Nano-Engineering Theme Areas

National Institute for Nano Engineering

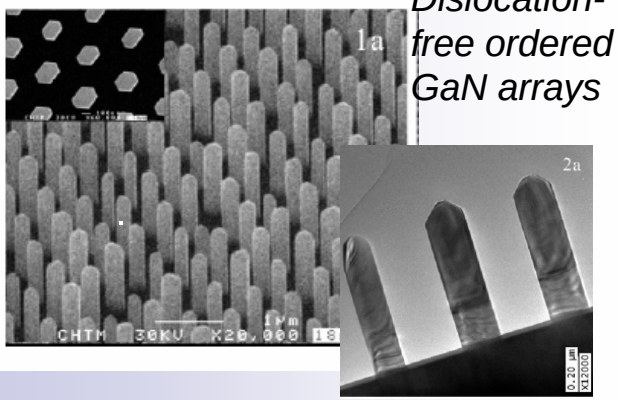
- **Nanoelectronics and Quantum Information Processing**
  - **Nano-electronics and photonics for the 21st Century**
  - **Atom Chip Device Engineering for Cold Atom Quantum Information Science and Technology**
  - **Self-assembly to direct manipulation of nanostructures on length scales from atoms to microns**
  - **Developing a Thermal Microscopy Platform for In-Situ Thermal/Thermoelectric Structure-Property Studies of Individual Nanotubes and Nanowires**
- **Nanomaterials Manufacturing**
  - **Nanocomposite Materials Design: Scientific Understanding and Control of Rheology, Assembly and Functionality**
  - **Phase Imprint Lithography for Large Area 3D Nanostructures**
  - **Nano-Engineering by Optically Directed Self Assembly**
  - **Stress-Induced Chemical Detection Using Flexible Nanoporous Metal Organic Frameworks**
  - **Electrostatic Microvalves Utilizing Conductive Nanoparticles for Improved Speed, Lower Power, and Higher Force Actuation**
  - **Interfacial Property Control of Elastomeric Nanocomposites**
- **Energy Nanotechnologies**
  - **Nanoengineering for Solid State Lighting**
  - **CO2 Reduction Using Biomimetic Photocatalytic Nanodevices**
  - **Optimized Nanoporous Materials**
  - **Fundamentals of Synthetic Conversion of CO2 to Simple Hydrocarbon Fuels**
  - **Improving Electronic Structure Calculations to predict Nanocatalyst Functions**
- **Nano-Bio – future activity of investment…..**

Sandia National Laboratories

Nano-electronics and photonics for the 21st Century

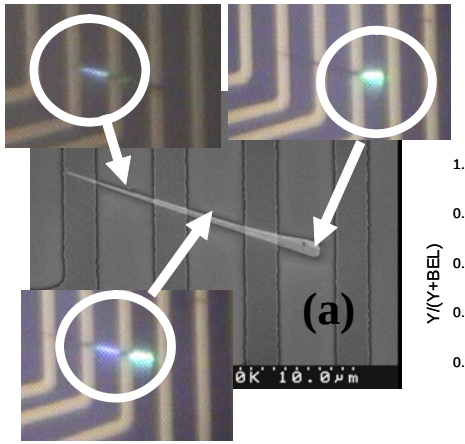
PI: Alec Talin

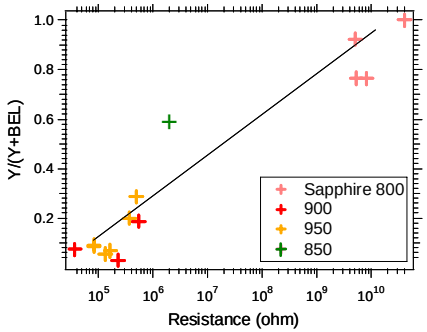
National Institute for Nano Engineering



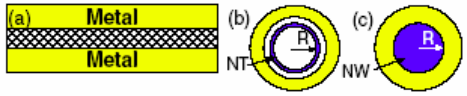
Dislocation-free ordered GaN arrays

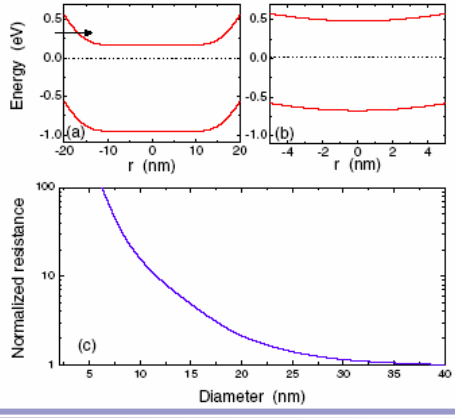
Ordered growth and integration





GaN and Ge NW devices for electrical/optical characterization





modeling contact resistance in nanotubes and nanowires

Leonard & Talin, PRL 97, 2006

State-of-the-art fabrication, test, and modeling of nanodevices

hp invent

Yale

UNM

Sandia National Laboratories

Nanoscale circuit simulation

Sandia National Laboratories

Atom Chip Device Engineering for Cold Atom Quantum Information Science

Matthew G. Blain, Peter D.D. Schwindt (Co-PI's)

