Polymerforschung – Perspektiven

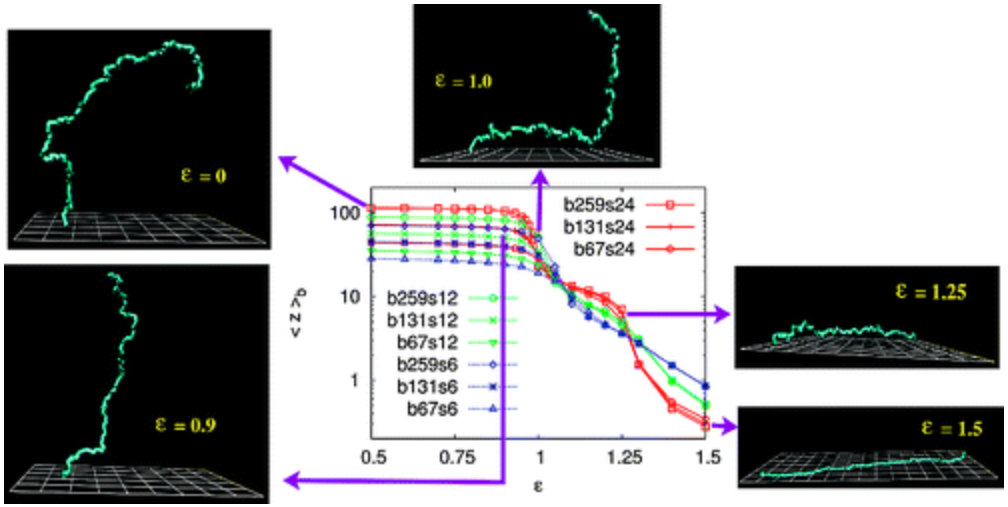
K.Kremer

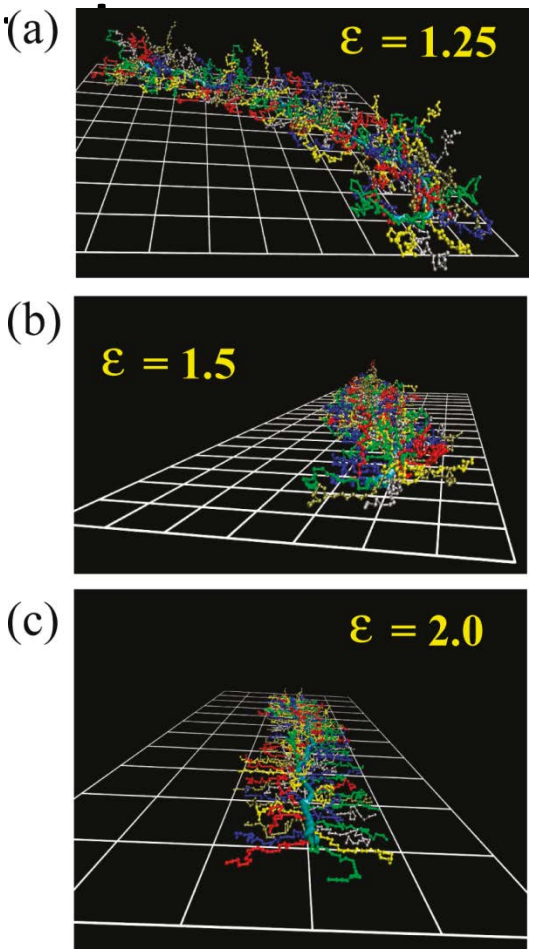
- Classical generic models, Scaling concepts
- Role of “new” chemistry, functional systems
- Glasses
- Polymer electronics
- Processes

