Computer Simulations of Polymers For Materials and Energy Applications

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Research Group and Projects

Theme: Computer simulations and models to address how the synthetic chemistry controls the self-assembly and properties of polymeric, colloidal and biological materials

Students, Postdocs & Ongoing Projects

Dr. Ben Hanson: Multiscale simulations of properties of polymer nanocomposites membranes.

David Trombly: Behavior and properties of protein-polysaccharide mixtures.

C. Mahajan: Properties of direct methanol fuel cell membranes.

Thomas Lewis: Dendrimer-DNA complexes for drug delivery applications.

Gunja Pandav: Self-assembly of protein-like polymers.

Dr. Victor Pryamitsyn: Simulations of properties of polymer nanocomposites.

Dr. Arun Narayanan: Simulations of properties of organic solar cells.

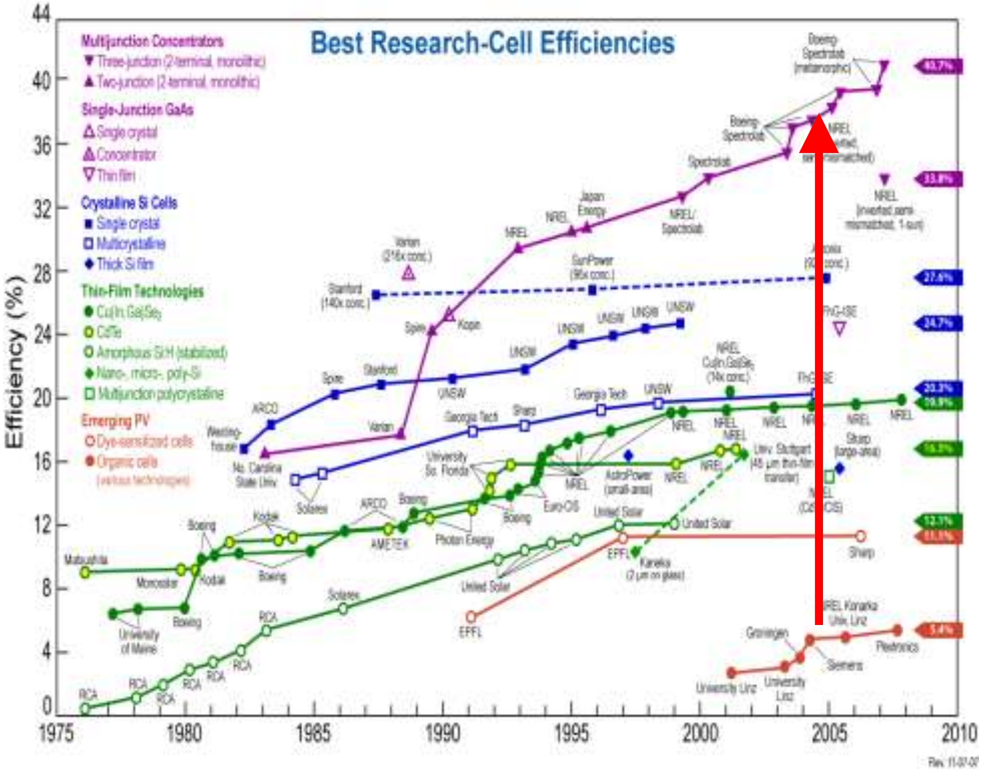
Molecularly Directed Design of Organic and Polymeric Solar Cells and LEDs

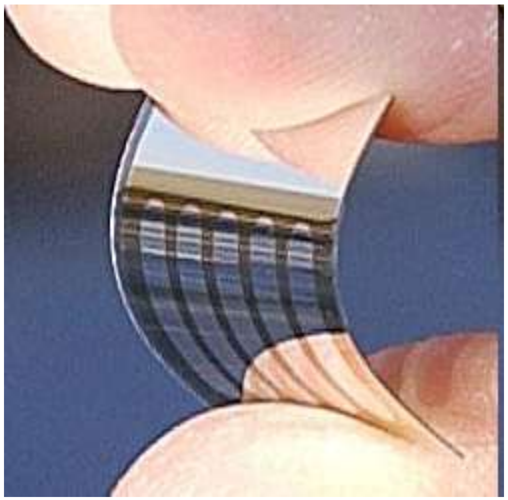
(A collaboration with Prof. Rachel Segalman, UC Berkeley and Prof. Lynn Loo, Princeton University)

Advantages of Organic Solar Cells

- Even though Si based cells have higher efficiencies, they are extremely expensive.

- Polymer solar cells are cheaper to manufacture, easy to process, and are flexible.