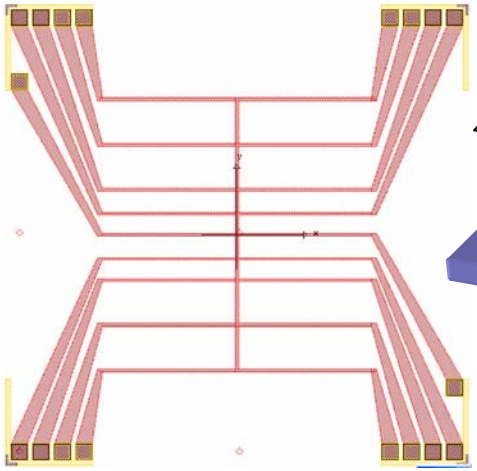
National Institute for Nano Engineering

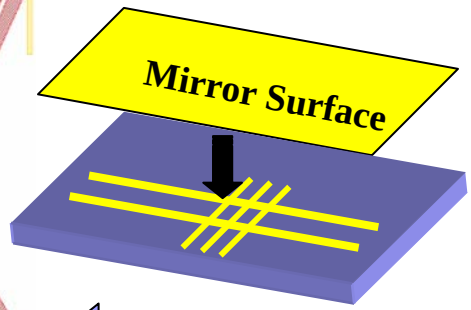
Project Goals

Integrate chip based cold atom magnetic traps with nano and micro scale optical waveguides, resonators, or cavities to realize atom chips with integrated atom optics.

Apply these integrated atom optics chips to perform photon-atom coupling for experiments in quantum information

Highlights





Fabrication in Progress

Atom Chip Design Complete

Technical Approach

- **Design mirror MOT atom chip**
- **Fabricate hemispherical recesses with nanoscale roughness factors for high finesse optical cavities**
- **Calculate magnetic fields for designs**
- **Fabricate the mirror MOT atom chip designs and characterize performance**
- **Develop custom package for atom chips to accommodate requirements of atom experiment**

Partners

•Prof. JM Geremia
Quantum Measurement and Control Group, Department of Physics and Astronomy UNM

•Prof. Hideo Mabuchi
Physics and Control & Dynamical Systems, CalTech/Stanford

Sandia National Laboratories

“Bottom-up” meets “top-down”: Self-assembly to direct manipulation of nanostructures

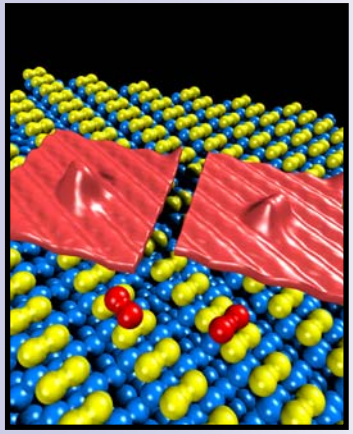
PI: Brian Swartzentruber

National Institute for Nano Engineering

Partners:
Franz Himpsel – UW-Madison
(University Partner)
Jim Hannon – IBM Yorktown Heights
(Industry Partner)

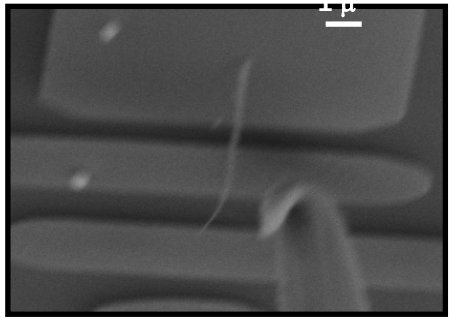
Novel nano-manipulator inside of SEM provides ‘top-down’ construction & characterization of unique nanostructures

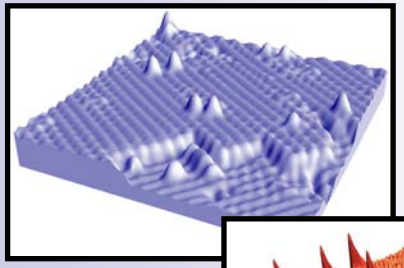
- Direct and precise control over placement of individual nanostructures
- Positioning with respect to each other

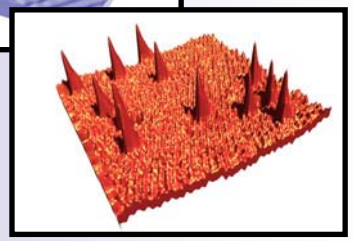


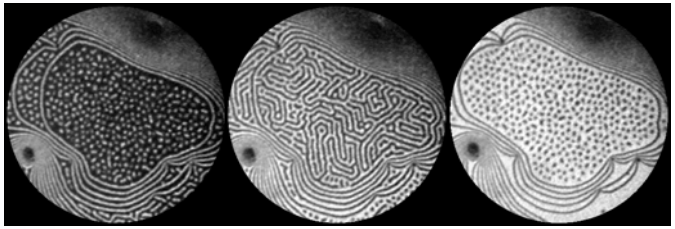
Combination LEEM-STM allows direct imaging of surface features on length scales from atoms to microns.

