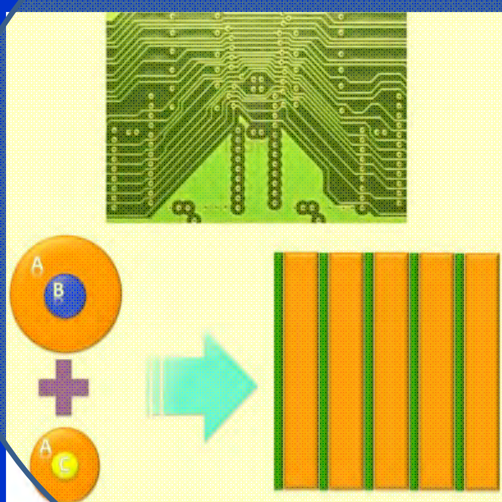
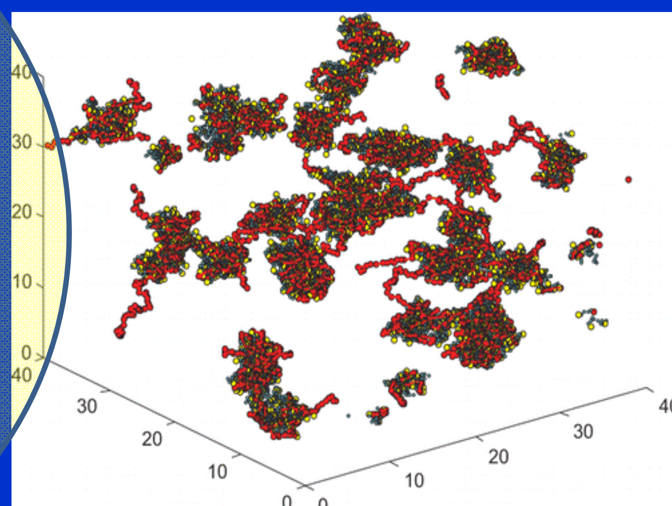
Modeling and computer simulations of polymer materials

Structure of Multicomponent Polymers

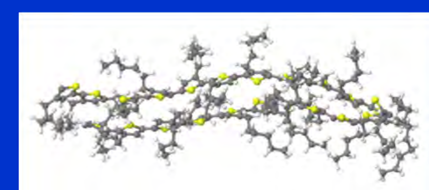
Lithography Applications

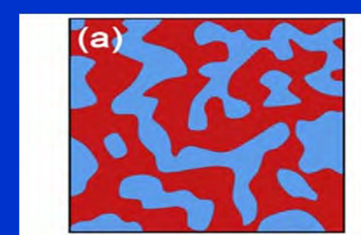


Protein-Polymer Mixtures



Morphology Control in Organic Solar Cells



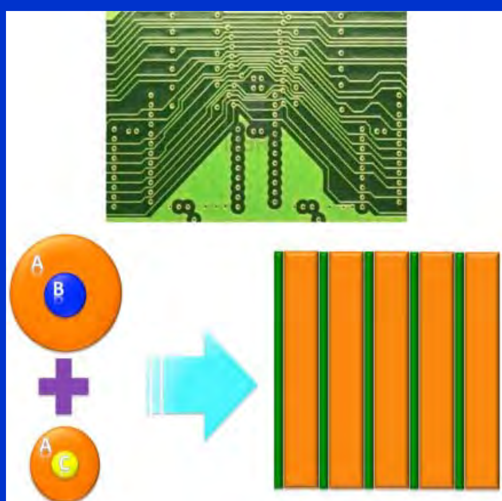


Ellison and Willson – Control surface interactions to facilitiate next generation semiconductor applications

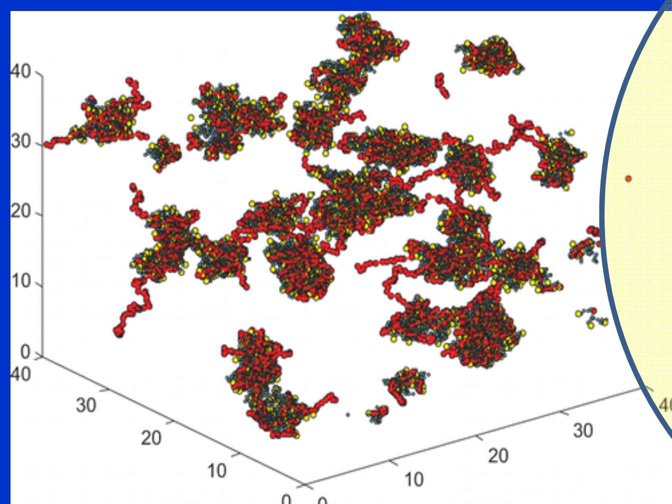
Modeling and computer simulations of polymer materials

