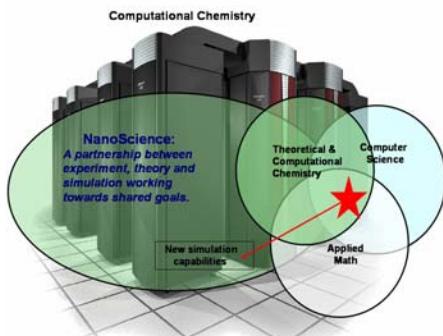


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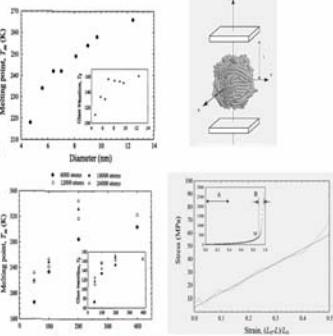
Atomic-scale methods provide information on the structure, dynamics, and thermodynamics of the system.
 Molecular dynamics (MD), mechanics (MM), Monte Carlo
 Large-scale normal-mode analysis (NMA).

Ab Initio (DFT-MD) methods used to compute electronic and molecular structure, and to obtain interaction potentials, activation energies for transitions, and electronic spectra as input into MD, Kinetic MC, coarse grain approaches.

NWChem, CPMD, CASTEP, VASP, new Wavelet based method

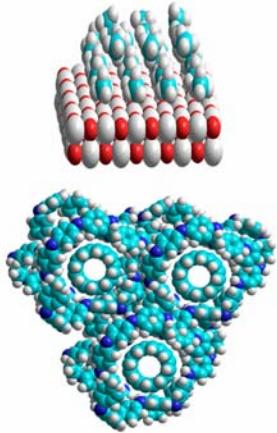
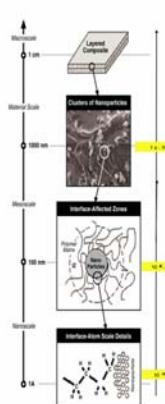
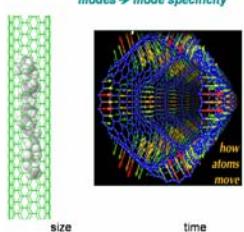
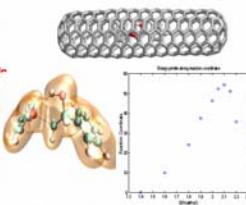
Heuristic methods provide complementary ways to perform efficient optimization and modeling based on experimental or simulation data
 Computational neural networks, evolutionary algorithms

All codes are implemented in parallel and run on ORNLJCS resources



Effects of Nano-Confinement

Reactions involving: dissociation, association, re-arrangements
 • Thermal decomposition, polymerization, isomerization, etc.
 • Classically the reaction kinetic inhibited by confinement; quanti predicts enhanced rates
 examine coupling to vibrational modes → mode specificity



Using Nano-Confinement to Tailor Semiconducting Polymers: New Generation Optoelectronics

Goal: To make polymer analogues of inorganic semiconductor quantum dots without specialized synthetic chemistry

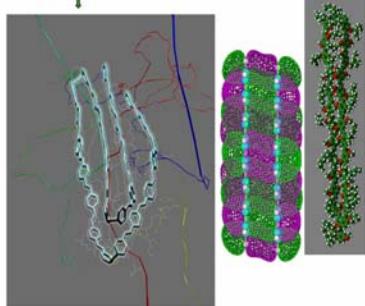
Issues:

- Control of chain organization and alignment
- Optimization of photophysical properties

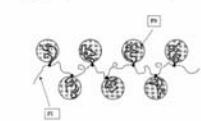
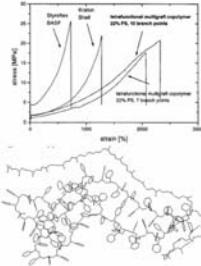
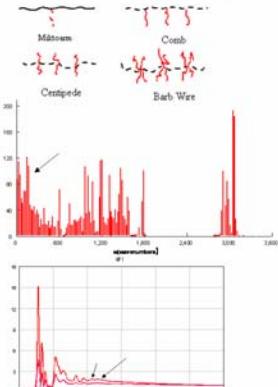
Applications: Electronic paper, luminescent clothing, display technologies, photovoltaic devices, light emitting diodes, field-effect transistors, solid state lasers, biomedical imaging...brighter, thinner, lighter, faster

Key Breakthrough: single molecule nanoparticles generated from dilute solutions of semiconducting polymers – Simulations show how 3-D confinement and solvent can lead to self-organization into the optimal structure!

The nanoparticles act like single (z-oriented) atoms - signature of quantum dot behavior



Results
 • Optimized photophysical properties by using dilute solution to generate single molecule nanoparticles
 • Photostability and spectral bandwidth superior to inorganic quantum dots under ambient conditions!



References: Sumpter, et. al. J. Phys. Chem. B 109, 7671 (2005); Polymer News 29, 302 (2004); Macromolecules 37, 6132 (2004); Nanolett 3, 603 (2003); J. Am. Chem. Soc. 126, 3376 (2004); Polymer 44, 4389 (2002); Macro. Theory Simul. 11, 711(2002); Polymer 44, 3761 (2003); Polymer Sci. B. (in press 2005)