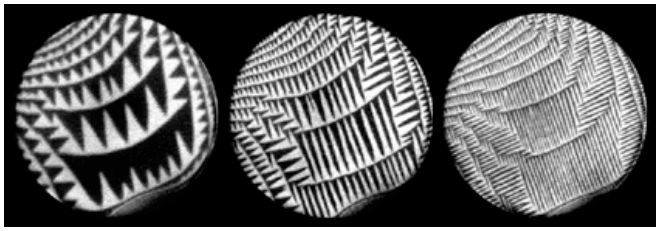
- Investigate ‘bottom-up’ generation of surface nanostructures
- Find templates for 3-d nanostructures

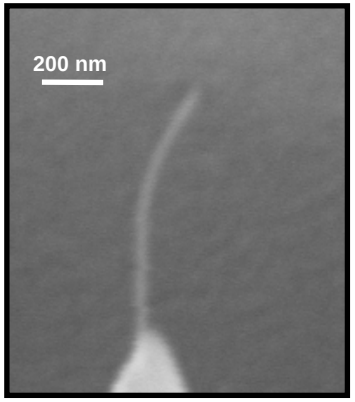












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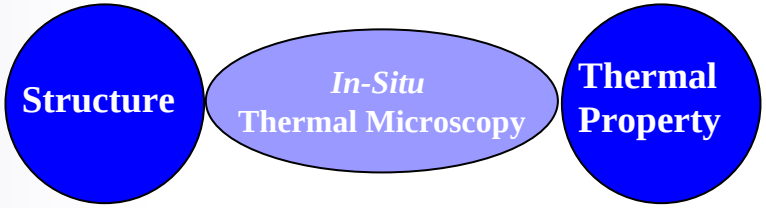
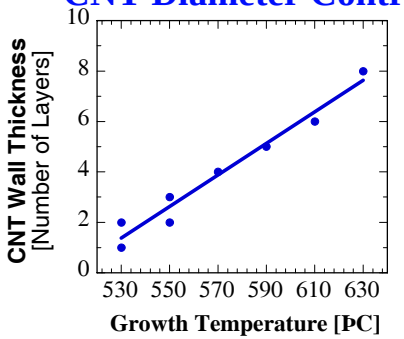
Developing a thermal microscopy platform for *in situ* thermal/thermoelectric structure-property studies of individual nanotubes and nanowires

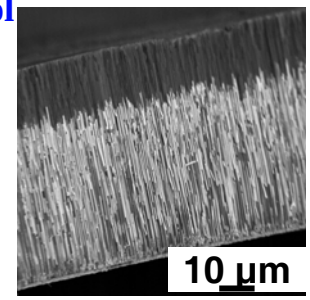
PI: Huang



- **Materials synthesis**
  - CVD growth of CNTs with different diameters, defects
  - Bi nanowires with different diameters, defects; electrochemical deposition in AAO templates
- **Platform design, structure-property characterization**
  - *Wall-by-wall peeling and stretching of CNTs*
  - *Electron-beam, ion-beam modifications*
  - *Post growth thermal annealing of Bi nanowires (crystallization, gb's, etc.)*
- **Computer modeling** *Ab initio* calculations
  - Self-consistent non-equilibrium Green's function (NEGF)

CNT Diameter Control





BiSb nanowires

Partners

Nanocomposite Materials Design

PI: C.J. Brinker & R. Schunk

National Institute for Nano Engineering

Controlling nanoparticle synthesis and processing: functionalization, rheology, dispersion & patternability, robustness

NanoParticle Flow Consortium

P&G

BASF The Chemical Company

Medtronic Alleviating Pain · Restoring Health · Extending Life

CORNING

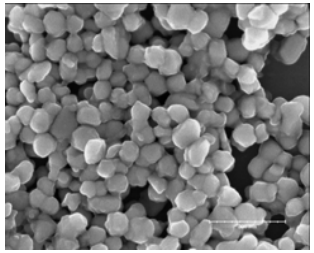
3M

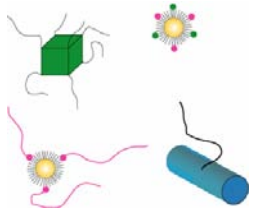
Boston Scientific Delivering what's next.

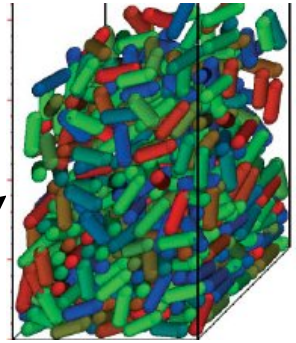
DOW CORNING

UNM

THE UNIVERSITY OF TEXAS AT AUSTIN

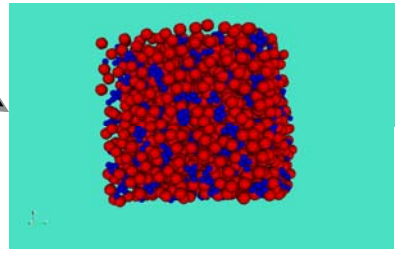




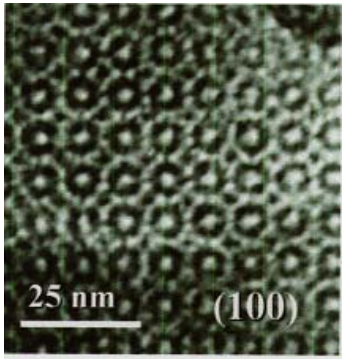


Rheology

Multi-scale predictive Simulation - e.g. coating, casting…



Dispersion stability



Surface self-assembly (membrane)