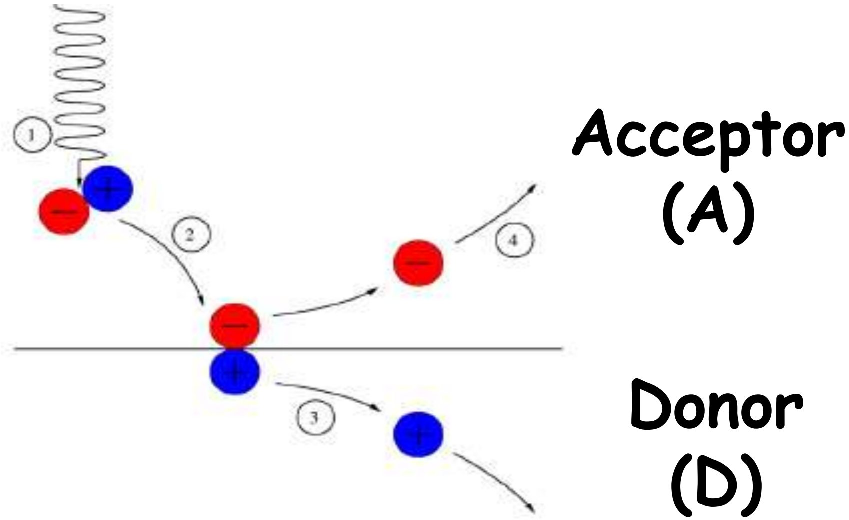




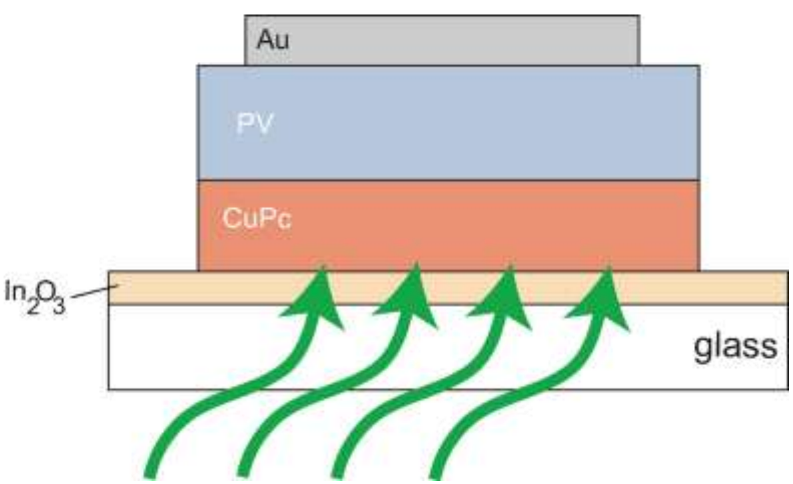
Polymer Solar cells:
Efficiencies ~ 5-6 %

Morphology Requirements

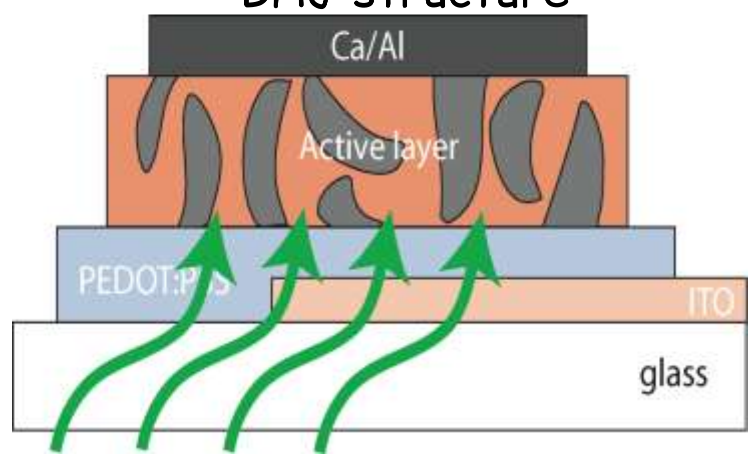
- ❑ Photogeneration leads to bound electron-hole pair called as exciton.
- ❑ Continuous interface between donor and acceptor between the electrodes (heterojunction)
- ❑ Lengthscale of phase separation ~ exciton diffusion length (10-20 nm)



