Task Title: *(Task Number: 425.042)*

Dispersion, Bioaccumulation, and Mechanisms of Nanoparticle Toxicity

The University of Texas at Dallas

Departments of Chemistry and Molecular & Cell Biology; Alan G. MacDiarmid NanoTech Institute

PIs:

- **Steven O. Nielsen (PI)**
- **Rockford K. Draper (co-PI)**
- **Inga H. Musselman (co-PI)**
- **Paul Pantano (co-PI)**
- **Gregg R. Dieckmann (co-PI)**

Graduate Students:

- **Udayana Ranatunga** — **PhD candidate (100% funded)**
- **Blake Wilson** — **PhD candidate (100% funded)**
- **others TBA**

Undergraduate Students:

- **Tyler Hughes, others TBA**

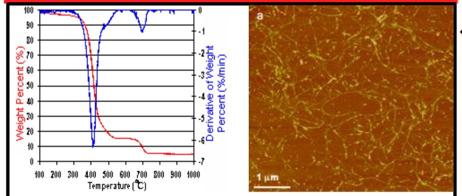
Senior Personnel:

- **Ruhung Wang** — **Research Associate**
- **Bob Helms**

Dispersion, Bioaccumulation, and Mechanisms of Nanoparticle Toxicity

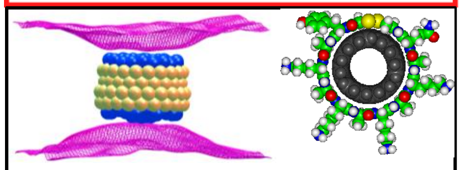
Nanoparticle material

Chemical & Physical Characterization



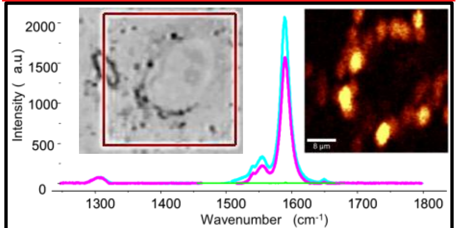
TGA of CNT starting material; AFM of biocompatible material

Computational Modeling & Predictions



CNT – bio interactions

Biological Testing



in vivo localization of CNTs using Raman

ESH Management

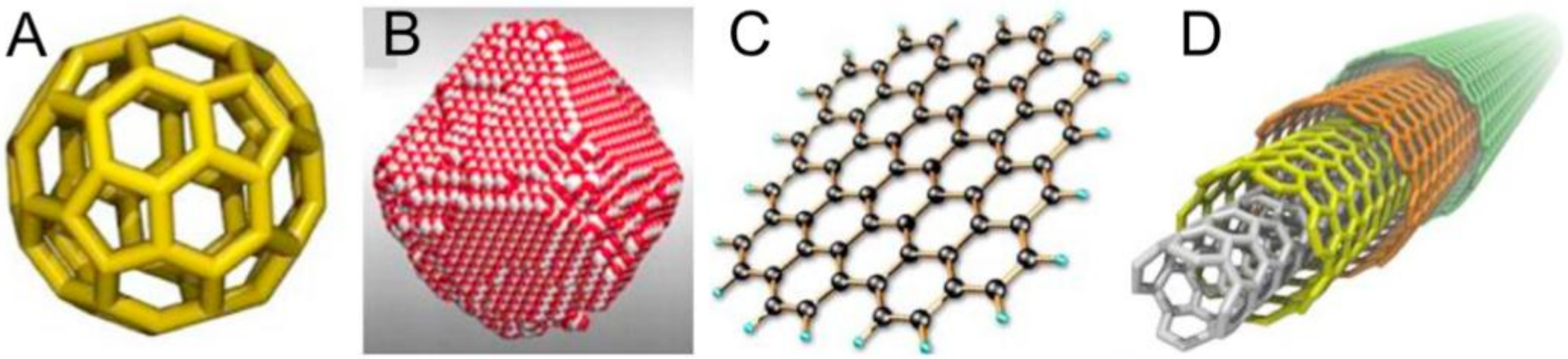
Research Description

Focus on two key determinants of nanotoxicity:

