Responsive Nanocomposites

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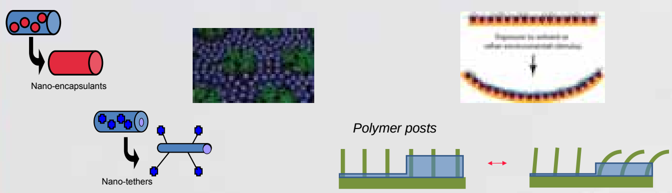
Problem

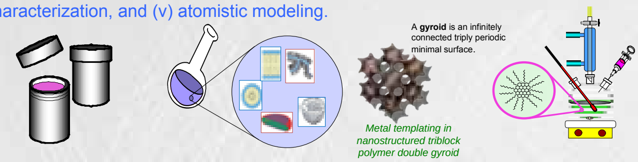
Materials need to change their properties based on changing environmental conditions.



Combine novel nanosynthetic routes with polymeric incorporation directed by computational calculations to develop both predictive capabilities and nanocomposites that can be altered by external stimuli.

Approach

Multi-pronged approach: (i) synthesis of nanomaterials (see below), (ii) functionalization of the nanomaterial, (iii) assembly, (iv) structural and functional characterization, and (v) atomistic modeling.



The external stimuli studied will focus initially on temperature or water stimuli where:

(i) the 'active responsive nanocomposites' will automatically change (shrink/swell) upon exposure or

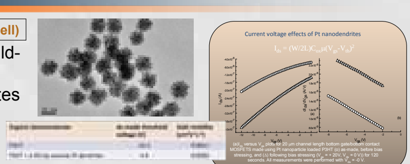
(ii) the 'applied responsive nanocomposites' where temperature or water in combination with an applied stimulus (i.e., a microwave or magnetic field) effects the final change.

Soft Templating – Shelnutt (UNM, Cornell)
Electrospinning – Boyle (Florida,Texas (Austin), Washington, UNM, HMC)
Graphene Functionalization – Lambert (Texas (Austin), UNM)
Polymer Interfacial Assemblies (nano 'grass') – Brinker (UNM, Harvard)
Computational Calculations – Grest (Clemson, Columbia)

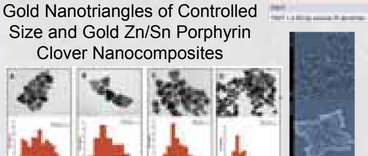
Results

Soft Templating – Shelnutt (UNM, Cornell)

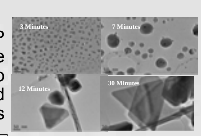
Enhanced Mobility in Organic Field-Effect Transistors (OFET) Containing Platinum Nanodendrites



Gold Nanotriangles of Controlled Size and Gold Zn/Sn Porphyrin Clover Nanocomposites

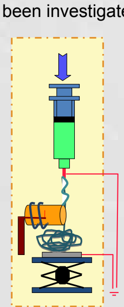


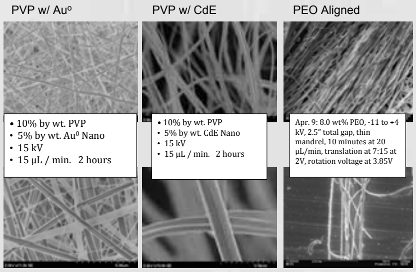
Copper NP coalescence leads to plates and wires



Electrospinning – Boyle (Florida,Texas (Austin), Washington, UNM, HMC)

Electrospinning of responsive polymers with a variety of nanomaterials have been investigated





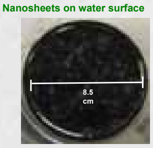
Spindle used to align wires: controlled deposition and release.

Higher NP loadings necessary to see response

Results (cont'd)

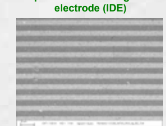
Graphene Functionalization – Lambert (Texas [Austin]), UNM)

Self-Assembled Nanosheets on water surface

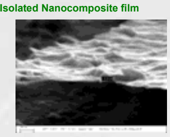


- Nanosheets up to cm in 2-D and < 100 nm thick form at the liquid-air interface upon UV photo-reduction of TiO_2-GO
- Nano-composites are photo-responsive
- Ongoing work is aimed at understanding the assembly process
- Recent work has proven that we can generate photocurrent (nA) from these films

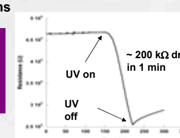
Deposited on Inter-digitated electrode (IDE)



Isolated Nanocomposite film



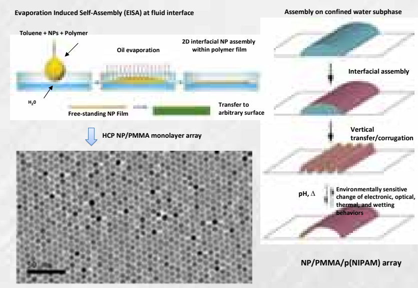
UV photo-reduction of TiO_2-GO used to prepare a partially reduced graphene-TiO_2 composite that self-assembles at the liquid-air interface: photoresponsive in nature.



T. N. Lambert *et al.* *J. Phys. Chem. C.* **2009** *113 (46)*, 19812-19823.

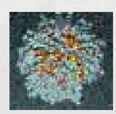
Polymer Interfacial Assemblies (nano 'grass') – Brinker (UNM, Harvard)

By incorporation of responsive hydrogel polymers and conducting interfacial self-assembly on patterned hydrophilic/hydrophobic substrates, we expect to create NP composites that undergo predictable 3D deformations in response to pH and temp.



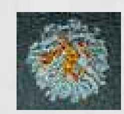
Computational Calculations – Grest (Clemson, Columbia)

Molecular Dynamics Simulations of Functionalized Nanoparticles



squalene

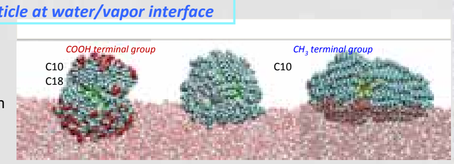
- Large-scale atomistic MD simulations
  - + structure of functionalized nanoparticles in solution
  - + resolve the interactions between them
- 5-, 10- and 20-nm silica nanoparticles coated with polyethylene oxide oligomers in water
  - + developed and tested effective methodologies for extracting forces between nanoparticles
- $Si(OH)_3(CH_2)_{10}CH_3$ alkylsilane-coated silica nanoparticles
  - + decane, $C_{24}H_{50}$ and $C_{48}H_{98}$ and squalene
- Determined entanglements between coated nanoparticles and polymer matrix using new primitive path analysis



decane

Alkanethiol gold nanoparticle at water/vapor interface

- Small changes in functional groups effect interactions
- Surrounding (solvent, polymer) or interface play important role in determining nanoparticle structure



Significance

*Ground-breaking responsive nanocomposites will enable rapid development of nanobased elastomeric systems.

- Any system with polymeric material will benefit (CINT, NW, etc): for example, reliability of these nanocomposites (a.k.a, seals, gaskets, parachutes, and wire insulation) under variable conditions.
- Graduate students will be trained to connect the synthesis of nanoparticles with their use in practical and important materials through NINE (SNL) program and our industrial partners.
- Responsive nanocomposites with defined properties are of interest to several collaborators: GoodYear™ (tires), Exxon/Mobil™ (polymers) and Intel™ (packaging, chips).*

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