Structure of Multicomponent Polymers

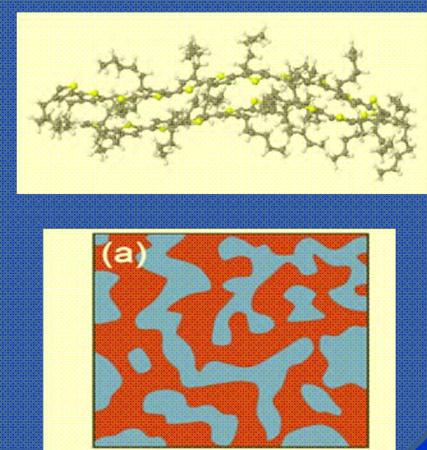
Lithography Applications



Protein-Polymer Mixtures



Morphology Control in Organic Solar Cells



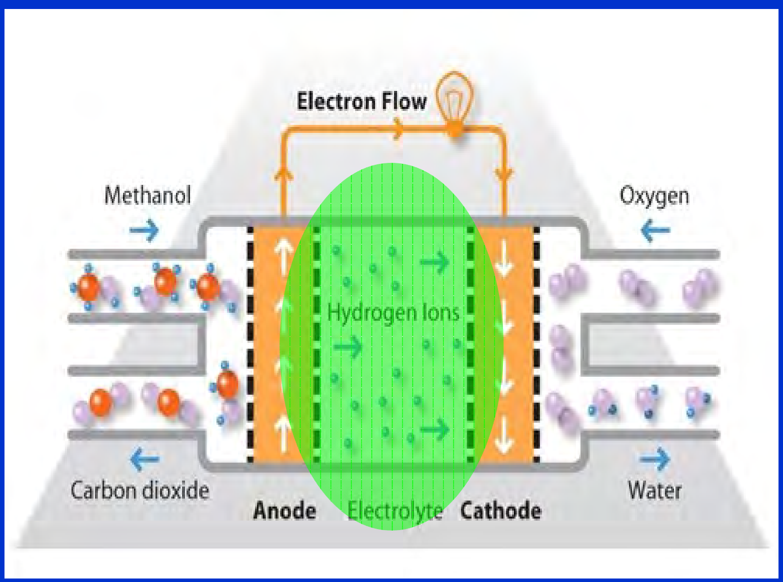
Verduzo (Rice) – Design block copolymer additives to enhance efficiencies of solar cells.

Modeling and computer simulations of polymer materials

Transport Properties of Polymer Materials

Modeling and computer simulations of polymer materials

Transport Properties of Polymer Materials



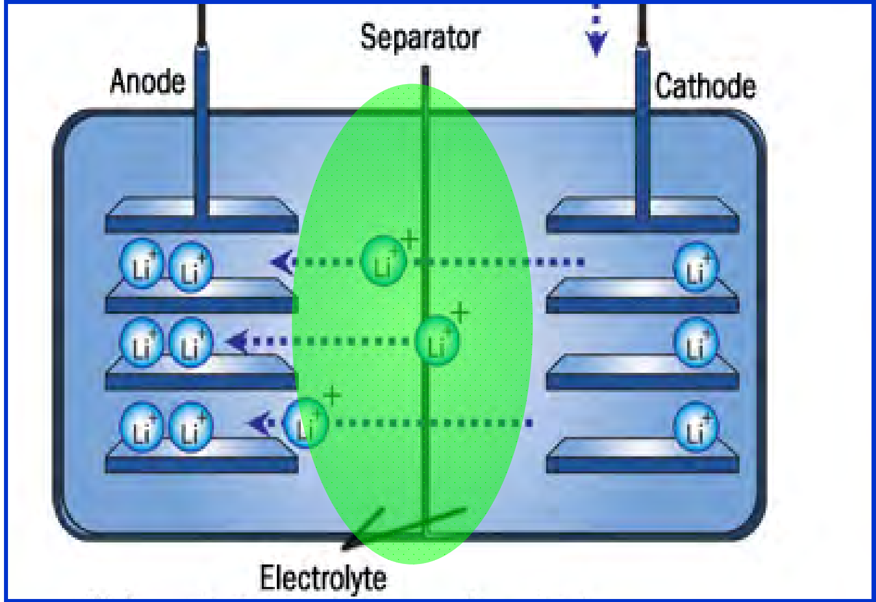
Methanol Fuel Cells

Water, Protons, Methanol

- Influence of morphology on membrane properties?
- Optimize the membrane design?