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Phase Imprint Lithography for Large Area 3D Nanostructures

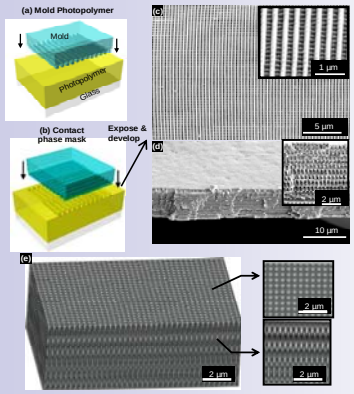
PI: Greg Bogart

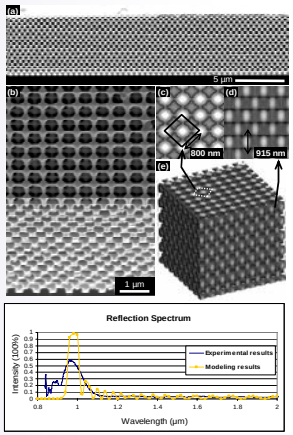
National Institute for Nano Engineering

Objective: To develop lower cost methods and infrastructure suitable for generation of large area 3D nanostructures for use in micro fluidics, photonics, sensors, fuel cells and battery devices, catalyst supports, data storage materials, density gradient systems, biodegradable drug delivery, and scaffolding for cell growth.

Approach:

- **Use modeling and experimental data to devise structure design, predict and improve device performance, and drive scaling techniques for low cost, large area fabrication.**
- **Polymer development is used to improve device structure functionality, stability, and improve phase mask performance.**
- **Atomic layer deposition (ALD) is used to improve functionality for application across different platforms.**





Partners:

University partners: Prof. Elizabeth Dirk, UNM

Prof. Christos Christodoulou, UNM

Prof. John A. Rogers, UIUC

Industrial partners : Dow Corning

Sandia National Laboratories

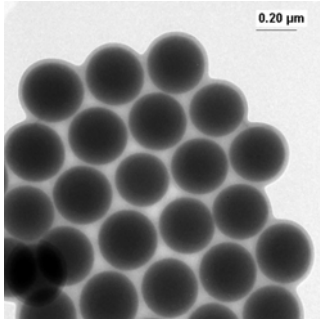
Methods, modeling, and results

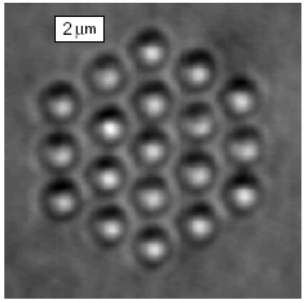
Laser Tweezers for Optically Directed Self-Assembly

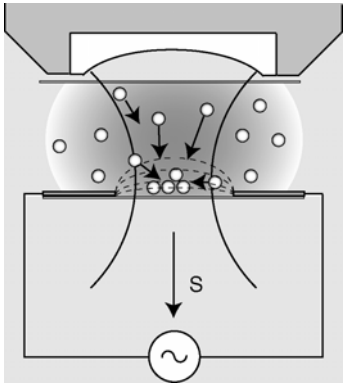
PI: Anne Grillet

National Institute for Nano Engineering

- **Develop highly ordered structures using laser tweezers to optically direct assembly of nanoparticles**
  - **Synthesis and functionalization of nanoparticles (CINT)**
    - Nanoscience of particle chemistry applied to engineer ordered structures
  - **Measurement of interaction potentials for nanoparticles**
    - HOT will enable testing and study of *aspherical* particles
  - **Engineering and Testing of photonic materials**
    - Particle level manipulation using laser tweezers
    - Directed assembly with external fields







Synergistic benefit for Sandia discrete element modeling efforts for nanoparticle suspensions funded through LDRD, DOE ASCR, NNEDC and the Nanoparticle Flow Consortium CRADA – Corning, BASF, Procter & Gamble, ICI Starch, 3M