1) **the nanoparticle colloidal state (well-dispersed vs. aggregated)**
2) **the bioaccumulation of nanoparticles**

dispersants: control colloidal state

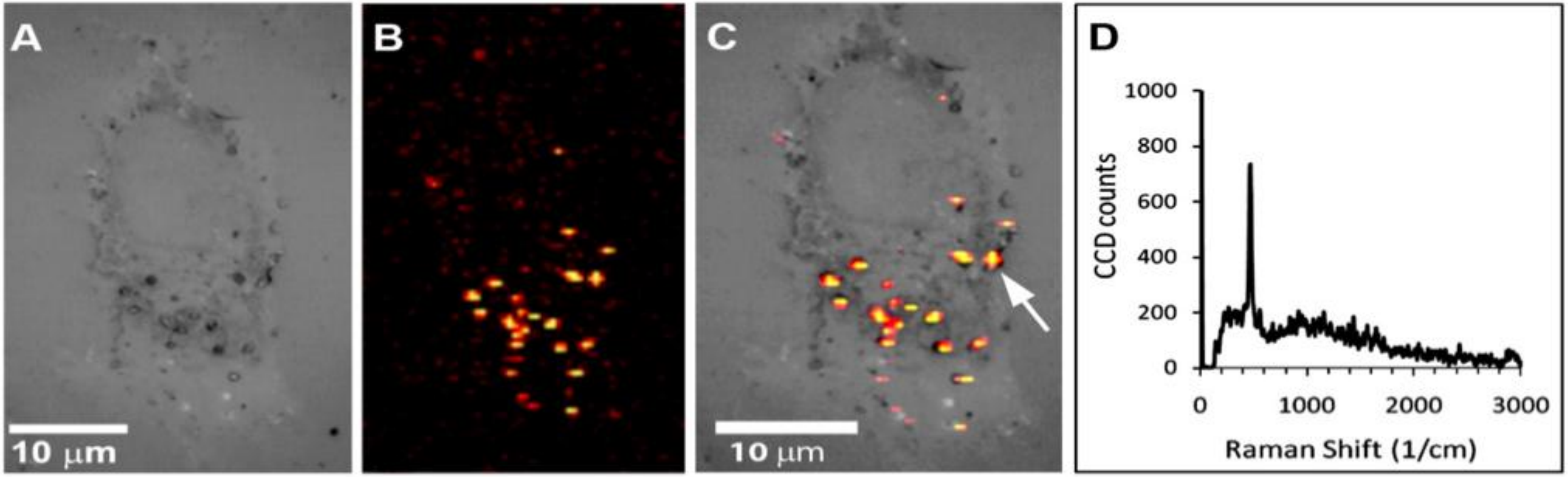
→ **use computational modeling to identify dispersants for a range of nanoparticles**



carbon spheres | **ceria** | **graphene, graphene oxide** | **carbon nanotubes**

Research Description

- **evaluate dispersant performance** (some break down upon sonication)
- **validate modeling data with experimental techniques**



Overall objective: reveal relationships among

- **nanotoxicity mechanics**
- **role of nanoparticle dispersion**
- **nanoparticle size**
- **bioaccumulation**

and provide a rational basis for managing and remediating nanotoxicity.

