Research in Materials for Energy Conversion and Storage

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Research in Materials for Energy Conversion and Storage

Interdisciplinary research thrust combining departments across the colleges of engineering and science.

- **Batteries for energy storage**
  - Modeling Si surface for anode reactions

- **Superconductors for energy transmission**
  - Coated conductors

- **Thermoelectrics and solar energy**
  - Nanowires for thermal energy
  - Microbial Fuel Cells

- **Fuel cells**
  - SOFC and its reliability test

- **Experimental and modeling**
  - YBCO + CeO2 thickness (µm)
  - Critical current density (MA/cm²)

- **Nanowires for thermal energy**
Solar cell efficiency has been greatly improved by hybridization between photovoltaic and thermoelectric devices, K.T. Park et al. submitted.
SiGe nanowires with high ZT value

Long ZnO nanowire for high temperature TE

Nanostructures improves thermoelectric efficiency

Mg$_2$(Si,Sn) solid solution thermoelectric materials have cheap, abundant and non-toxic constituents.

High ZT at 400-500 C range
High Power & Long Life Li-ion Battery

LiCoO$_2$ core-
Li$_3$VO$_4$ shell

- Overcome the overcharge problem
- Improve cycling performance and C-rate capability

Power generation with wastewater

3D electrode

- CNTs
- Stainless Steel Mesh
- Highway for electrons transfer;

Power density (mW/m$^2$)

<table>
<thead>
<tr>
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<th>Power density (mW/m$^2$)</th>
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<tbody>
<tr>
<td>Bare SS mesh</td>
<td>0.4</td>
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<tr>
<td>SS-CNT</td>
<td>433.2</td>
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Flexible Power Generation & Cooling

Engineering thermal and electrical transport with nanomaterials

TE behaviors of polymer composites

Air stable p- and n- junction modules

The testing modules produced ~6 mV voltage with ~25 nW generated power upon ~22°C temperature differences [3].

Engineering carrier concentration

The value of power factor was improved by ~5.5 times after adjusting PANi/CNTs samples.
NanoBio Systems Lab

*at the interface of micro/nano technology and life sciences*

**Research interest**

Solving grand challenge problems in the broad area of energy and health

[ENERGY]

- Microbes as biorefineries for electricity, fuel, and fine chemical production
  - Microbial Fuel Cell: Harvesting electricity from wastewater
  - Photosynthetic Microalgae: Producing transportation-grade oil in ponds
- Development of microfluidic lab-on-a-chip systems that can accelerate R&D in renewable bioenergy sector

[HEALTH]

- Development of microfluidic lab-on-a-chip systems for remote healthcare and point-of-care diagnosis, cancer diagnosis and prognosis, microphysiological systems for drug/toxicity screening, infectious disease, antibiotic resistance
Projects in Energy

Microbial Fuel Cell
- Harvesting electricity from wastewater
- Develop high-throughput screening platforms
- Develop new nanomaterial electrodes
- Funded through Bill and Melinda Gates Foundation, NSF, and QNRF

Microalgae as a Photosynthetic Refinery
- Transportation-grade oil production from microbes
- Develop microalgae lab-on-chip photobioreactor platform for genetic screening leading to scalable biofuel production
- Funded through the Emerging Frontiers in Research and Innovation (EFRI) grant from the NSF (US $2M)

Funding for the NanoBio Systems Lab is being provided by:
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More than 80 journal articles in HTS related work
Nanostructured coated Superconductors for power transmission

More than 50 journal articles
Vertical Aligned Nanocomposite Multifunctional nanocomposites

More than 20 journal articles
Thin Film Solid oxide fuel cells for energy conversion

Nanostructured ceramics for nuclear energy applications
More than 10 journal papers.

More than 30 journal articles
Microelectronics and optoelectronics
By inserting CeO$_2$ nanolayers in YBCO matrix, YBCO $J_c^{sf}$ maintains a high value and does not follow the thickness-dependence.


Pinning in high temperature superconductors heteroepitaxial second phases in YBCO films with a $1.5 \times 5 \times$ increase in $J_c$.

Solid oxide fuel cells

La$_{0.5}$Sr$_{0.5}$CoO$_3$/Ce$_{0.9}$Gd$_{0.1}$O$_2$ VAN film as cathode-electrolyte interlayer

Solid oxide fuel cells
Single cells with LSCO/CGO VAN interlayer show 2-3 times enhancement in power density.

Solid Oxide Fuel Cells (SOFCs)
Ideal candidates for smart-grid energy storage and electrical load leveling because of:

- High electrical and cogeneration (i.e. combined heat and power) efficiencies of 50-60% and 80-90%, respectively.
- The highest volumetric and gravimetric energy densities of any energy generation technology.
- Backwards operation producing fuel and oxidant and using electricity. Later, they can resume normal operation, producing electricity from fuel and oxidant.
Other advantages of SOFCs or ceramic fuel cells:

- Extracting energy from biogas, gasoline, natural gas, jet fuel, syngas, hydrogen, or any oxidizable fuel.
- Lower CO$_2$, NO$_x$, SO$_2$, volatile organic compound (VOC), and particulate emissions compared to conventional fossil fuel technologies.
- Low costs from of ~$150/kW.
- Life time extended up to 40,000 hours.