Modeling and
computer simulations
of polymer materials

Transport Properties of Polymer Materials



Battery Electrolytes

Cations and Anions

Water Purification

Water and Salt

We study…

Fundamental mechanisms underlying properties

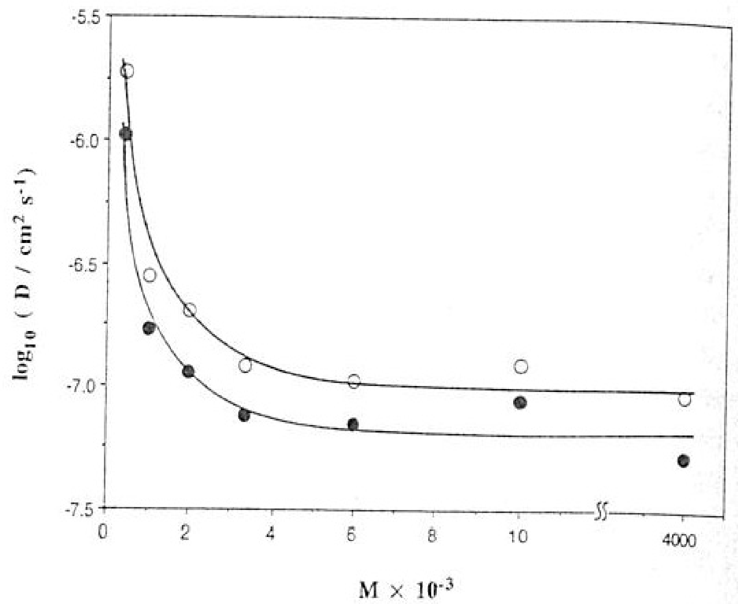
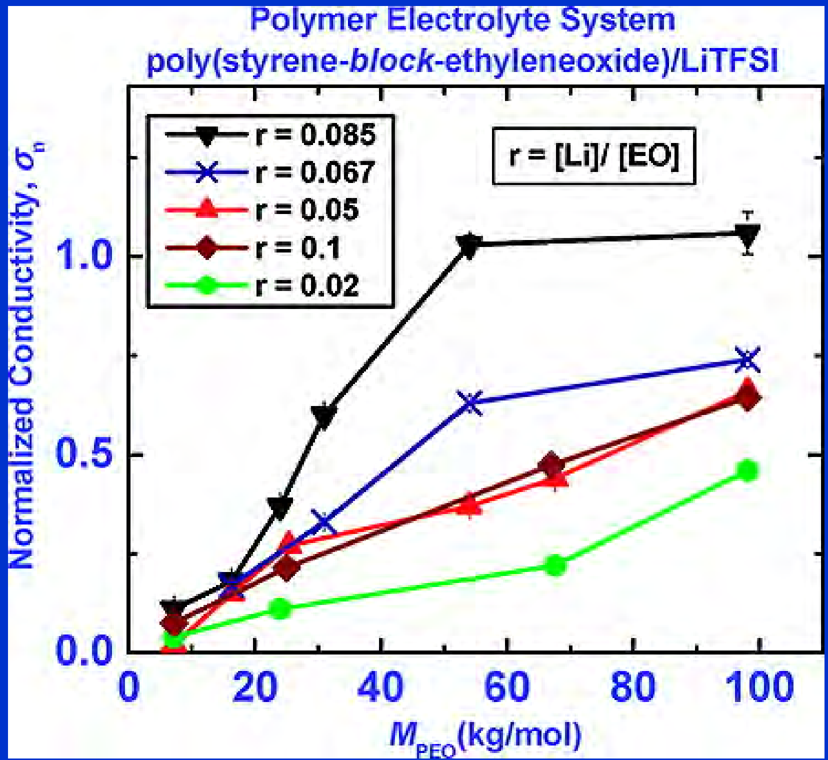


