Materials Science and Engineering: The Science of Stuff

February 28, 2017

Ultrafast Optics and its Applications

Michelle Sander
Assistant Professor

Electrical & Computer Engineering
Materials Science & Engineering
BU Photonics Center

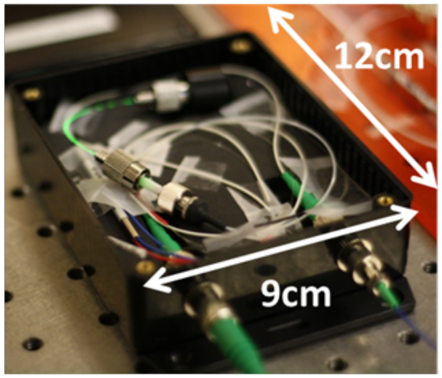
Ultrafast Optics and Femtosecond Laser Development

Laser Physics

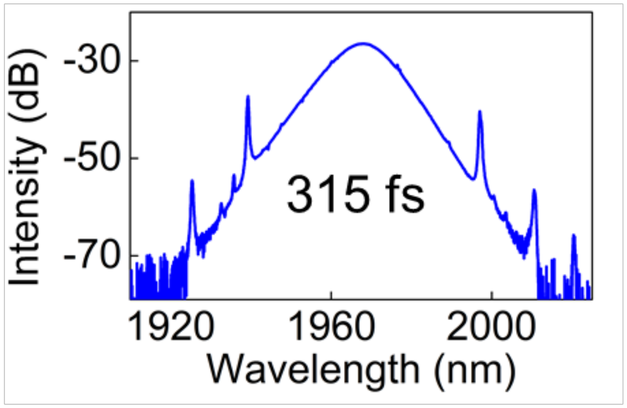
Nonlinear Optics

Pulse Dynamics

Compact, all-fiber design



Thulium/Holmium Lasers



Novel Optical Materials

Novel Characterization Techniques

Broadband Emission 1.7 – 2.1 μm

Eye-Safe Regime

LIDAR

Spectroscopy