Challenges:

Improving SOFC materials properties and microstructures to allow low temperature (200-500°C) SOFC operation and the associated benefits of improved thermodynamic efficiencies, longer service lifetimes, rapid start-up times, and cheaper balance-of-plant costs.

Lifetime of SOFC is in many cases limited by their mechanical failures!
Research is focused on understanding and improving mechanical properties of SOFC’s materials and components.

Approach:
The mechanical reliability of the SOFC is determined by the stress distribution and the stochastic distribution of strength. Therefore, the probability of failure of SOFC components is determined by the area where two distribution curves overlap.

Example I: Residual Stresses

Residual stresses in Ni-YSZ/YSZ bilayer after reduction as a function of temperature.

Compressive stresses in YSZ electrolyte can reach 600 MPa!
Example II: Mechanical Properties of Electrolyte

Doped oxides with fluorite structure show lowest elastic moduli, strength and fracture toughness due to anelastic relaxation of defect at near operating temperatures of SOFC. The decrease in mechanical properties can be controlled by controlling the type and concentration of dopants.

Example III: Thermal Cycling of Anode

Left: Decrease of characteristic biaxial stringent of Ni-YSZ Cermet anode material with the number of thermal cycles up to 800 °C.

Right: SEM of the Ni-YSZ Cermet anode material: Red– YSZ, Dark Blue – Ni Light Blue – residual NiO.
Professor, Department of Chemical Engineering, and Materials Science and Engineering Program

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Research interests: first-principles computational materials design and evaluation; applications to catalysis, electrocatalysis, gas separations.

Recent/current topics: fuel cell electrodes, battery electrodes and electrolytes, CO₂ capture; catalyzed growth of single-walled carbon nanotubes
• **Fuel cell electrodes**: design and evaluation of alloy materials for efficient oxygen-reduction electrocatalysts (DOE/BES 2001-2012)

• **Battery electrodes**: design and evaluation of new cathode materials based on metal-phtalocyanines (AFOSR 2002-present)

• **Battery electrodes and electrolytes**: analysis and evaluation of silicon anodes for Li-ion batteries; investigation of electrolyte stability on Si anodes; design of alternative electrolytes (BATT-DOE 2013-2017)

• **CO₂ capture and separation from flue-gas mixtures**: evaluation and design of new materials for CO₂ separations from flue-gas mixtures containing N₂, water, and acid impurities (ARPA-E 2010-2012)

• **CVD synthesis of single-walled carbon nanotubes**: analysis and evaluation of synthesis variables towards selective growth of single-walled carbon nanotubes with specific chiralities (DOE/BES 2006-present)
**Recent results**

**Dealloying of nanoparticles**

→ porous fuel cell catalysts


**Metal dissolution in acid medium**

Functionalized Si surface plays critical role on solid-electrolyte interface of Li-ion batteries

Balbuena et al, work in progress

**Catalyzed growth of single-walled carbon nanotubes**

Gomez-Gualdron and Balbuena, Carbon, 2013

**CO₂ captured in molecular trap**

Li, Yu, Lu, Sun, Sculley, Balbuena, and Zhou, Nat. Comm., 2013
Jorge M. Seminario

- Fox Professorship
- Professor of Chemical Engineering
- Professor of Electrical and Computer Engineering
- Professor of Materials Science and Engineering
- seminario@tamu.edu
- http://research.che.tamu.edu/groups/Seminario/index-1.html

**Research interests**
Nano and Molecular Electronics, Nanotechnology, Nanosensors, THz Molecular Systems, Digital Signal Processing, Quantum Chemistry, Energetic Materials and Transition Metals, VLSI for Nanoelectronics, Molecular Dynamics Simulations, Atomic and Molecular Physics

**Current topics**
- NanoSensors for chemical, biological, and nuclear agents.
- Silicon based battery electrodes
On-going projects -- 2013

• **Identifying the Presence of Uranium and/or Plutonium:** Developing graphene nanoplasmonic sensors to determine trace amounts of uranium and/or plutonium. Argonne National Lab

• **First Principles Modeling of SEI Formation on Bare and Surface/Additive Modified Silicon Anode:** analysis and evaluation of silicon anodes for Li-ion batteries; investigation of electrolyte stability on Si anodes; design of alternative electrolytes. Lawrence Berkeley National Lab

• **Near and Far-Field Interfaces to DNA-Guided Nanostructures from RF to Light waves:** Exploiting the Spectrum Develop of nanosensors based on DNA and CNT for chemical and biological agents using most of the electromagnetic spectrum. MURI/ARO Program
Design of Nanosensors for Fissile Materials in Nuclear Waste Water

Jorge M. Seminario

Two prototypes I, II being fabricated

SiN
Au
Graphene

SiO₂
Au

Si

UO₂(NO₃)₂(H₂O)₃ [1–10 ppm]

UO₂(NO₃)₃(H₂O)₂ [1–100 ppm]

PuCl₂(H₂O)₆²⁺ [100 ppt]
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