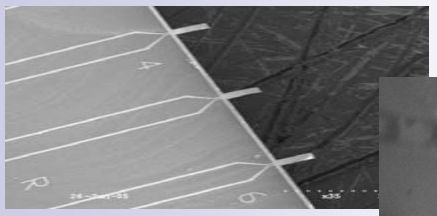
Sandia National Laboratories

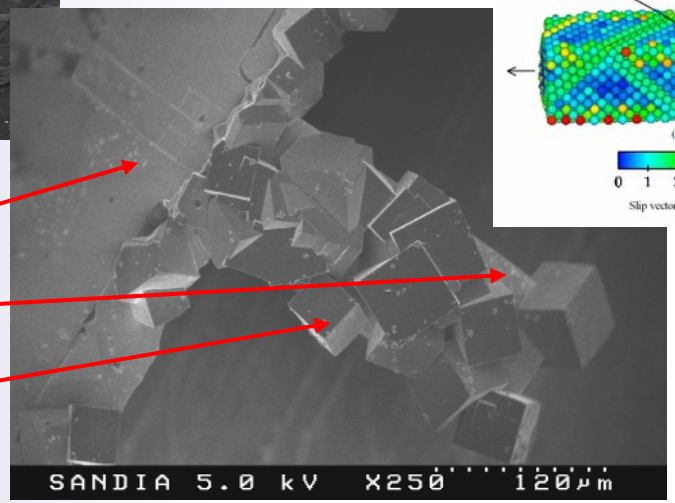
Stress-Induced Chemical Detection Using Flexible Nanoporous Coordination Polymers

National Institute for Nano Engineering

PI: Mark Allendorf

- MEMS devices, specifically static microcantilevers, can provide solutions to the most demanding sensor applications through orthogonal sensing of surface stress and heat.
- ***Recognition chemistries are needed to achieve sub-ppb sensitivity and selectivity required by these applications!***
- Structural flexibility in coordination polymers enables stress-induced detection with exceptional sensitivity in microcantilevers
- ***Challenge: Discover the link between nanopore chemistry and mechanical stress to enable a rational design process***

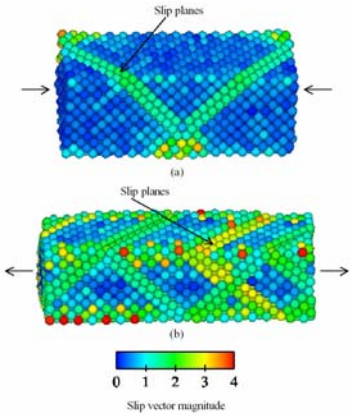




Uncoated region of device

Cantilever surface

Cantilever coated with zinc-carboxylate CP



Connecting chemistry and mechanical engineering via high-level computations and experiment

Georgia Institute of Technology

LUNA INNOVATIONS

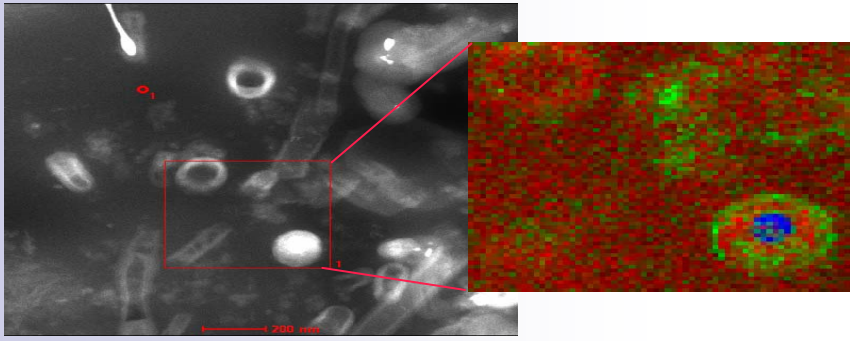
Sandia National Laboratories

Interfacial Property Control of Elastomeric Nanocomposites
PI: Tim Boyle

National Institute for Nano Engineering

Objective: Develop fundamental understanding of, and control over, nanocrystal elastomer interactions for polymeric nanocomposites limits necessary materials advances.

Approach: Combine novel synthetic routes with advanced nanoscale characterization, and molecular models to develop a predictive capability of elastomer (liquids and solids) nanomaterial interfacial behavior.



The University of New Mexico

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GOODYEAR

United Technologies

PURDUE UNIVERSITY

Impact

Understanding of interfacial phenomena to enable rapid development of nanobased elastomeric systems.

Sandia National Laboratories

Electrostatic Microvalves
PI Chris Apblett

National Institute for Nano Engineering

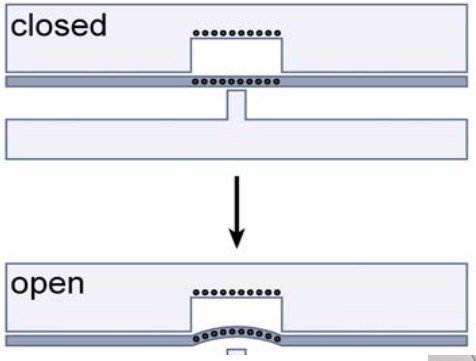
Goal:

COMBINE the speed and low power of electrostatic actuation with the performance of pneumatic actuation in microvalves

Key Features:

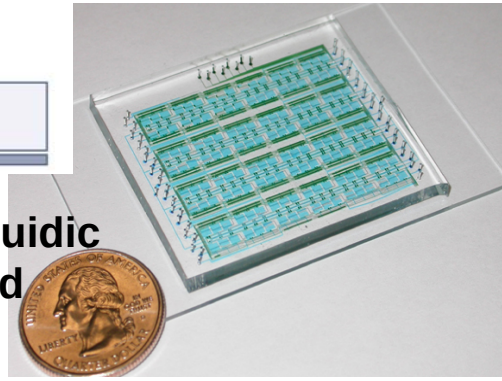
- **Computer analysis of microvalve actuation for optimal performance**
- **Fabrication of microvalves in single and array modes**
- **Use of Microvalves in microfluidic array to demonstrate superior speed and sealing**