Biomedical Treatment/Surgery

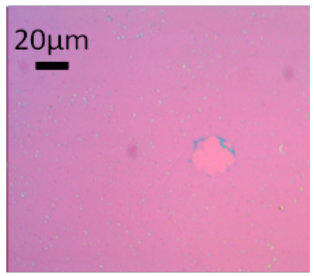
Micromachining

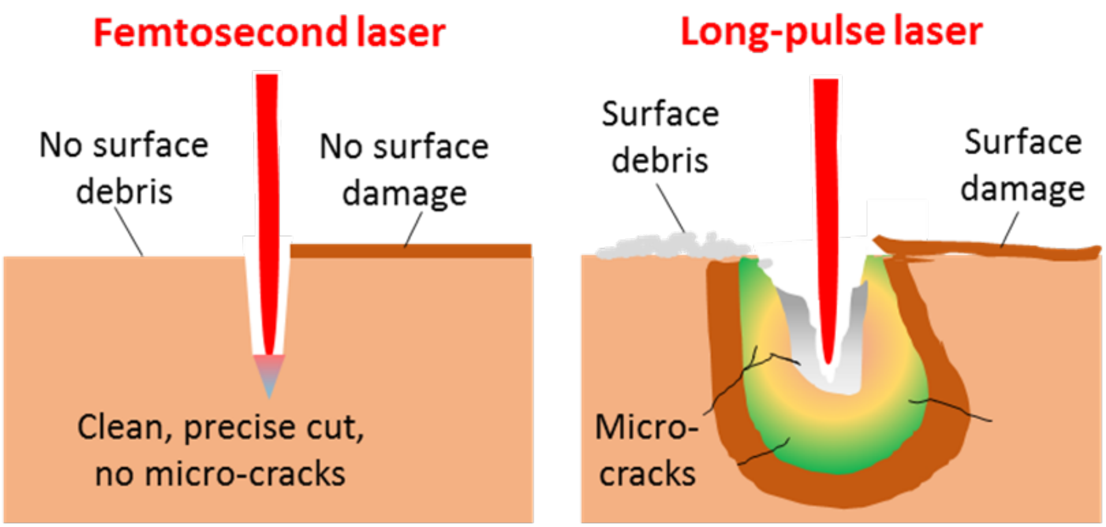
Precision Metrology

Frequency Combs

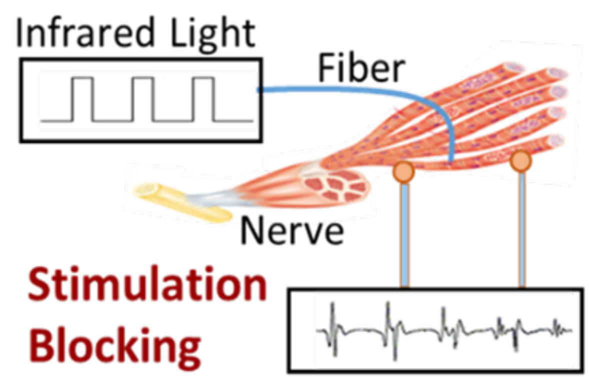
Ultrafast Material Interaction

Graphene Micromachining



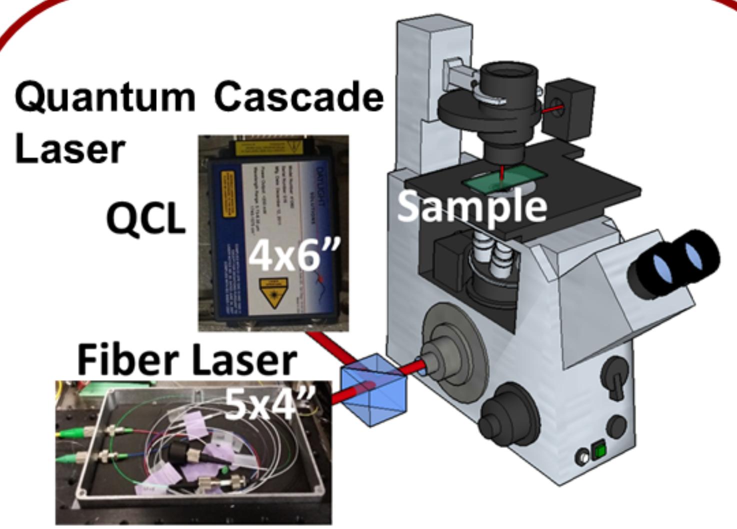


Infrared Nerve Stimulation

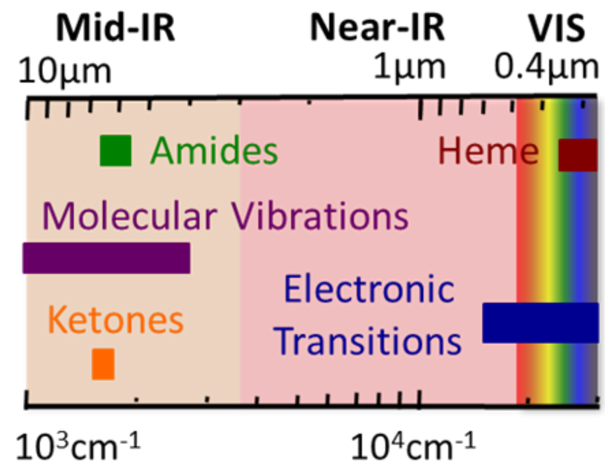


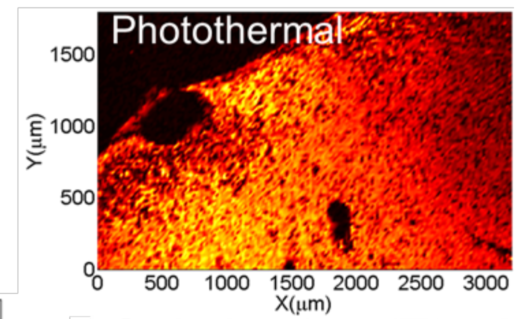
- High spatial selectivity
- No electrical stimulation artefacts

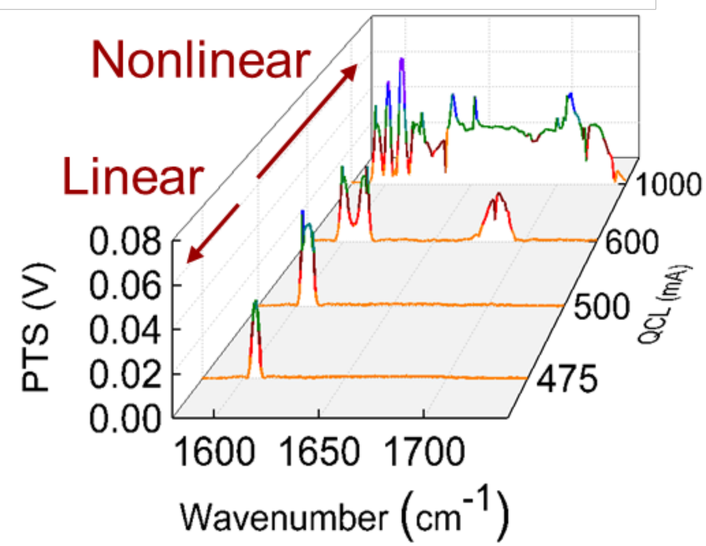
Mid-Infrared Vibrational Photothermal Spectroscopy and Imaging: Chemical/Biological Characterization