Classical generic models, Scaling concepts

- Search for critical exponents, scaling

Transition from research focus to research



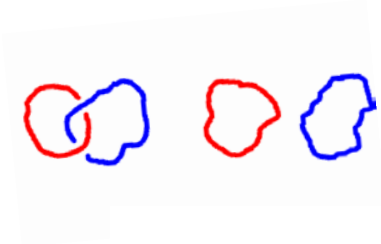


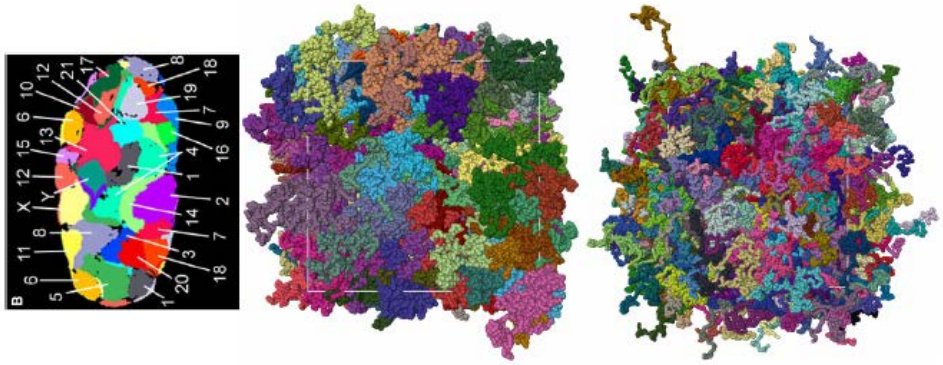
Structure of Bottle Brush Polymers on Surfaces: Weak versusStrong Adsorption
Hsiao-Ping Hsu, Wolfgang Paul, and Kurt Binder, JPCB 2011

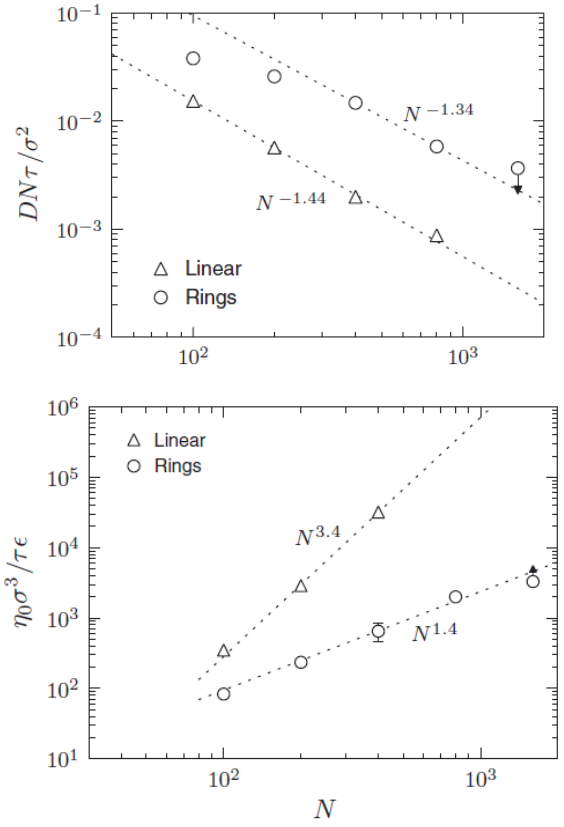
Classical generic models, Scaling concepts

