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# Modeling of Macromolecules at Multiple Scales

## S&T Campaign: Materials Research
*Materials Manufacturing Science*

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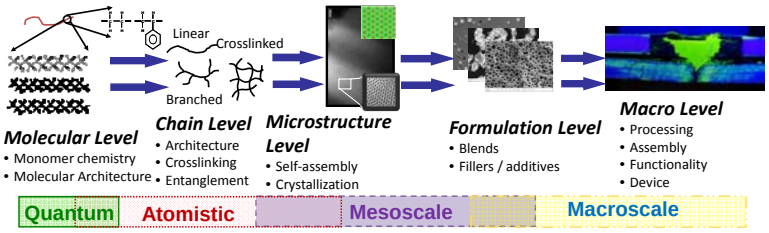
## Research Objective

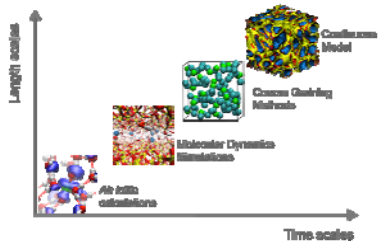
- Develop novel algorithms and methodologies to accurately and efficiently predict properties of macromolecules and multifunctional materials
- Perform simulations at Quantum, Atomistic and Mesoscale level of multiscale research to predict novel properties and explain observed phenomena
- Complement experimental research in development of novel materials with superior protective and multifunctional properties




## Challenges

- Bridging spatial and temporal scale
- Achieving accurate calculation of intermolecular interactions and entropy consideration of polymer conformations
- Reconciling computed thermo-mechanical processes at very high frequencies with experimentally available data at low rates (strain, cooling)
- Transferability of optimized DFT, atomistic and coarse graining methods across various chemistries and properties
- Methodology to simulate processes under external fields

### Scale Bridging Methods

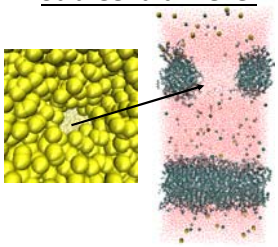



Transfer of information between different scales

### Heterogeneous Polymers Networks

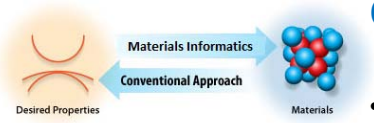
Mechanical and Thermal Properties of Polymer Networks with Heterogeneities and controlled defects

### Effects of Blast at the Sub-Cellular Level



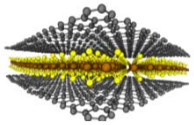
Coarse-grained and atomistic modeling to elucidate damage from blast TBI

### Materials Informatics




Design materials for desired properties

### 2D materials

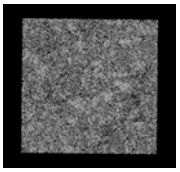


Mechanical and Electronic Properties of 2D materials and composites

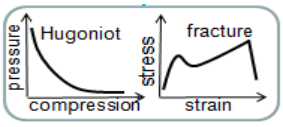
## ARL Facilities and Capabilities Available to Support Collaborative Research

- Peta-flop supercomputer resources of DoD
- ACAPP: ARL Center for Advanced Polymer Processing, (synthesis, characterization, fabrication) POC: Joseph Lenhart
- Unique software and expertise developed and validated at ARL and partially available in the LAMMPS and CP2K programs:
  - simulation of branched, entangled, semicrystalline and thermo-reversible gels and polymers
  - dynamic and mechanical processes at high strain rates
  - DPD method (DPD-mSRP) with bond repulsion for polymer mechanics
  - systematic, polarizable coarse graining
  - heterogeneous polymer networks and entangled polymer systems
  - biological system modeling
  - accurate, reactive atomistic potentials for hydrocarbons
  - fitting fast, order N DFTB method to achieve DFT accuracy
  - materials informatics to design materials with desired properties
  - diffusion wavelets for coarse graining
- Computational-Experimental collaborative research

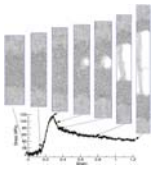
### Structure and Property Prediction



Structure and properties of materials

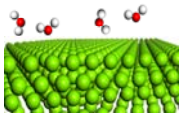


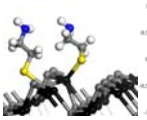

### Fiber Processing



Modeling the effect of processing conditions: Temperature, Pressure, Strain

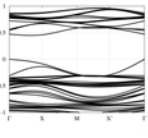
### Surface Science

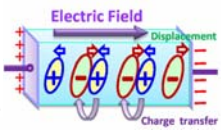




Understanding surface reactions and electronic properties

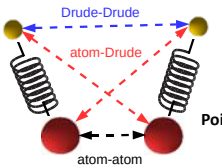
### Electron Transport

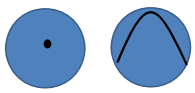




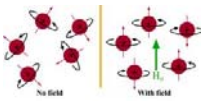

Develop accurate and efficient methods

### Electric and Magnetic Fields



Point vs. Smeared Charge Distribution



Behavior under applied field

Polarizable Force field and Functionality Development

## Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration

- Novel methods and algorithms to conquer the length and particularly the time bottleneck of polymer simulations
- Robust algorithms to optimize force-fields at the atomistic scale and systematically coarse grain towards the mesoscale
- Macro-scale (continuum) simulations that utilize lower level atomistic or mesoscale data
- New, order-N DFT concepts for solid state simulations

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