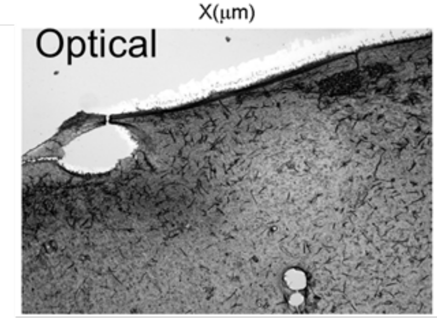


- Robust, non-destructive, compact, eye-safe, label-free
- Pump/Probe with high brightness mid-IR QCL
- High sensitive near-IR detection
- Low optical powers ~ 1mW









Advancing High Energy Density Batteries Through Controlled Mass Transport

Emily Ryan

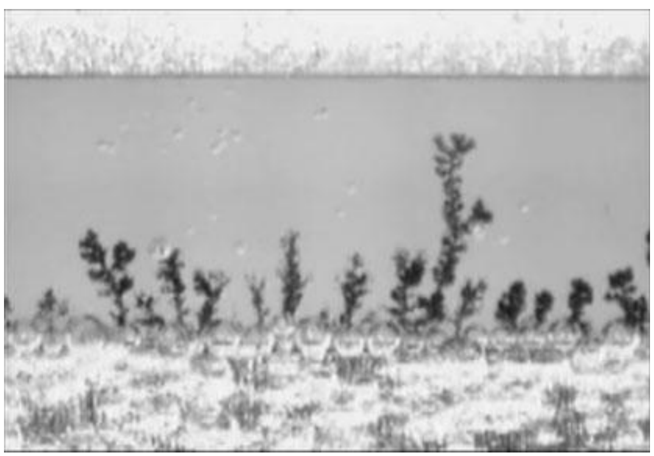
Assistant Professor

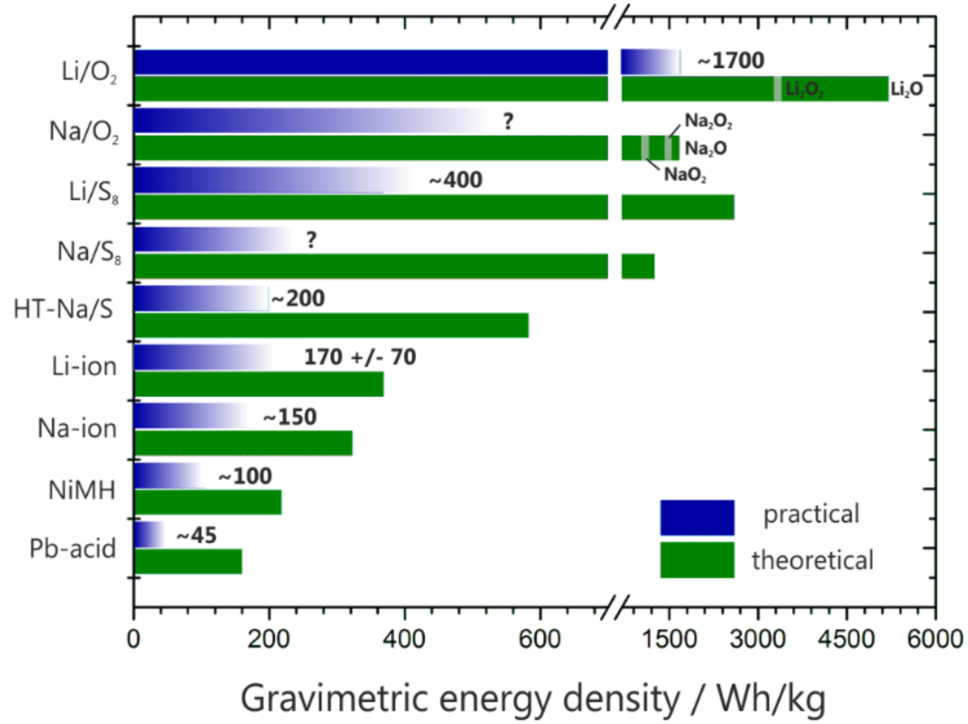
Mechanical Engineering

Materials Science & Engineering

High Energy Density Lithium Batteries

- Challenges
  - Interfacial Stability
  - Material properties
  - Long-term performance
    - Degradation with cycling