- Search for critical exponents, scaling

Transition from research focus to research tool







Chicken nucleus -- melt on rings -- melt of liner polymers

Grosberg, KK et al, 2012

Classical generic models, Scaling concepts

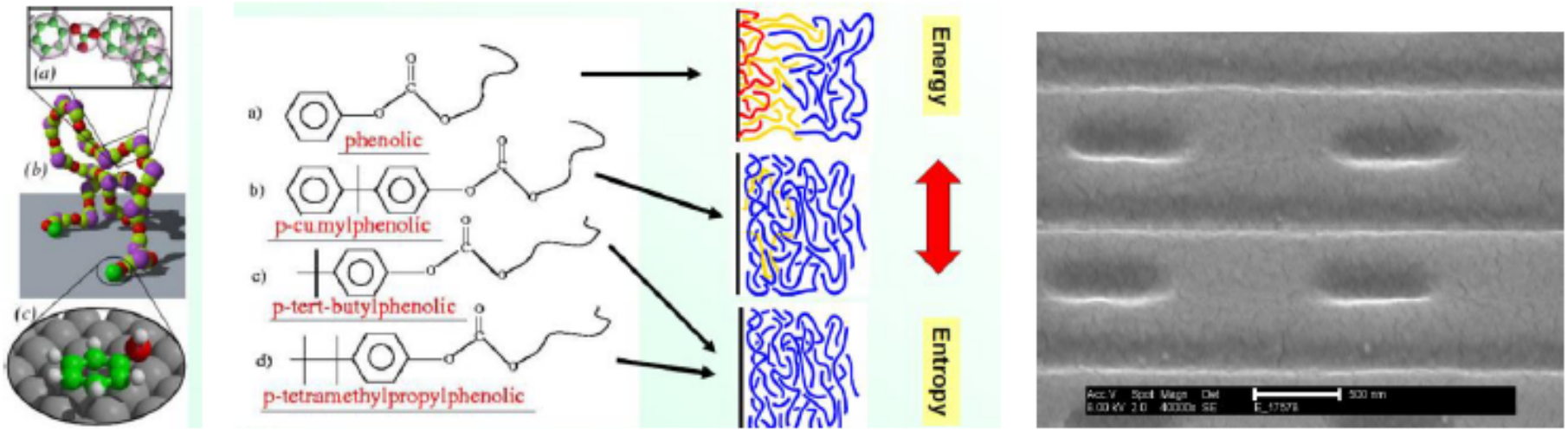


Fig. 3: Illustration of a coarse grained simulation of polycarbonate with all atom resolution for the interaction with a Ni surface. Depending on chain ends, the morphology is dominated by irreversible sticking of chain ends or entropy dominated packing of chains close to the surface. (JACS 2005). On the right hand side is electron microscope image of a DVD shown with the data pits and the guiding grove for the laser beam shown. The scale bar corresponds to 500nm.

Leon, Delle Site, KK, JACS 2005

Role of “new” chemistry, functional systems

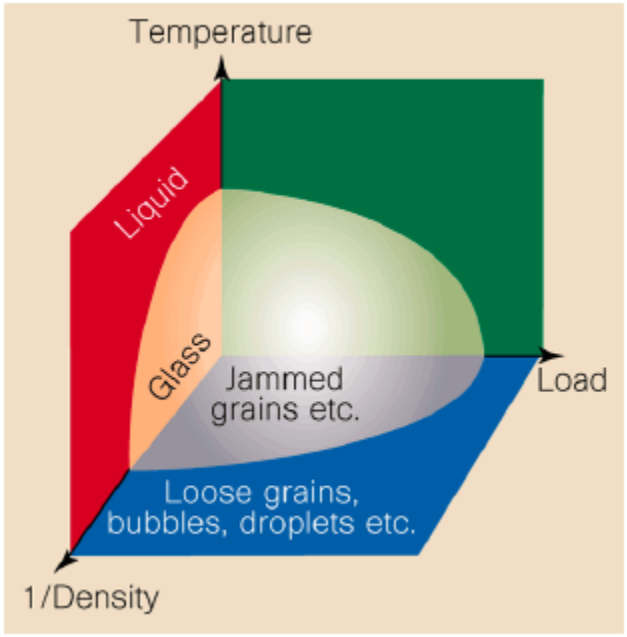
- For functional systems, new chemistry needed
- Links to bio related methodologies/models
- Hierarchical assemblies…

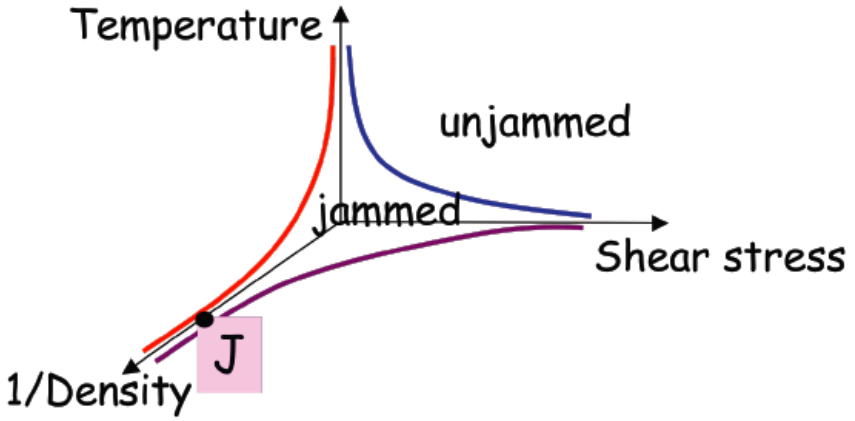
BUT

- Does industry want new polymers?
- What can be done with known, accepted chemistry?
- Which role could physics play here?

