Multiscale Molecular Simulations of PV Encapsulants

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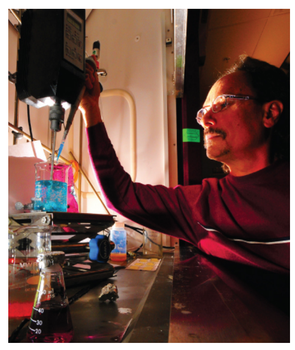

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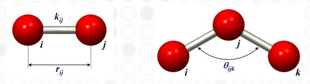
Overview

- Molecular simulations can provide important information about nanoscale structure and phenomena in PV encapsulant materials with atomic-level detail not currently accessible to experimental techniques
- The atomic-level detail of molecular simulations are useful for studying local packing of the polymer, as well as the interactions and dynamics of additives (e.g., UV absorbers) and contaminants (e.g., H_2O or O_2) within the polymer
- Molecular simulations are a cost-effective route for efficient high-throughput screening of potential encapsulant materials
- A multiscale approach combines quantum mechanical (QM) calculations and atomistic and coarse-grained molecular dynamics (MD) simulations to capture a broad range of length and time scales
- Results from the molecular simulations can be passed to simulation models at higher lengths scales, such as meso or continuum techniques
- This capability leverages open source tools like Sandia's LAMMPS MD package and NREL's STREAMM toolkit to setup, run, and analyze molecular simulations

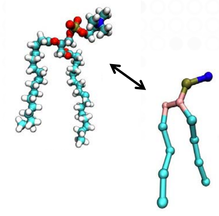
Molecular Modeling

- MD techniques follow classical dynamics using Newton's law ($F = ma$), by updating the positions of particles using the net forces on the particles
- Potentials are described using force fields with terms for bonded interactions (e.g., bonds and angles) and nonbonded interactions (e.g., van der Waals)

$$U = U_{\text{bond}} + U_{\text{angle}} + U_{\text{dihedral}} + U_{\text{nonbond}}$$

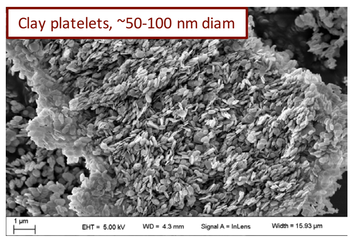


- QM techniques approximate the wave function following Schrödinger's equation ($H\psi = i\hbar\,\partial\psi/\partial t$) to consider quantum effects
- We can move between different scales using fine-graining or coarse-graining techniques to capture different features and phenomena
- Chemically-specific coarse-grained models can be derived from atomistic models with techniques like iterative Boltzmann inversion and force matching



Polymer/Clay Nanocomposites

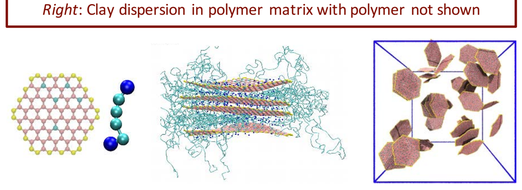
- Sandia and Texas A&M are working on inexpensive, transparent polymer/clay nanocomposites with layers of polymers and oriented clay platelets
- Tailoring the clay particles and polymer matrix controls the barrier properties, composite integrity, and fire retardancy



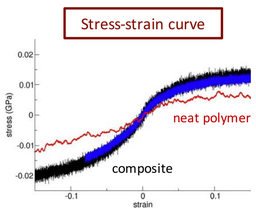
**Sandia*: Margaret Gordon, Erik Spoerke, Eric Schindelholtz, Ken Armijo, Rob Sorensen,
Texas A&M: Jamie Grunlan, Kevin Holder, Shuang Qin

- Chemically-specific coarse-grained models of polymer/clay nanocomposites can yield insight into material processes (e.g., encapsulation, intercalation, and exfoliation) and resulting material properties

Left: Coarse-grained model; *Middle*: Example of polymer intercalation; *Right*: Clay dispersion in polymer matrix with polymer not shown



Stress-strain curve

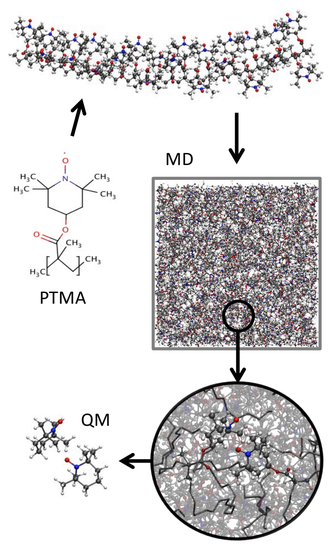


*JL Suter, D Groen, PV Coveney, *Adv. Mater.*, **2015**, *27*, 966-984; *Nano Lett.*, **2015**, *15*, 8108-8113