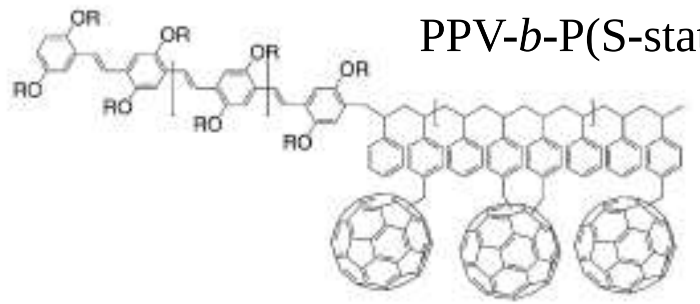
Bilayer structure



BHJ structure

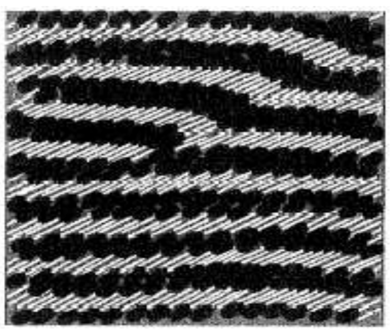


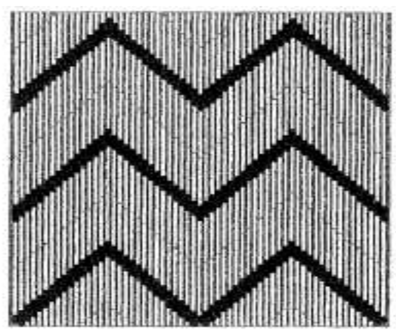
Semiconducting Block Copolymers

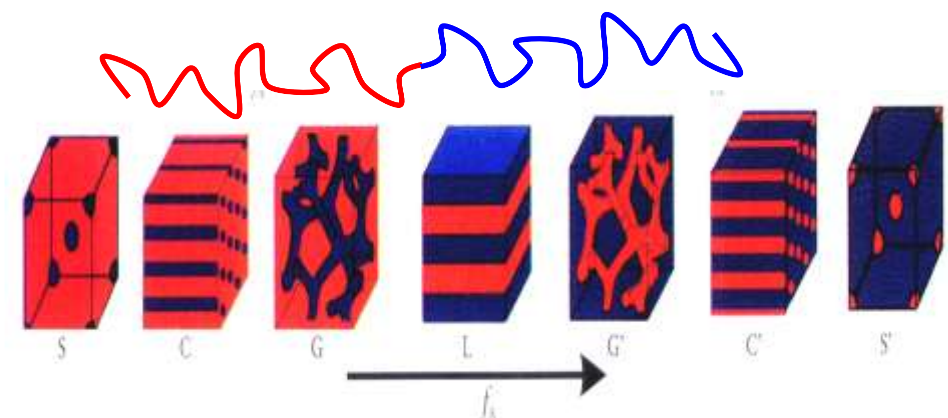


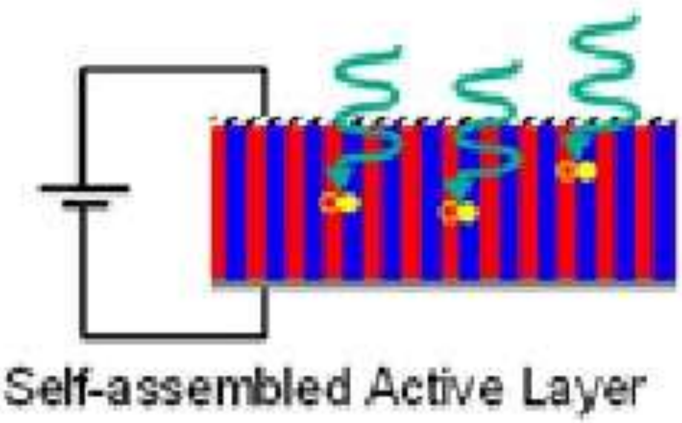
PPV-*b*-P(S-stat-C_{60})

- Such polymers self-assemble into complex morphologies







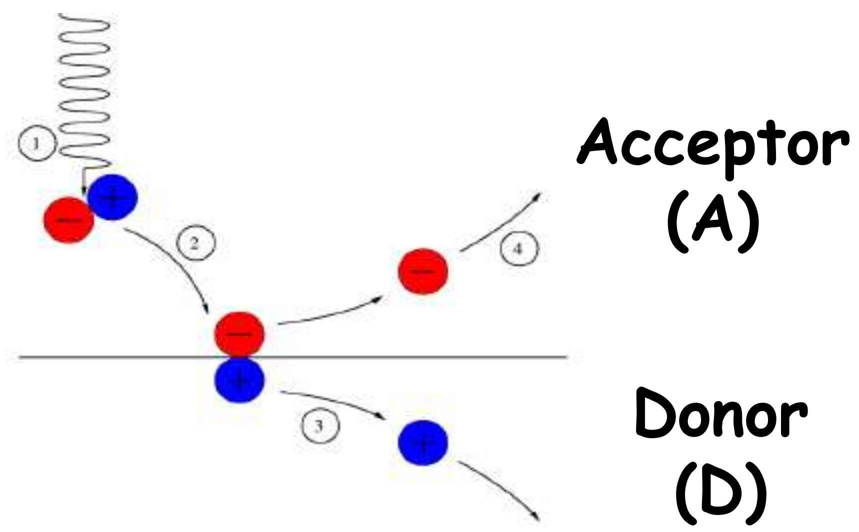


- Mechanisms underlying such self-assembly ?

- Model or predict the statistical mechanics of such morphologies?

Transport/Device Models

- Photogeneration leads to bound electron-hole pair called as exciton.
- Continuous interface between donor and acceptor between the electrodes (heterojunction)
- Lengthscale of phase separation ~ exciton diffusion length (10-20 nm)



- Fundamental statistical mechanical models for such transport processes and the impact of different morphologies ?

- Identify optimum morphologies and materials for organic solar cells and LEDs ?

Tools of The Trade