Glasses

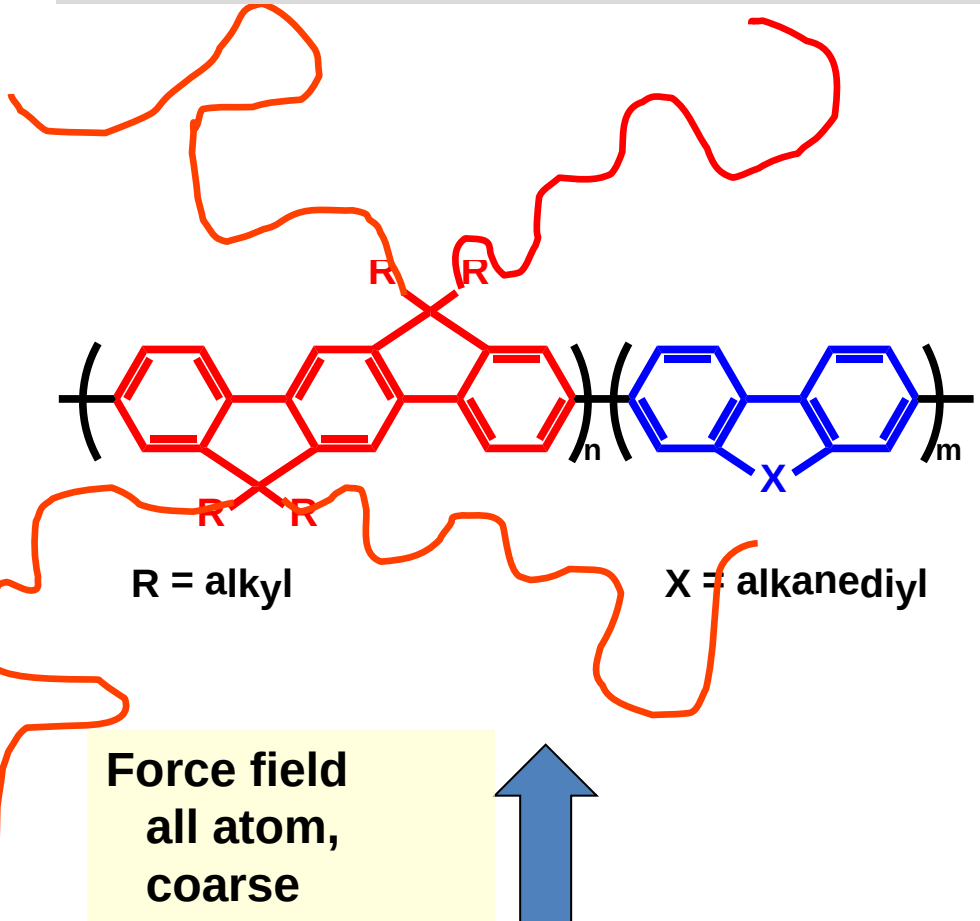
- Classical mode coupling etc approaches still fashionable, but… (real progress over the last 20 years?)
- New, alternative views, (Nagel, Liu, Weitz, Chandler..)
  so far restricted to collodial systems, applicable to polymers??





"Jamming phase diagram" (*A. J. Liu and S. R. Nagel, Nature 396, N6706, 21 (1998).*) The jammed region, near the origin, is enclosed by the depicted surface.

