CFN Scientific Themes

Peter Sutter
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Center for Functional Nanomaterials
CFN Scientific Themes

CFN-Based Research:

- **Nanocatalysis** (Peter Sutter, psutter@bnl.gov)
- **Electronic Nanomaterials** (Charles Black, ctblack@bnl.gov)
- **Soft- & Biological Nanomaterials** (Oleg Gang, ogang@bnl.gov)
- **Electron Microscopy** (Yimei Zhu, zhu@bnl.gov)
- **Theory & Computation** (Mark Hybertsen, mhyberts@bnl.gov)

Focus - **Energy Applications**: Functional nanomaterials for exploiting renewable energy sources, energy storage, utilization.
Nanocatalysis

Leader: Peter Sutter (psutter@bnl.gov)

Nano-Catalysis - utilize phenomena at the nanoscale to achieve improved activity, selectivity, resistance to poisoning.

- Increased surface/volume ratio.
- Electronic structure, charging.
- Availability of specific active sites.
- Dynamically changing active sites.
- Alloying, tuning of composition, strain.
- Cooperative/proximity effects, spill-over.

Focus - In-Situ Microscopes & Probes

Interrogate individual nanostructures …

- In relevant environments: realistic pressures & temperatures.
- With combined spatial, temporal, and spectral resolution.
Transition Metals: Oxidation Catalysis

**CO Oxidation Catalysis:** Identification of oxygen-rich structures on the catalyst [Ru(0001)]; mechanism & reactivity of nano-catalysis.
Electronic Nanomaterials

**Leader:** Charles Black (ctblack@bnl.gov)

Explore nanostructured materials for enhanced or novel optical/electronic properties (esp. *energy conversion*)

**Science program:**
- Photovoltaics
- Photochemistry
- Nanoplasmonic structures

“**The Sun is a singular solution to our future energy needs**”

**But:** Enormous gap between potential and current use of solar energy

⇒ Need *conceptual breakthroughs* through high risk/high payoff research

http://www.sc.doe.gov/bes/reports/abstracts.html
Improved photovoltaic conversion:

- **Increase** junction surface area
- **Decouple** junction absorption length from carrier diffusion length
- **Provide** high mobility pathways for charge extraction

**Fabrication challenge:** nano-features ⇔ macro-device
Templated Self Assembly

**Idea:** Use natural patterns to create large-area materials with controllable nm-scale heterogeneity.

- Large area patterning (~cm²)
- Small feature sizes (<20nm typical)
- Periodic with high density (>10¹⁰/cm²)
- Reasonable size uniformity (std. dev. ~10%)
- All dimensions tunable with nm-scale precision
- Flexible material choices

![Image of template and final structure](image-url)
Soft- & Biological Nanomaterials

**Leader:** Oleg Gang (ogang@bnl.gov)

**Challenges:**

- Control of nano-object **positioning and orientation.**
- Assembly of **large scale systems/devices** w. designed architectures.
- Building **hierarchical structures.**
- Dynamic (re-configurable, responsive, self-repaired…) systems?

**Soft/ Biomimetic Approach for Building Nanoscale Systems:**

Utilize/adopt biological structures with **recognition interactions** and **regulated behavior** for the control of non-biological nano-objects

Use a rich phase behavior of soft systems for assembling functional nano-components

Apply assembly approaches to **build functional nano-systems** for applications in energy transfer, catalysis and sensing.
Electron Microscopy

Leader: Yimei Zhu (zhu@bnl.gov)

Hitachi HD2700C Dedicated scanning TEM
Analytical STEM (EELS)

FEI Titan 80-300 Environmental TEM
In-situ experiments at elevated pressure & temperature

JEOL 2100F High resolution analytical TEM
Analytical TEM (imaging, EDS)
Analytical STEM

Analytical STEM: Nanoprobe EELS

Twin boundary

Twin interior

Intensity

oxygen K-edge

Energy Loss (eV)

520 525 530 535 540 545 550
Theory & Computation

Leader: Mark Hybertsen (mhyberts@bnl.gov)

Expertise in theory & computation:
- Bonding, structure & reactivity
- Electronic states, transport & optical properties
- Assembly & emergent pattern formation

Current research projects:
- Mechanism & design: Oxygen reduction reaction on nanocatalysts (Ping Liu)
- Catalyzed water oxidation by solar irradiation of band-gap-narrowed semiconductors (Jim Muckerman)
- Bonding, electronic states and electron transport at metal-organic interfaces (Mark Hybertsen)
Catalytic Activity of Pd$_3$Fe Nanocrystals

**Pd-Fe alloy nanocrystals for ORR:**
- Peak Oxygen Reduction Reaction activity observed for Pd$_3$Fe/C
- Comparable to Pt/C (Shao, Sasaki & Adzic, JACS, 2006)

**Analysis of O binding:**
- Volcano variation of ORR activity with calculated O-binding energy
- Pd$_3$Fe(111) predicted to be less active than Pt:
  Over strong O-binding at the Fe-Pd hybrid sites (BE$_O$<-3eV)

**Key result:** Pd ML/Pd$_3$Fe(111) predicted more active than Pt with a moderate O-binding

*Shao, Liu, Zhang, & Adzi, J Phys Chem B, 2007*
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