Actutate-to-open



Putting new microvalve concept

With existing microfluidic platform for improved performance



Technical Approach:

Use of conductive nanoparticles within a flexible matrix to maintain high conductivity throughout range of valve motion

Technical Challenges:

- **Particle to particle contact must be maintained in order for valve to operate correctly**
- **Valve must be small and robust enough to be integrated into microfluidic platform**
- **Use of microarray to grow proteins for TEM analysis must survive TEM environment (microarray as well as proteins)**

Team Members:

Sandia National Laboratories: Microdevice Fabrication Group, Materials Characterization Group, Multiphase and Nanoscale Transport Group

University of Illinois at Champaign-Urbana Kenis Microfluidic Group

ITN Energy Systems New Products Division

Sandia National Laboratories

Nanoengineering for Solid State Lighting

PI: Mary Crawford

National Institute for Nano Engineering

Objective: to achieve significant energy efficiency advances in Solid State Lighting (SSL) through application of nanoengineering and nanoscience to InGaN-based semiconductor materials and LEDs

Strategic Partner: Rensselaer Polytechnic Institute including Professor Fred Schubert, Professor Christian Wetzel and Professor Shawn Lin

Description of Effort: Two subtasks address major technical challenges to achieving energy efficient LEDs across the visible spectrum

(1) Nanoscale engineering to enhance light extraction of LED materials and devices

→ novel nanostructured graded index materials

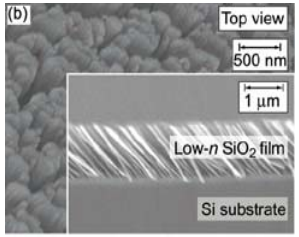
→ advanced light extraction strategies (e.g. photonic lattice and surface plasmon approaches)

(2) Nanoscience studies of InGaN to improve internal quantum efficiency (IQE)

→ study and control of nanoscale InGaN materials properties that impact luminescence processes

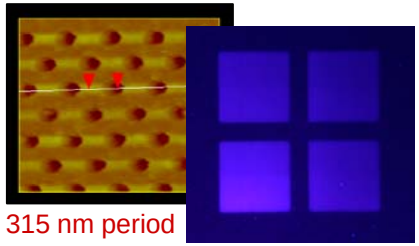
→ focus on critical challenges of low efficiency green materials and "efficiency droop" at high currents

Novel graded index films based on dielectric nanorods



Low index dielectric nanorod arrays through oblique angle deposition

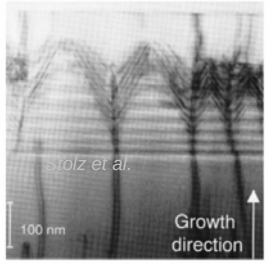
Photonic lattices for light extraction



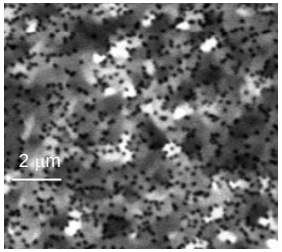
315 nm period

Light extraction from 2 x 2 lattice array

Investigation of nanoengineering of "V-defects" on threading dislocations for enhanced IQE of InGaN



TEM image of V-defects in InGaN multi-quantum wells



Top view cathodoluminescence image of InGaN QWs with V-defects

Potential Impact: achieving LED efficiency goals set by the SSL roadmap would enable U.S. electricity consumption to be reduced by 10% (50% reduction of electricity for lighting), saving ~$25B/ year