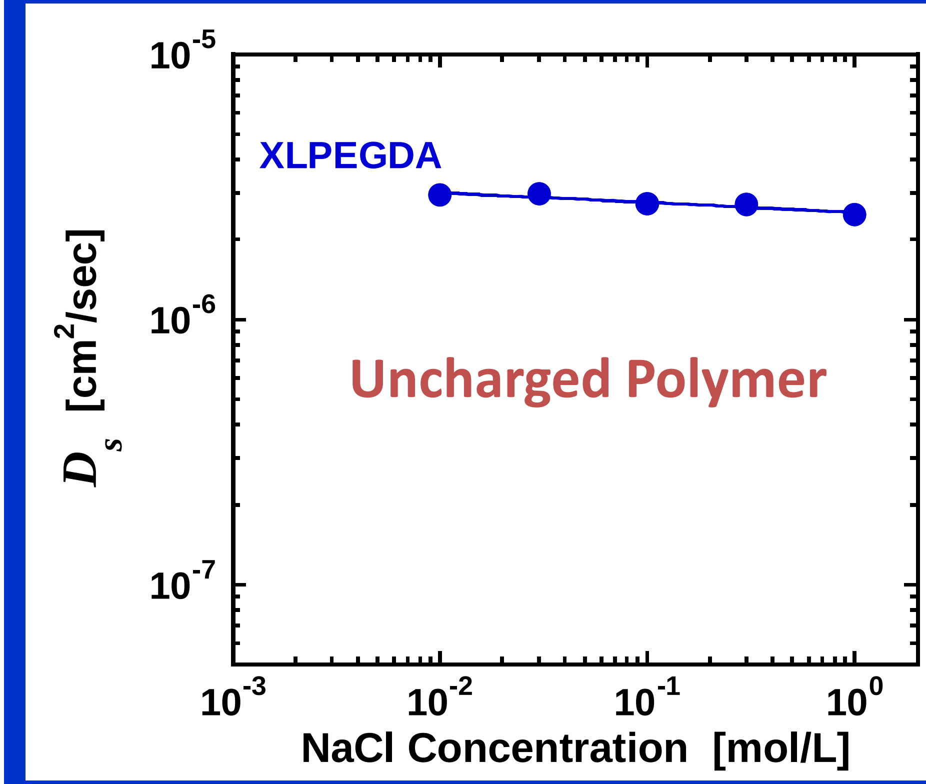
Fig. 6. Variation of $\log_{10}D$ for ^7Li in PEO–$LiCF_3SO_3$ with an ethylene oxide to lithium ratio of 20:1 at 70°C (●) and 90°C (○) as a function of molecular weight, *M*.