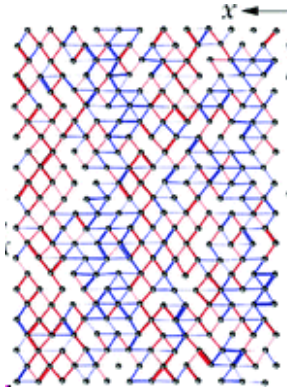
Polymer electronics



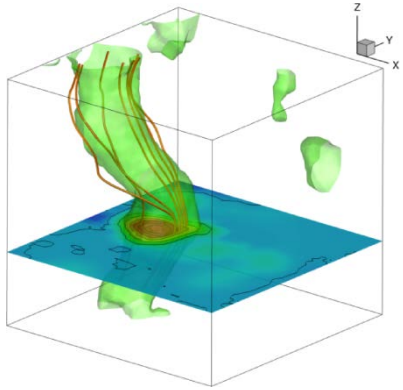
R = alkyl

X = alkanediyl

Mobility matrix

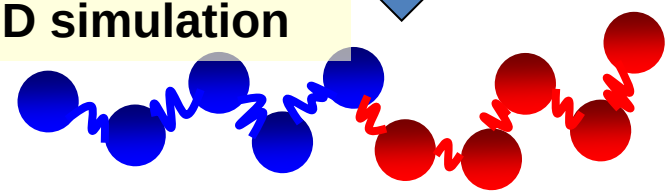


Flux filaments



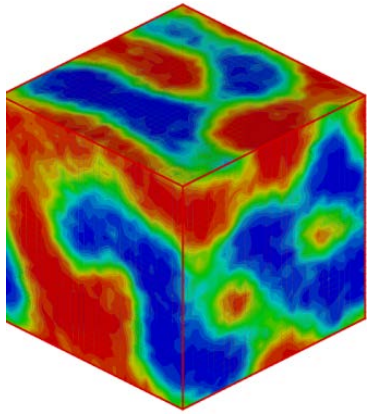
Kinetic MC
Quantum Chemistry

Force field
all atom,
coarse
grained
MD simulation

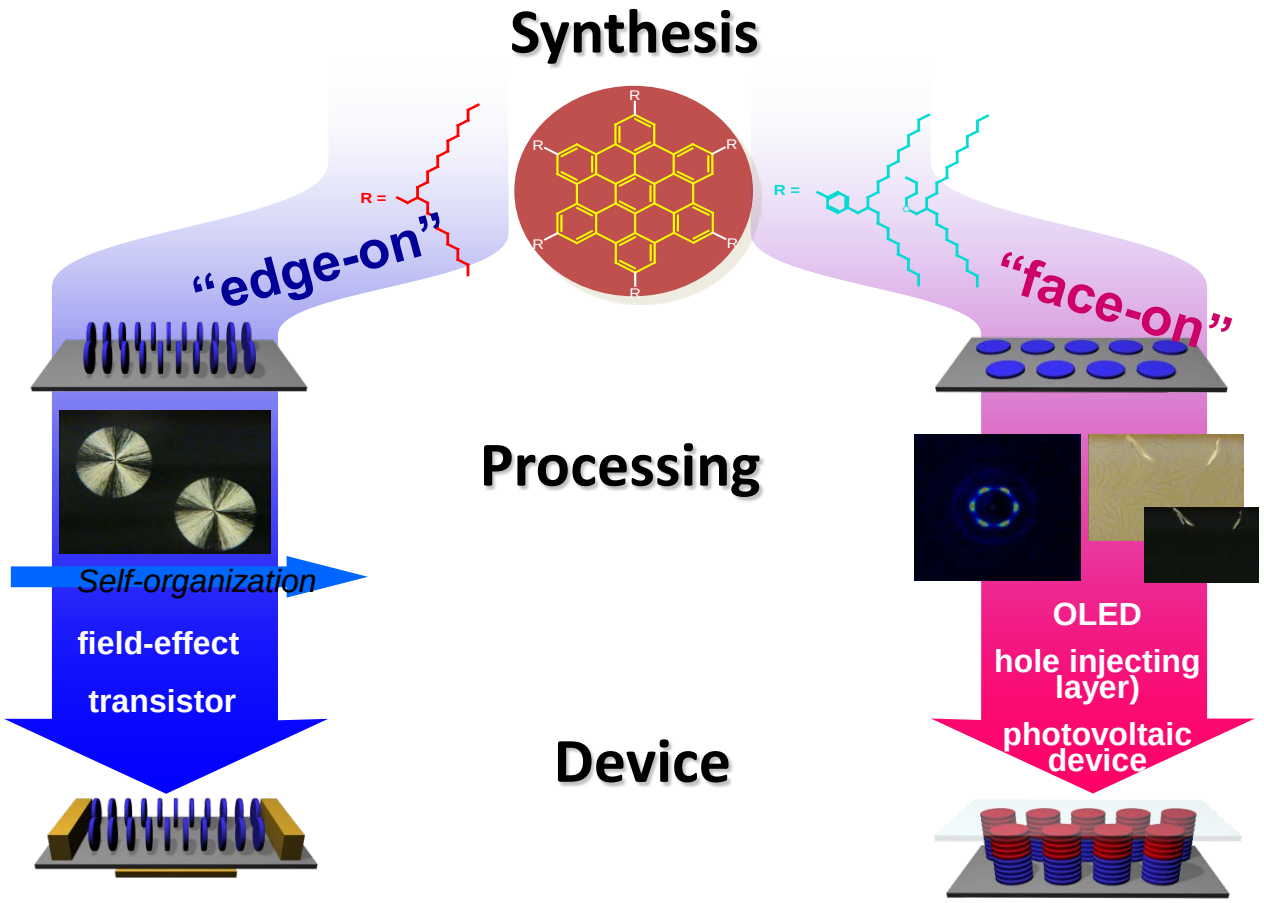