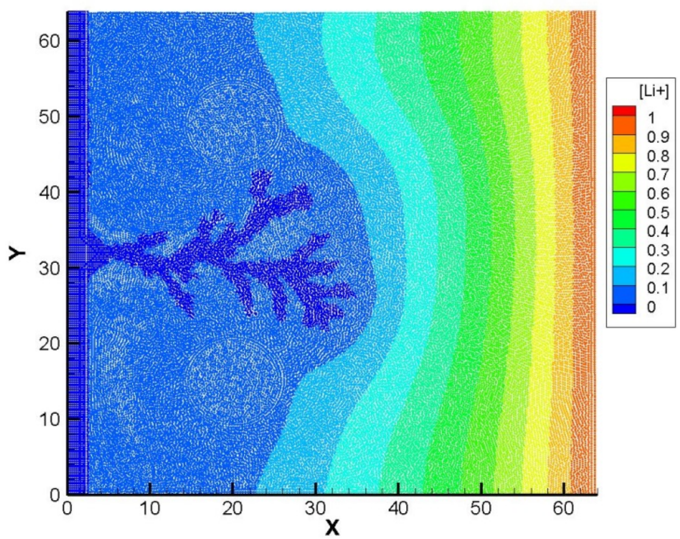




Images from:
https://www.extremetech.com/mobile/217191-new-lithium-air-battery-could-drive-huge-performance-gains
https://mitechnews.com/new-products-contracts/u-m-researchers-study-dendrites-suspected-causing-smart-phone-battery-fires-create-batteries-store-10-times-energy/

Computational Modeling of Dendrite Growth at the Anode-Electrolyte Interface

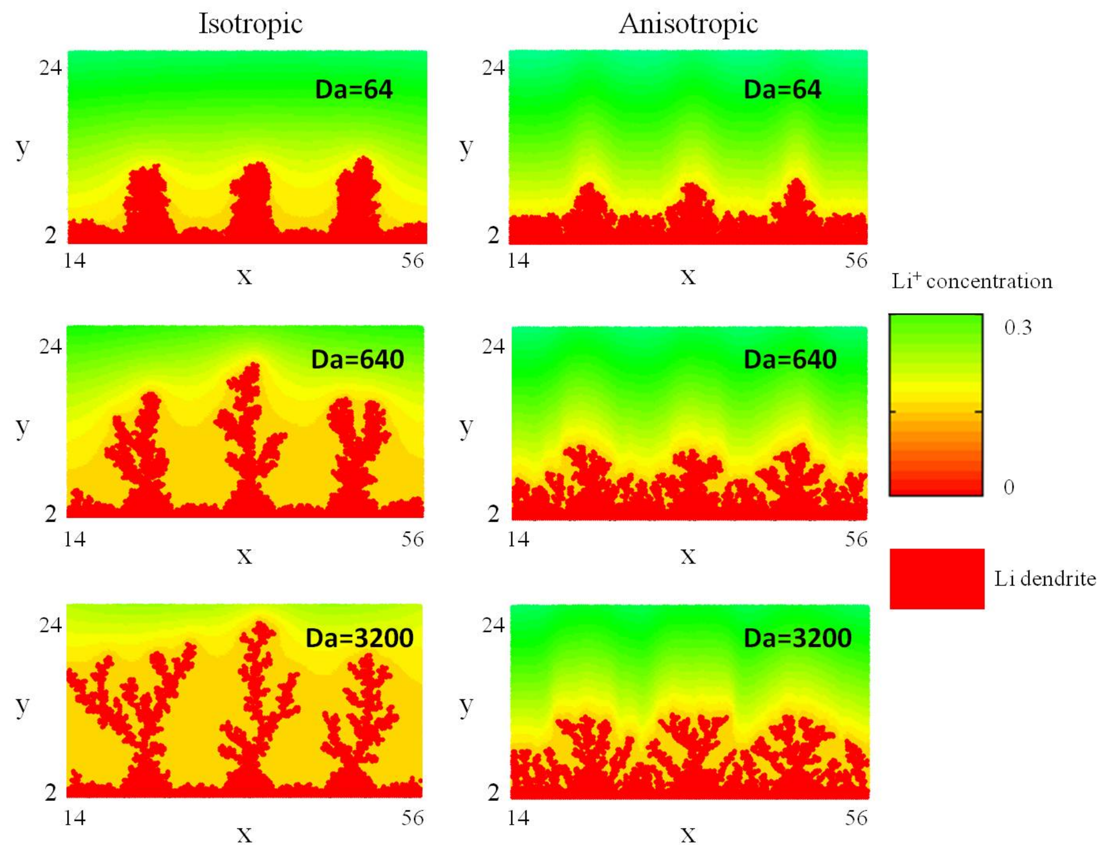
- Lagrangian particle based model of dendrite growth
  - Reactive transport: diffusion, convection, surface reactions
- Investigating driving forces for growth and morphology changes
- Design novel electrolytes to suppress growth
  - Controlled mass transport through electrolyte
  - Materials informatics for materials discovery