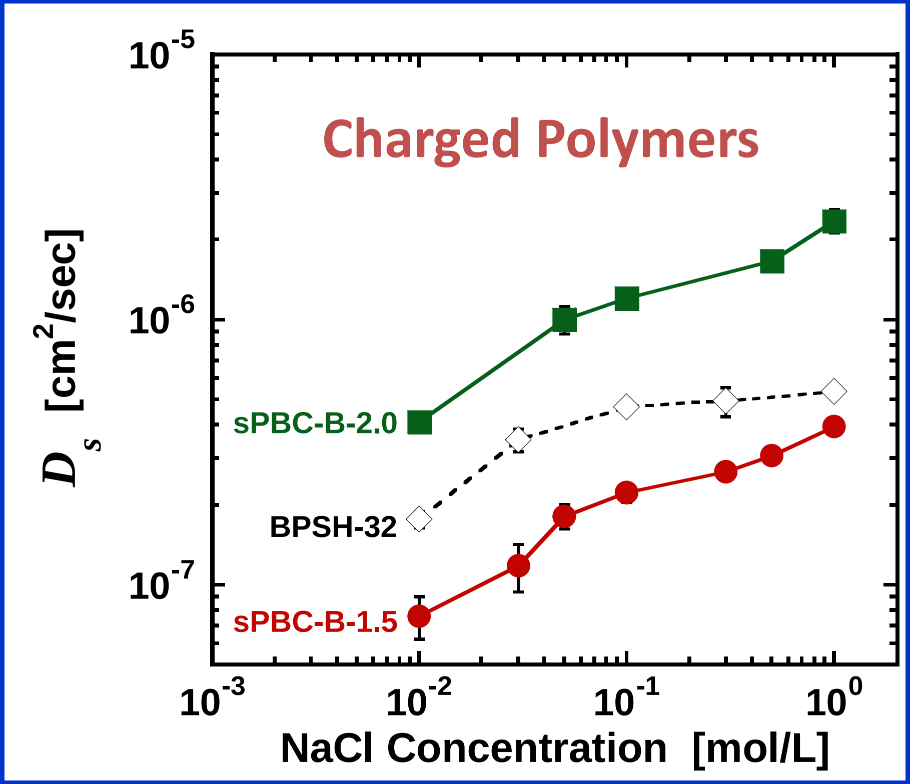


Lithium Ion Conductivities in Battery Materials

We study…

Fundamental mechanisms underlying properties

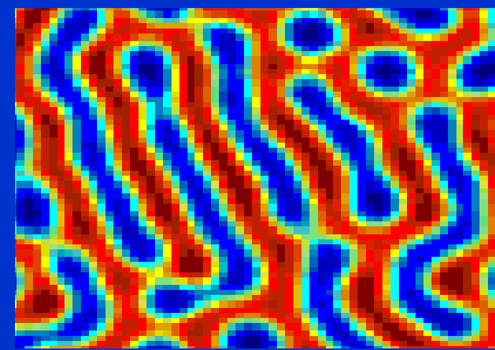




Salt Diffusion in Reverse Osmosis Membranes

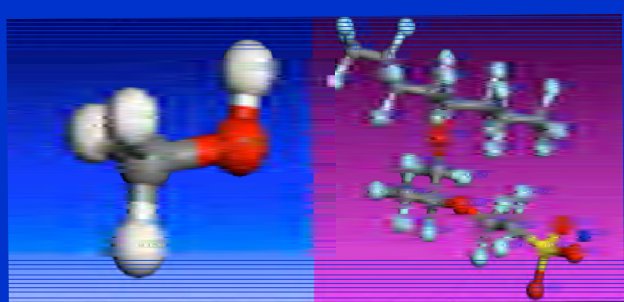
Through…

Computer Simulations and New Methods



Coarse-grained Scale

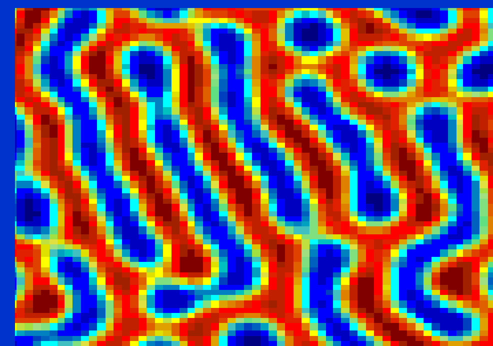
Coarse-graining Techniques



Atomistic Scale Simulations

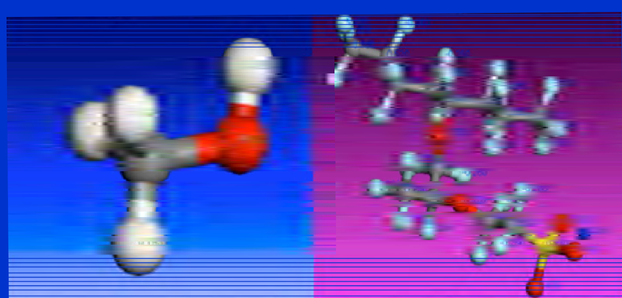
Through…

Computer Simulations and New Methods



Coarse-grained Scale

