Introduction to Nanoscience & Molecular Engineering (NME)

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Cognitive Approach towards Product Engineering Involving both Molecular Engineering and NanoScience

Example from Overney’s Lab in Collaboration with IBM
Thermomechanical Nano-Writing, Ultrahigh Density Pattern

Thermomechanical ultrahigh density storage in polymers. Recording density: > 1 Tb/cm² (1000 Gb/cm²)

A possible alternative to magnetic recording, which is approaching a physical barrier (i.e., the superparamagnetic limit of 100 Gb/in²).

Involves sophisticated macromolecules that utilize nanoconstraints
Nanomanufacturing graphene oxide aerogel with optoelectronic tweezers

MSE Pauzauskie, Pete
Nanoconstrained Molecular and Systems Engineering and Physical Sciences

ChemE Overney, Rene
Growth of Transparent Conducting Oxide Films

Biology Nemhauser, Jennifer
A diversity, focused on homing endonuclease and genome engineering, algal biofuels and potential new pilots focused on human metabolic disease.

MSE Luscombe, Christine
Quantum dot nanophotonics

EE Lin, Lih
Metabolic engineering of bacteria for biofuels production

ChemE Lidstrom, Mary
Nanomag

Biochemistry Baker, David
Lipid bilayer nanodiscs for drug delivery, vaccine development and membrane biophysics.

Biochemistry Daggett, Valerie
Protein folding, dynamics, design, and misfolding diseases

EE Fu, Kai-Mei
Quantum optics, quantum computation, magnetic sensing

PHYS Gundlach, Jens
Nanopore DNA Sequencing

BioE Kim, Deok-Ho
Unconventional nanolithography, cell-nanotopography interactions, nanostructured biomaterials

EE Klavins, Eric
Synthetic biology (building parts, components, and systems for genetically engineered organisms to living systems programmable).

Nanopore DNA Sequencing

MSE Krishnan, Kannan
Synthetic biology (building parts, components, and systems for genetically engineered organisms to living systems programmable).

Biochemistry Daggett, Valerie
Protein folding, dynamics, design, and misfolding diseases

ChemE Overney, Rene
Nanoconstrained Molecular and Systems Engineering and Physical Sciences

Pharmacology Chung, Jae-Hyun
Concentration of molecules on to a nanotip for disease diagnosis and drug discovery.

CHEM Chatterjee, Champak
Surface reactions in energy technology

Medicinal Atkins, William
Concentration of molecules on to a nanotip for disease diagnosis and drug discovery.

CHEM Pauzauskie, Pete
Synthetic biology (building parts, components, and systems for genetically engineered organisms to living systems programmable).

R.M. Overney University of Washington

Nanoscience and Molecular Engineering in Chem. Eng. at UW

• Adler (Electrochemical Engineering tied to Crystal and Electronic Structure)
• Berg (Colloids, Adhesion)
• Baneyx (Biotechnology and Protein Engineering)
• Castner (BioMedical, Protein Interaction)
• Hillhouse (Nanomaterial Assembly and Energy)
• Jeneke (Organic Electronics and Photovoltaics)
• Jiang (Molecular Design of Biocoatings)
• Lidstrom (Genomic and Metabolic Manipulation of Bacteria)
• Overney (Nanoscience based Molecular Engineering)
• Pfaendtner (Biomaterials and Molecular Physics)
• Pozzo (Colloids, Nanofabrication, Bio-separations)
• Ratner (Biointerfaces, Drug Delivery and Tissue Engineering)
• Schwartz (Electrochemical Materials and Interfaces, Nano/Microfabrication)
• Stuve (Electrocatalysis and Surface Science)
• Shen (Nanomaterials for Biomedical Applications)
• Yu (Nanomaterials and Functional Nanostructures)
Nanoscience & Molecular Engineering at the UW Campus

- **Center of Nanotechnology (CNT)**
  - established early 2010
  - Dual Ph.D. Program in Nanotechnology
  - NanoTech Facility

- **Institute of Molecular Engineering & Science (MoES)** – established early 2010
  - Strong Science with Engineering Focus involving both Nanoscale Principles and Molecular Engineering
  - The first of its kind in the United States
  - Impressive Infrastructure (e.g., MoES Building)
  - Intellectual Critical Mass to make a Transformative Impact in Science and Engineering
  - Truly Crossdisciplinary (in contrast to merely “Interdisciplinary”)

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Ph.D. Program in Nanotechnology

University of Washington

**Required:**
- Nanotechnology Courses outside home department (about 50 courses)
- Rotation in lab outside home department
- Thesis in nanoscale science & nanotechnology
- Nanotech seminar

**Options:**
- NanoTech User Facility
- Industry or PNW/L Internship
- Mentoring Program (Center for Workforce Development)
- Future Faculty Training Certificate
- Entrepreneurship in Technology Certificate
- NSF-funded IGERT Program

http://www.nano.washington.edu
Nanoscience and Molecular Engineering

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<th>Molecular Sciences</th>
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<th>Surface Sciences</th>
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<td>and Technologies</td>
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NanoScience & Molecular Engineering

- Rognitive engineering based on molecular designs and external constraints.