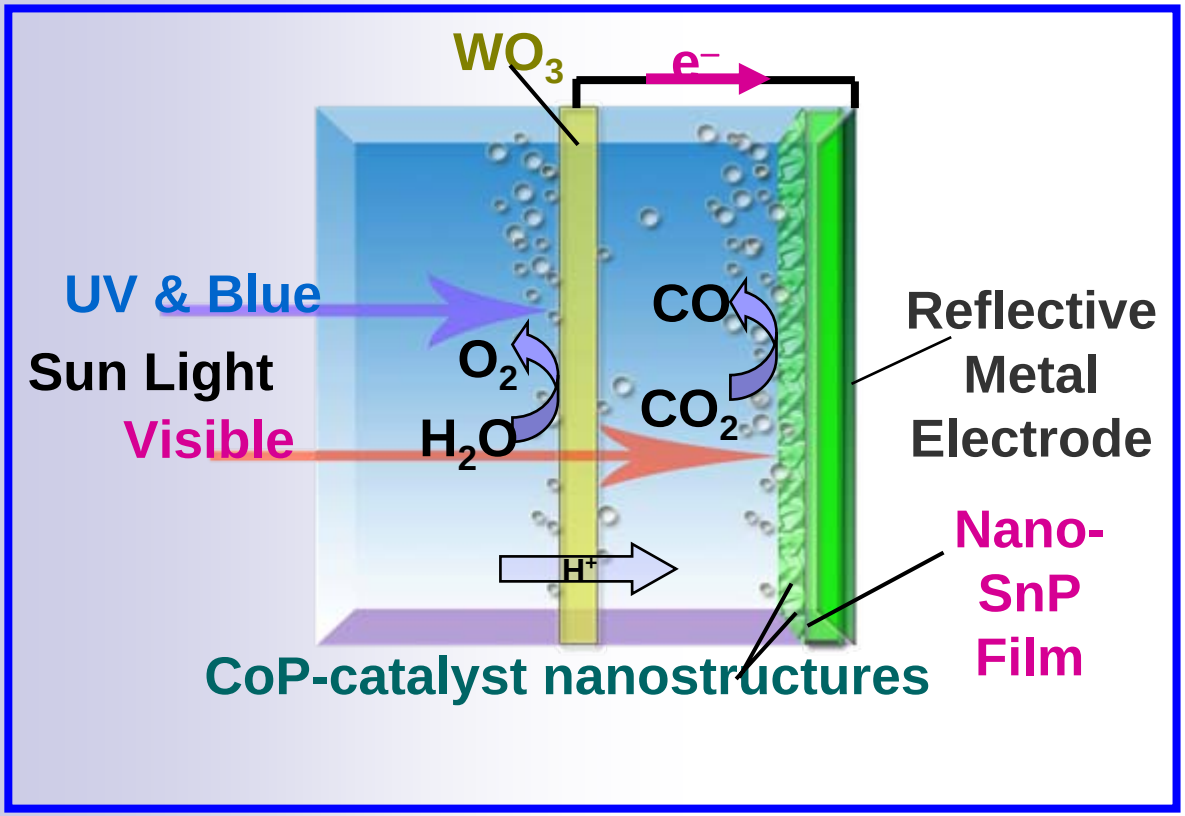
Sandia National Laboratories

CO_2 Reduction Using Biomimetic Photocatalytic Nanodevices

PI: Jim Miller

National Institute for Nano Engineering

Approach: CO_2 Recycling through Bio-inspired Photochemical Reduction to CO



Technical Objectives:
1.) To design, fabrication, and characterize photoactive catalytic nanostructures.
2.) Incorporate nanostructures into stand-alone device.

Partners

Praxair

UC Davis

Nanoexa

$$H_2O + CO_2 \Rightarrow CO + O_2$$

Nano-Macro Tandem Solar CO Cell

Sandia National Laboratories

Fundamentals of Synthetic Conversion of CO_2 to Simple Hydrocarbon Fuels

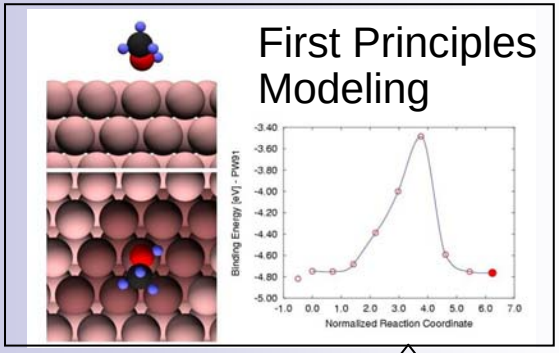
National Institute for Nano Engineering

PI: Rick Kemp

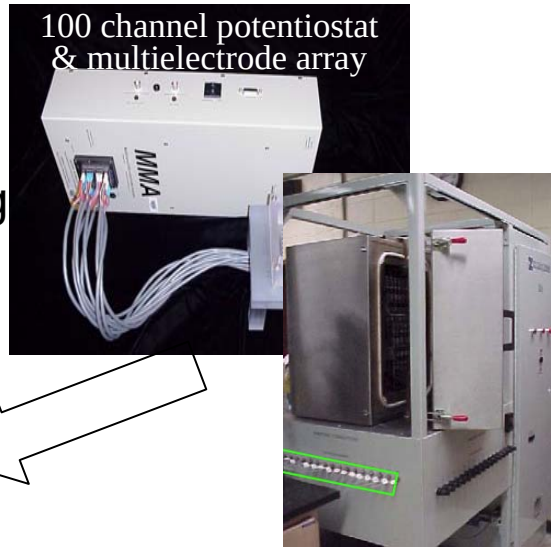
High Level Goal:

Waste CO2 Recycled and Chemically Converted to Transportation Fuels, Providing a Source of Sustainable Energy, While Simultaneously Limiting CO2 Emissions in the Atmosphere

- **Proposed Project Consists of Two Primary Technical Thrusts:**
  - **Process Analysis Task (Thermodynamic Analysis and Process Flows)**
  - **Theoretical Prediction, Preparation, and Evaluation of Nanocatalysts for the Conversion of CO_2 to Methanol (Used as Fuel Itself or Fuel Precursor)**



Materials Screening



Catalyst Preparation (SNL)….