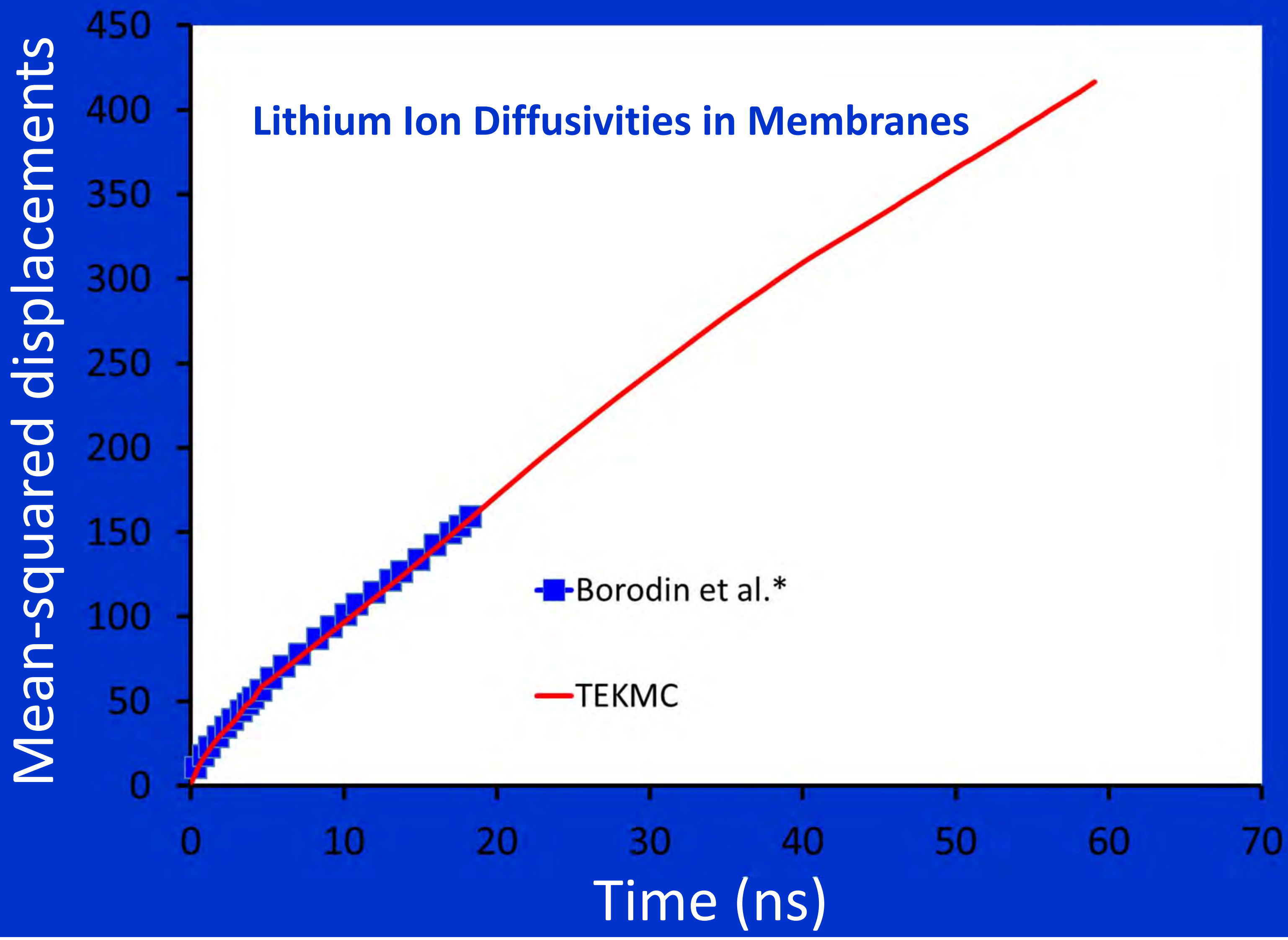
Fine-graining Techniques



Atomistic Scale Simulations

Through…

Computer Simulations and New Methods



Through…

New Models

$$\nabla.(\varepsilon\nabla\psi) = -(p-n)$$

Poisson's equation

$$\frac{\partial n}{\partial t} = D(\mathbf{E}) - R(n,p) + \frac{1}{q}\nabla[qn\boldsymbol{\mu}_{\mathbf{n}}.\mathbf{E} + k_B T\boldsymbol{\mu}_{\mathbf{n}}.\nabla n]$$

Electron (n)

$$\frac{\partial p}{\partial t} = D(\mathbf{E}) - R(n,p) - \frac{1}{q}\nabla[qp\boldsymbol{\mu}_{\mathbf{p}}.\mathbf{E} - k_B T\boldsymbol{\mu}_{\mathbf{p}}.\nabla p]$$

Hole (p)