MD, SCMF

Processing
Nonequilibrium

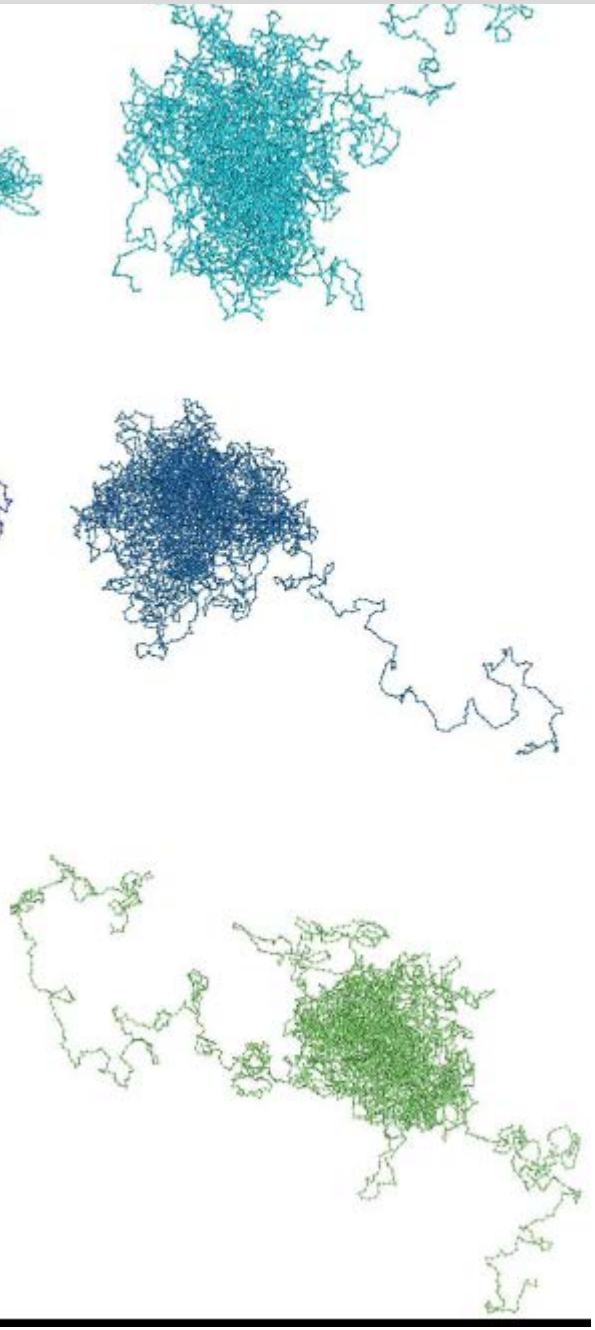


Function and Morphology - Processing

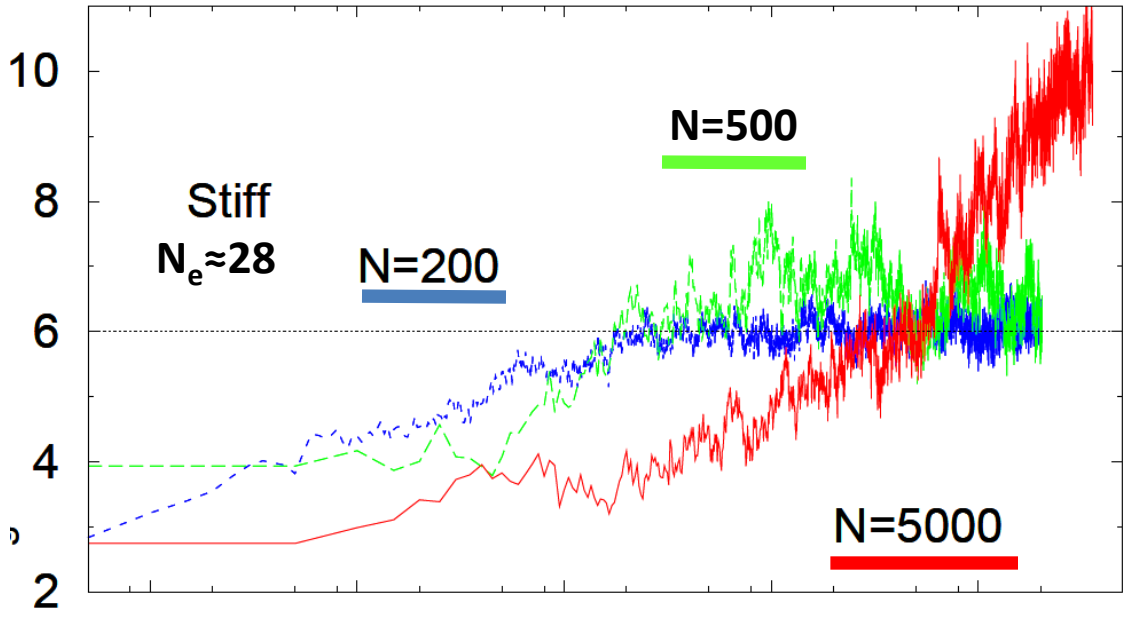


Predict and determine structure,
optimized for function,
- based on different experimental protocol
- based on chemical modification

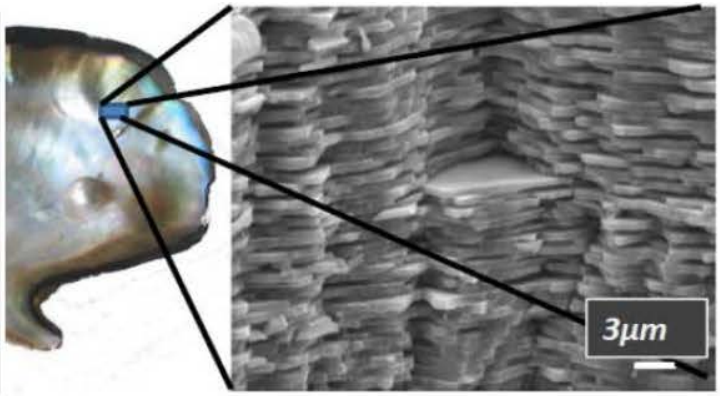
Morphology and Processing

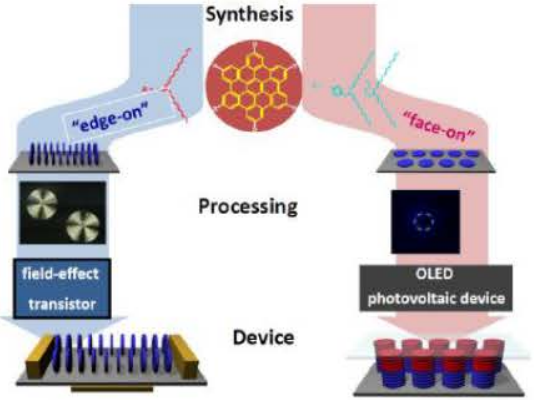


"Use" topological constraints:
Melt of collapsed
linear polymers



Processing


3μm


Synthesis
"edge-on"
"face-on"
Processing
field-effect transistor
OLED photovoltaic device
Device

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If you are in equilibrium

-- you are dead

(P. Pincus)