Transformative Impact in:
- Health
- Materials
- Energy
- Environment
- Consumer goods

Rational Molecular Material Engineering

Fundamentally motivated Molecular Designs

Material Analysis with molecular intrinsic insight

Experimentally Verifiable Molecular Simulation
Engineering with Constraints

- External Constraints
  - Interfacial Constraints
    - Field Constraints
    - Dimensional Constraints
  - Inter- and Intramolecular Constraints
    - Enthalpic Constraints
    - Entropic Constraints
- Impact of Constraints on Transport Properties
- Engineering Applications
  - Modern Material Characterization
    - Scanning Probe Methods

Modern Technology - Engineering with Constraints

- Engineering Applications
  - Fuel Cell
  - Membranes
  - Hardrive Lubrication
  - TeraBit Recording

- Inter- and Intramolecular Constraints
  - Bottom-Up
  - Self-Assembly

Energetics

- External Constraints

S. Sills, PRL 91(9), 095501, 2003
External Constraints

- **Interfacial Constraints**
  - Dewetting Velocity
  - Interfacial Cooling
  - M. He, PRL (2000)

- **Dimensional Constraints**
  - ~ 2 nm
  - ~ 10 nm
  - Polymer Nanorods
  - Size Selective Sorption Selective

- **Field Constraints/Gradients**
  - Glass Transition

Nanotools: Process Characterization

**Nano-Transport Properties in Membrane Systems** (Overney)

To optimize transport properties in membrane systems, a fundamental understanding of the molecular mobility is imperative. ➔ **Direct Nanoflux Analysis**

For many applications it is desirable to study nano-transport properties in parallel to material properties, e.g., polymer membranes used in fuel cell applications. Structure properties (e.g., ionic sub-domains) and transition properties (e.g., glass transition) are studied in situ with fluid mass transport.

**Structural Information**

- Ionic Clusters (T = 300 K)
- Nanoscopic probing revealed an unexpected rheological transition in Nafion (Dupont), about 30°C below the well known glass transition temperature, which is responsible for the currently widely used operating temperature.

- Glass transition
- Structural transition responsible for water transport
**Instrumentation and Bottom–up Design**

(Overy)

Nanocomposite (Silica/PTMSP): Reverse Selective Membrane

**Applications:**
- Lithium ion Solid State Batteries
- Hydrogen Purification

**Molecular Engineering: Self Assembling Chromophores**

Stabilized Self-Assembled “Polymer”

**Face-to-Face Phenyl/Perfluorophenyl Interaction**

\[ T = 24 \, ^\circ C \]

Stabilization Energy
\[ E = 4-6 \text{ kcal/mol} \]
\[ (~ 30 \text{ kJ/mol}) \]

**Gray, Overney, et al., Nano Letters (2008) 8, 754.**

**T-D. Kim et al., JACS (2007) 129, 488**

**R. H. Grubbs, J. Am. Chem. Soc. 1998**

**S. Coates, J. Phys. Chem. B 2003**
Molecular Dynamic (MD) Simulation

C_H_6

C_F_s

15 D

Relaxations, glass transition, crystallization
Self-assembly
Glass forming process
Local mass transport properties (membranes)
...

Interfacial and Dimensional Constraints

- Ultrathin polymer films
- Membranes
- Nanocomposites
- Organic LED materials
- Simple alkane liquids
- ...

Intra- and Intermolecular Constraints

- Side-chain and local backbone relaxations, critical energy barriers (polymers)
- Molecule-molecule interaction during structuring process (molecular glasses)
- Cooperativity and energy consumption, cooperative length scale
- Condensed organic materials
- Polymers (polyelectrolytes, conjugated polymers, dendritic-chromophore polymers, …)
- Molecular glasses
- Organic NLO materials
- Proteins
- ...

Materials

- Understanding phenomenological properties and processes (e.g., glass transition)
- Origin of frictional energy dissipation
- Cognitive approach to material engineering (e.g., towards increase in electro-optical activity in photonics)
- ...

Impact

Applications
- Energy (Storage, Conservation)
- Electro-Optics (Photonic Materials)
- Separation Membrane Technology (e.g., applied to hydrogen technology)
- Electronics (Transistors with Bio-mimetics)

NME Research in Overney’s Lab (Office BSN 245)