Radical Polymer Electrodes

- Atomistic simulations elucidated possible effects of morphology on electron-transport mechanisms in radical polymer electrodes
- Molecular models and MD simulations of PTMA were setup using STREAMM
- Two primary distances (4.5 and 6.5 Å) were identified as contributing to an effective electron transfer distance of 5.5 Å
- Inter-site couplings were computed between >10,000 pairs of sites with QM calculations, showing that electron transfer mostly takes place between sites on different chains

STREAMM's automated structure generation from monomer to oligomer to bulk material, and automated extraction of sub-regions for QM calculations



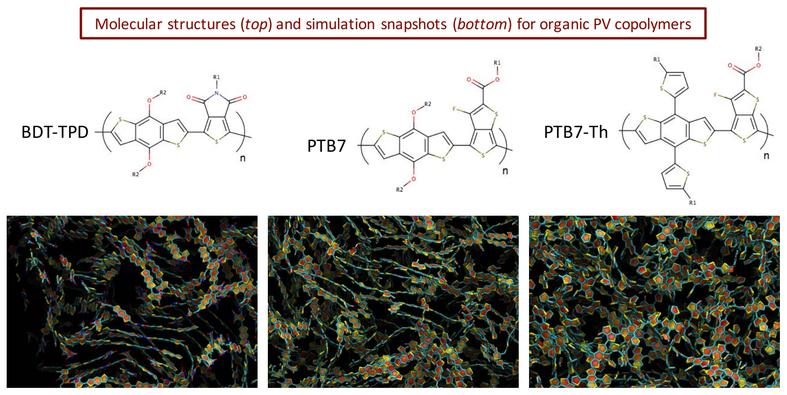
Top: N-N radial distribution functions; *Bottom*: Average inter-site electronic coupling

*TW Kemper, RE Larsen, T Gennett, *J. Phys. Chem. C*, **2014**, *118*, 17213-17220

Polymer Photovoltaic Active Layers

- Atomistic MD simulations were setup using STREAMM and performed in LAMMPS for three organic PV copolymers (BDT-TPD, PTB7, and PTB7-Th), with variations to the backbone and side-chain structure
- Aligned parallel chains with pi stacking were observed in BDT-TPD and PTB7, but not in PTB7-Th due to steric hindrance from the side-chain, which contradicts assumption made in the literature
- Transport in BDT-TPD and PTB7 likely occurs between parallel pi stacks, while transport in PTB7-Th likely occurs between orthogonal pi stacks

Molecular structures (*top*) and simulation snapshots (*bottom*) for organic PV copolymers

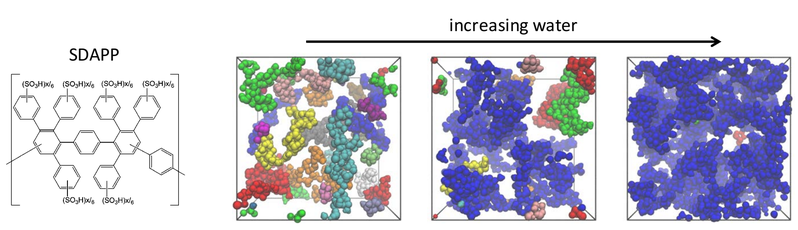


**NREL*: Travis Kemper and Ross Larsen

Ion-Containing Polymers

- Sulfonated polyphenylenes (SDAPP) show promise for proton exchange membrane fuel cells (PEMFCs) and vanadium flow batteries
- Little is known about the nanoscale structure of these amorphous polymers, which is not easily characterized with current experimental techniques
- Atomistic simulations yielded unique insight into the morphology of the ionic domains formed by the aggregation of water and ionic groups, specifically the size, shape, and connectivity, as well as resulting implications for ion transport
- As more water is added into the system, the ionic domains become more fully percolated and the domains become slightly larger and more spherical in shape, which would improve ion transport

Left: Molecular structure of SDAPP; *Right*: Ionic domains with disparate clusters shown in different colors



**Sandia*: Lauren Abbott, Amalie Frischknecht, Cy Fujimoto, Todd Alam, Eric Sorte

LAMMPS lammps.sandia.gov

Large-scale Atomic/Molecular Massively Parallel Simulator

- Open source classical molecular dynamics code
- Particle simulations at the atomic, meso, and continuum scales
- Inclusions of common potentials for hard and soft materials
- Efficient parallel simulations using spatial decomposition of domain space
- Modular framework for easy extension with new features and functionality

STREAMM streamm.nrel.gov

Simulation Toolkit for Renewable Energy and Advanced Materials Modeling

- Automated generation of candidate molecules for materials discovery
- Automated generation of initial conditions for molecular simulations
- Automated extraction of sub-regions for analysis and calculation of properties
- Integration with analysis and visualization algorithms
- Object-oriented framework for easy extension of the functionality to specific needs

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