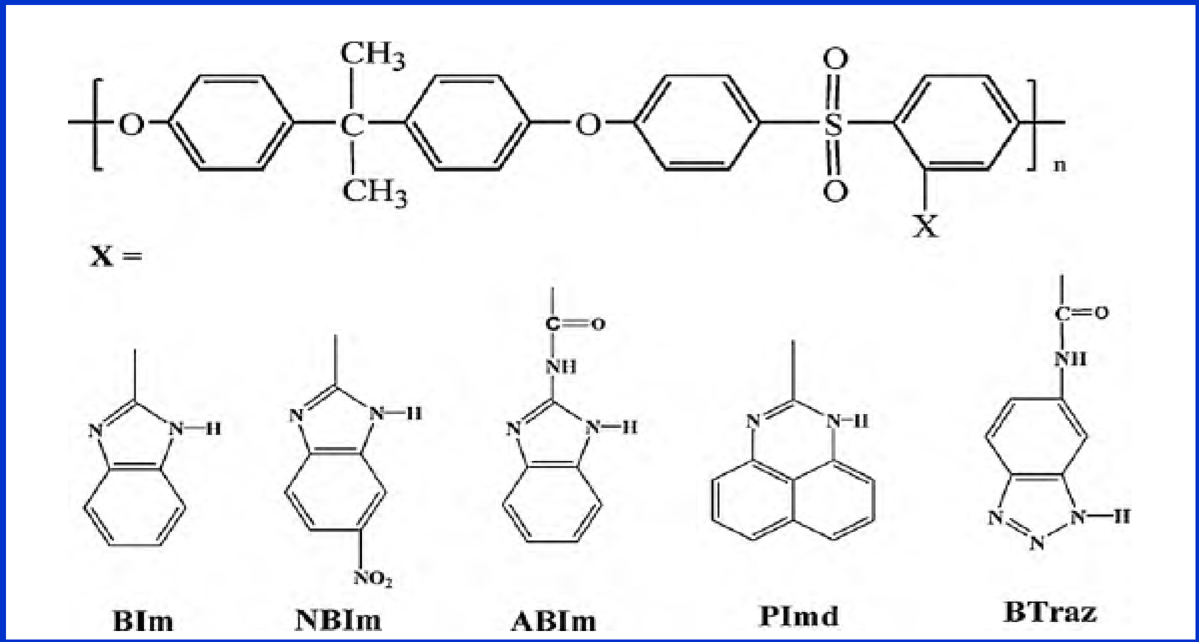
$$\frac{\partial x}{\partial t} = G(\mathbf{r}) + \frac{1}{4}R(n,p) - R_d(x) - D(\mathbf{E}) - \frac{1}{q}\nabla[-k_B T\boldsymbol{\mu}_{\mathbf{x}}.\nabla x]$$

Exciton (x)

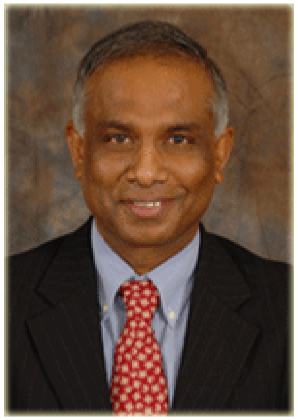
Model for device characteristics of OPV materials