bioaccumulation and toxicity

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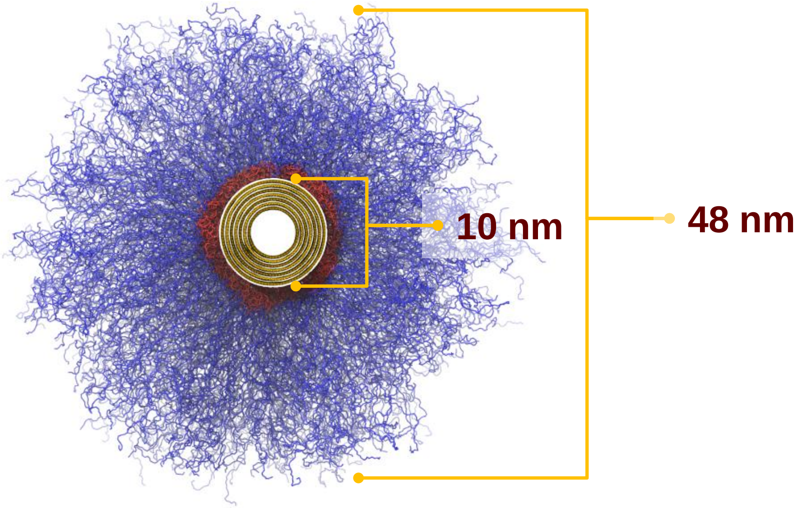
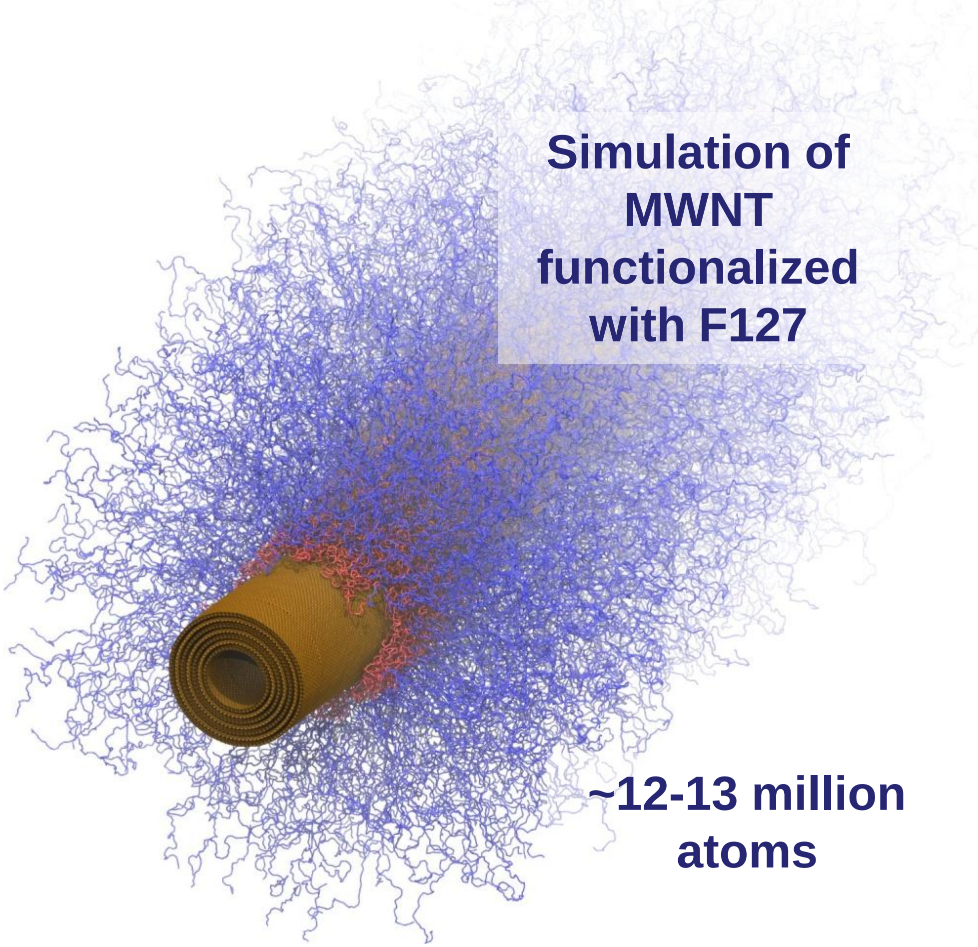
physical properties

Studying Pluronic-MWNTs with Molecular Simulation (from yesterday's talk)





- Simulations are too CPU intensive
  - Diameter of experimentally used MWNT ~10-20 nm
  - Too many atoms to simulate!
  - Need a more efficient approach

Molecular Simulation versus Predictive Molecular Thermodynamics Approach

Molecular Simulation:

inter- and intra-molecular forces → free energy

Strength: free energy emerges from the potential energy and the configurational entropy