- Nano Cu Prepared on Supports (*e.g.*, ZnO)
  - Nano-Cu Deposited on Electrodes

Partners

UV UW UNM

Sandia National Laboratories

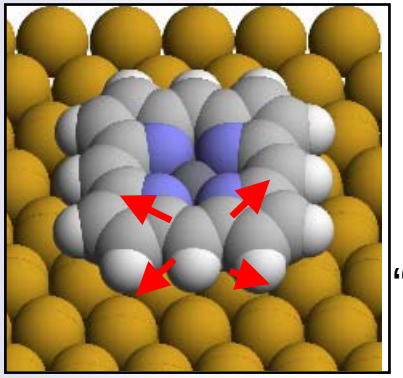
Electronic Structure Calculations to Predict Nano-optoelectronics and Nanocatalyst Functions

PI: Kevin Leung

Problem: Improve predictive capability for DFT methods to model nanocatalysis using transition metal complex or oxide, impact education and national security

Current challenges	Approach	NINE partner
photo-catalysist, e.g., Co-doped anatase	**quasi self-interaction corrected DFT (SIC-DFT)**	**Prof. Nicola Spaldin UCSB, Materials Dept.**
FeO, Fe-nanocatalyst	**self-consistent DFT+U**	**Prof. Nicola Marzari, MIT**

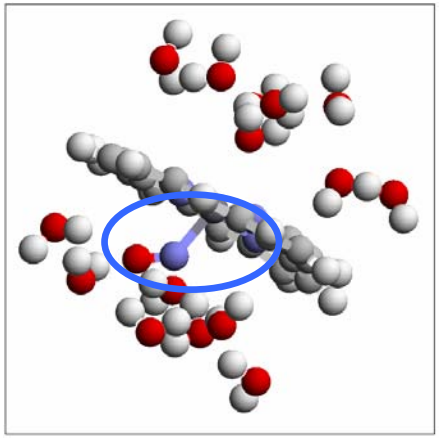
DFT+U success: porphyrin on electrodes: [Leung *et al.* JACS 2006]



$-E$

"Mn(III)" ➔ Mn(II)

on Au electrode



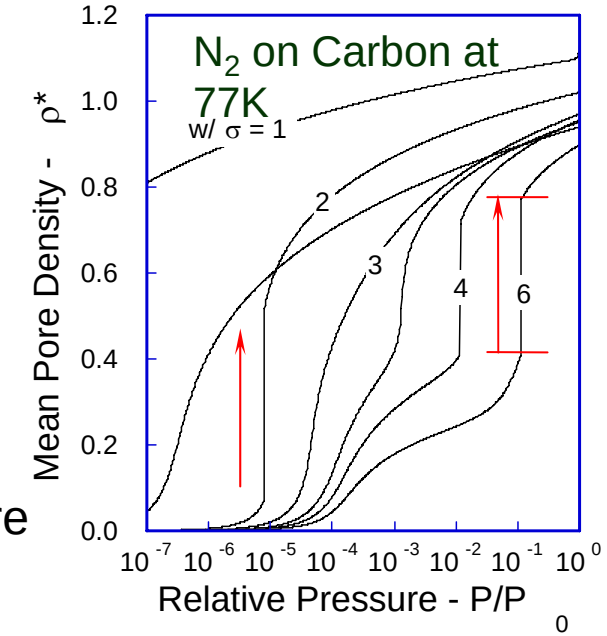
Further DFT+U improvement needed for NO gas sensor [Leung et al. 2007] **(pertinent to CO_2 reduction in water too!)**

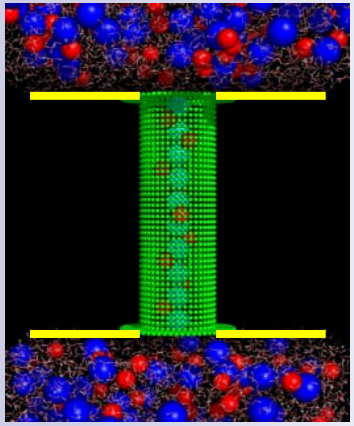
engage NINE partners to improve DFT modeling methods, help meet energy and environment challenges, e.g., via modeling CO2 sequestration reactions

Optimized Nanoporous Materials

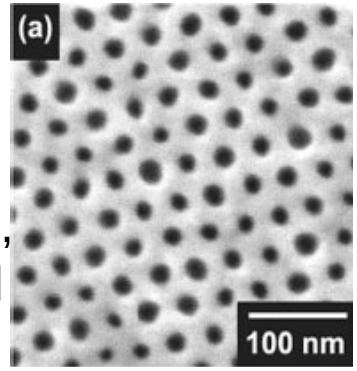
Dave RobinsonPaul Braun, Eric Luijten (UIUC)

The high surface areas of nanoporous materials permit high capacity storage of adsorbates or charge, or high surface reaction rates. However, transport through nanoscale channels slows dramatically as diameter decreases.





We parameterize transport properties for given materials using multiscale computational tools and design tiered pore layouts that allow both high capacity and rapid transport.



Applications in renewable energy storage, pulsed power

We develop soft bicontinuous templates, replace with inorganics, and iterate with more finely scaled templates.