Suppressing Dendrite Growth

- Reduce mixing near the electrode-electrolyte interface by inducing anisotropic transport properties
  - Maintains battery performance
  - Reduces dendrite growth
- Anisotropy

$$\frac{D_{yy}}{D_{xx}} = 10$$

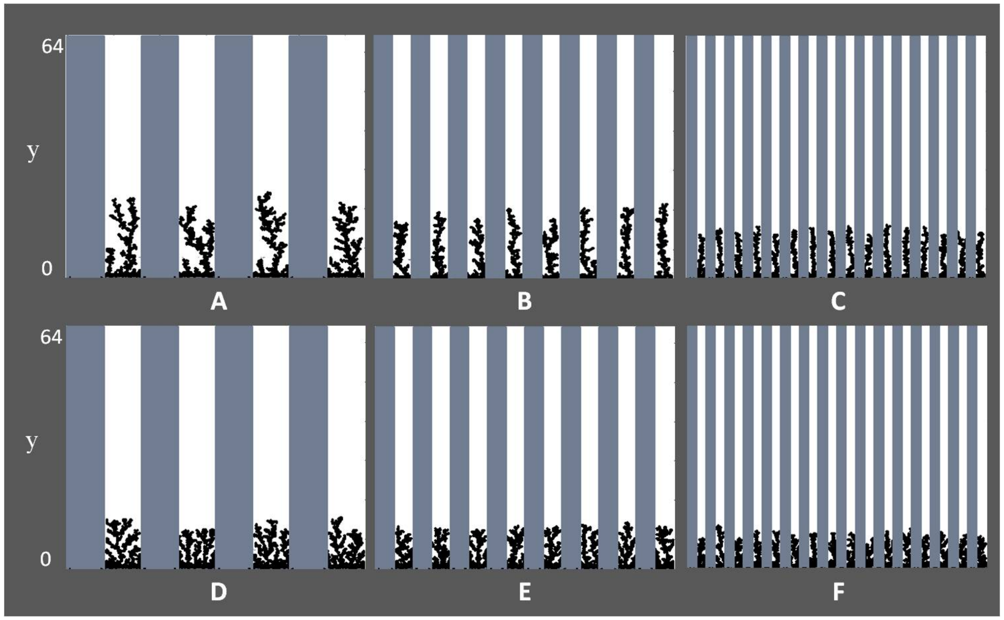


Designing Electrolytes to Suppress Dendrite Growth

- Controlling the transport properties in the electrolyte can control the growth rate and morphology of dendrites

Isotropic

Anisotropic



How can we translate these studies to enhanced battery performance?

- New electrolyte materials
  - Anisotropic transport properties
  - Low viscosity
  - Stable under battery operating conditions
- Structured electrolytes
  - Hybrid liquid-solid electrolyte
  - Force anisotropic transport
- Separation membranes
- New Materials
  - Materials Informatics