Weakness: accuracy of the forces

Predictive Molecular Thermodynamic Approach:

directly postulate the form of the free energy

Strength: free energy expression is physically motivated and can provide insight

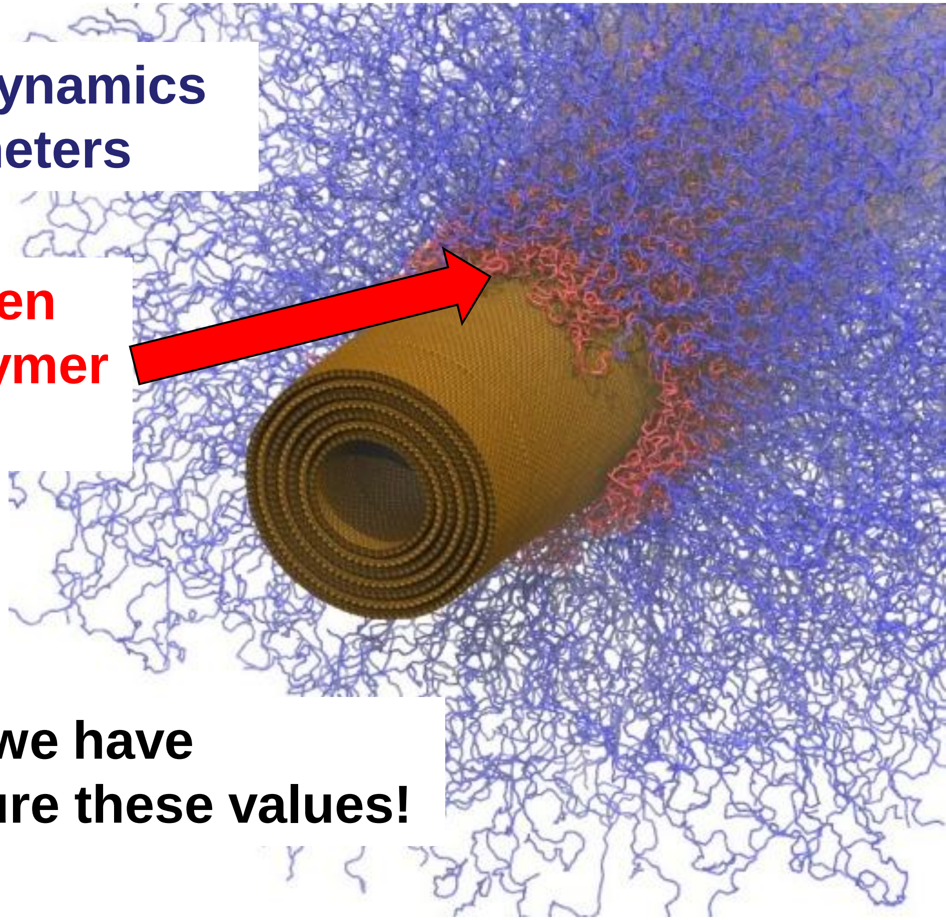
Weakness: terms may be missing from the free energy expression, or may be too simple or coupled in ways that are not accounted for

Molecular Simulation versus Predictive Molecular Thermodynamics Approach

Link between these approaches:

In the Predictive Molecular Thermodynamics Approach, there are unknown parameters

example: the surface tension between the hydrophobic block of the copolymer and the MWNT



the molecular simulation model we have developed can be used to measure these values!

ESH Metrics and Impact from 2011 ITRS Winter Meeting (Korea)

1. *Understand (characterize) processes and materials during development phase*
   - Carbon nanotubes, graphene/graphene oxide, metal oxide nanoparticles
   - Processing considerations, contaminants

2. *Use materials that are less hazardous or whose by-products are less hazardous*
   - Assess inherent nanomaterial ESH properties and by-products

3. *Make the factory safe for employees and the communities where we operate*
   - Develop procedures to separate by-products from benign materials
   - Develop dispersion strategies to manage ESH impact