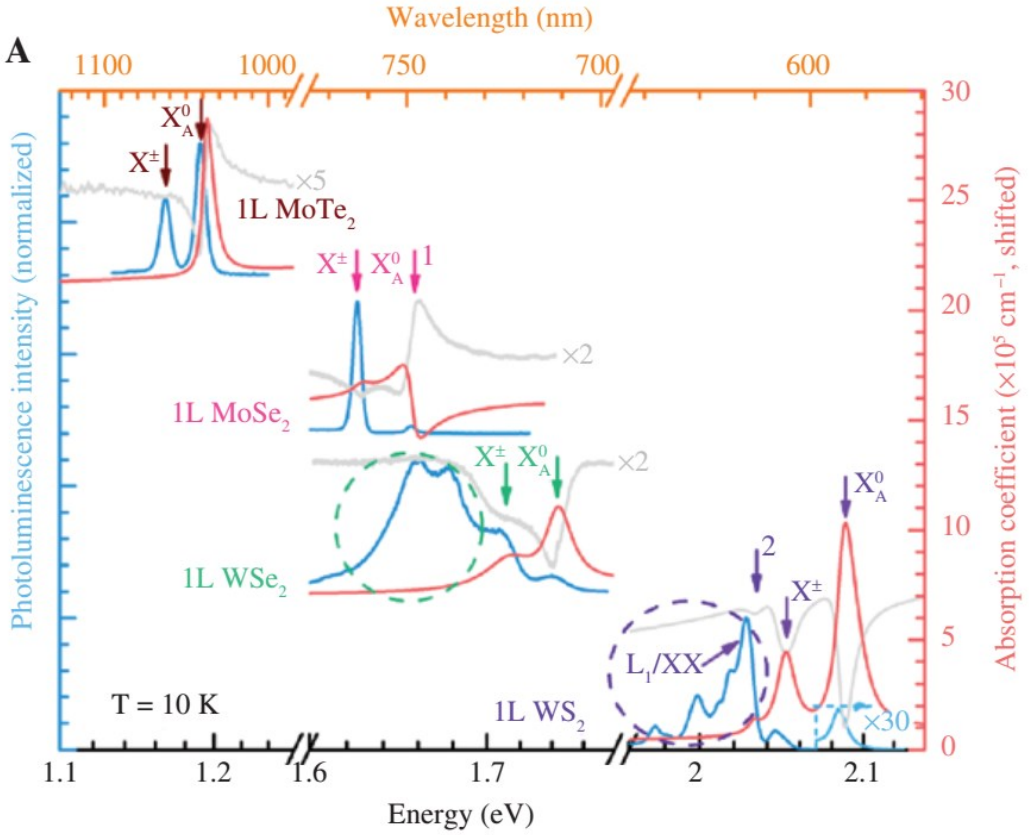
- H-aggregate formation was confirmed experimentally.
- Binding energy 460meV of Aggregates was confirmed.
- Difference in molecular packing of MCT and MH was confirmed.
- CT state observed for MCT:PCBM film with 37meV excitation energy

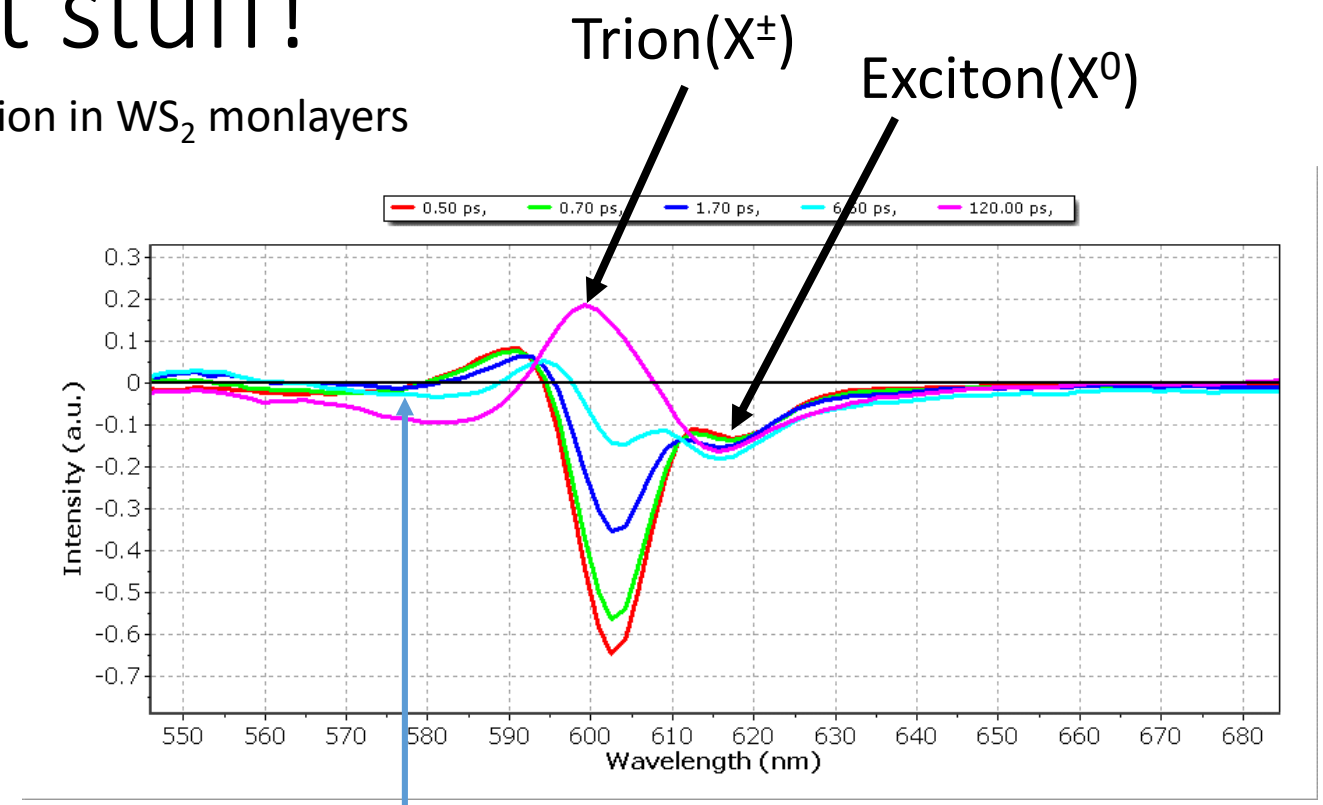
Sidechains control intramolecular interactions
and Charge transfer state formation

Thank you

Hot stuff!

Trion formation in WS_2 monlayers





Excitation