We predict…

Means to improve properties



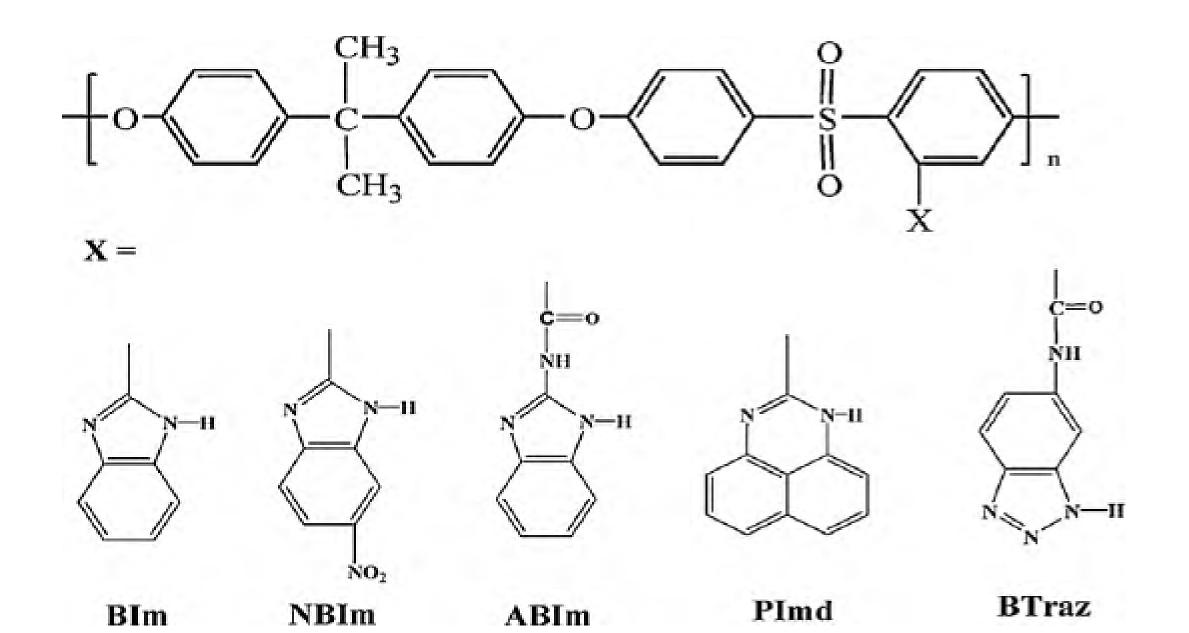
Base
ABIm ↓
BIm
BTraz
NBIm ↑
PImd

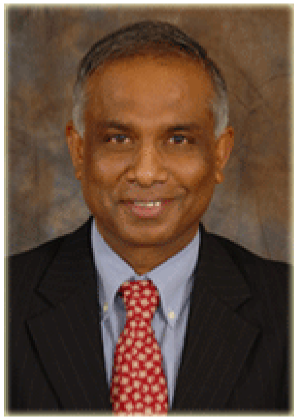


Manthiram, ME/CHE

We predict…

Means to improve properties





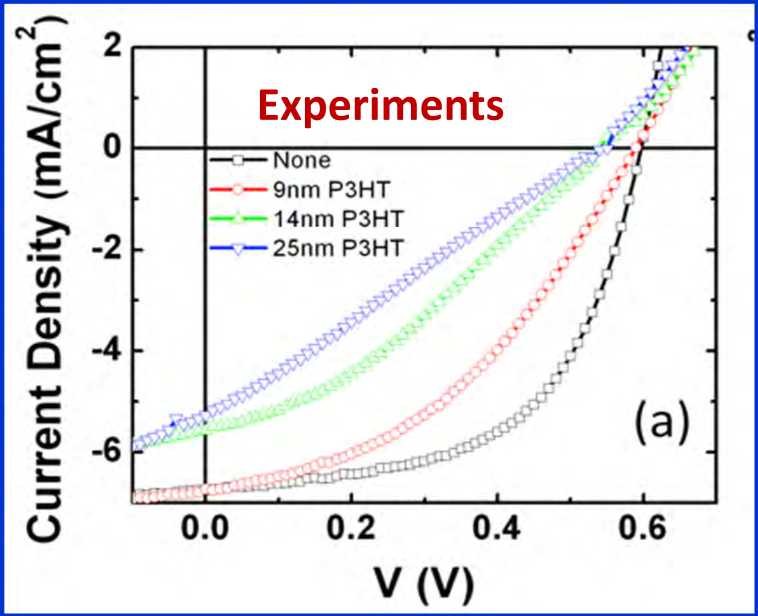
Manthiram, ME/CHE

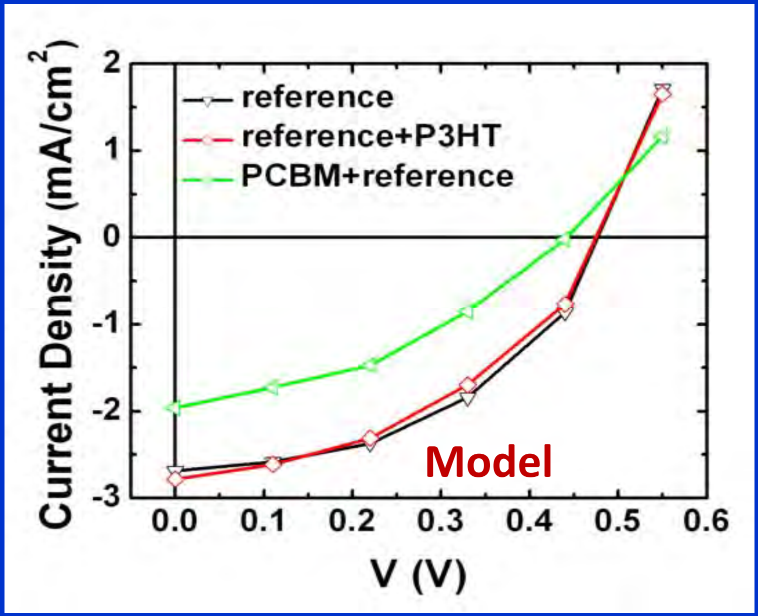
Base	Methanol Crossover Current Density (mA/cm²)
ABIm ↓	95
BIm	91
BTraz	87
NBIm ↑	87
PImd	77

We predict…

Mechanisms underlying experimental results

Lynn Loo, Princeton Univ





Where are we going?

Where are we going?