Organic Electronic Materials

Malika Jeffries-EL
Associate Professor

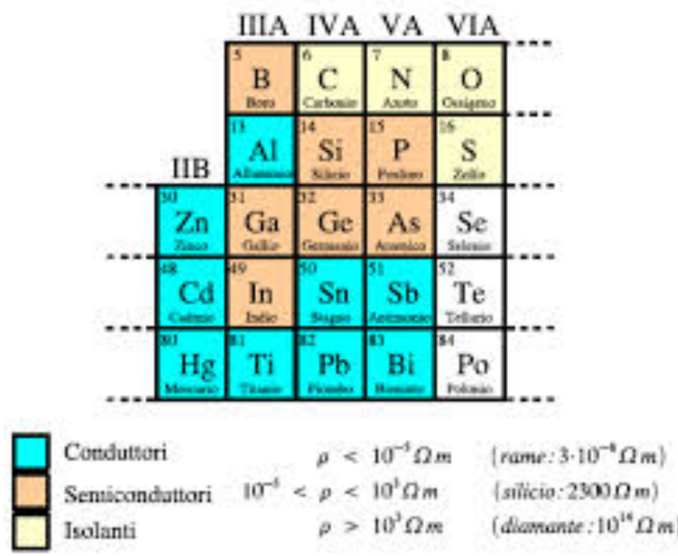
Chemistry

Why develop organic electronics?

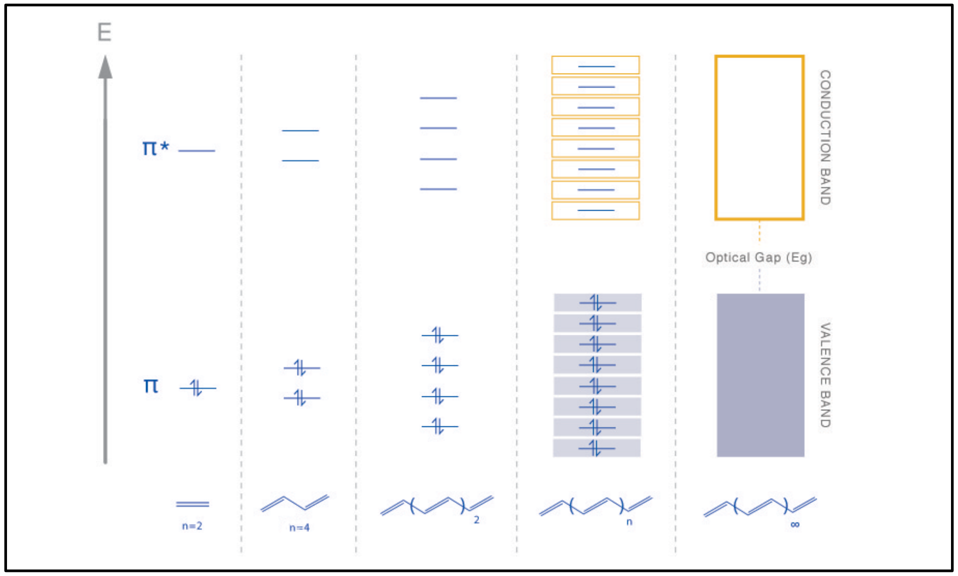
❖ Cellular Phones

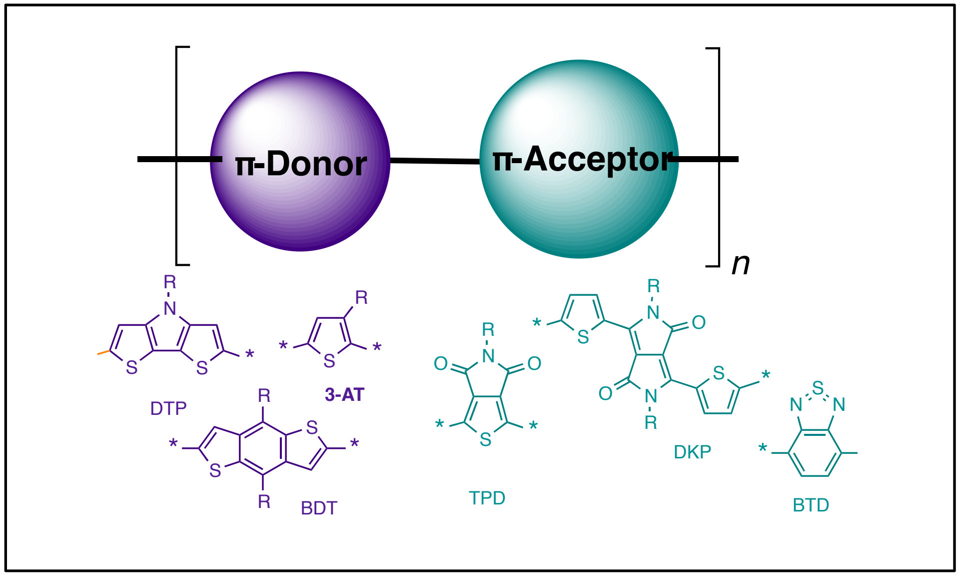
❖ Tablets

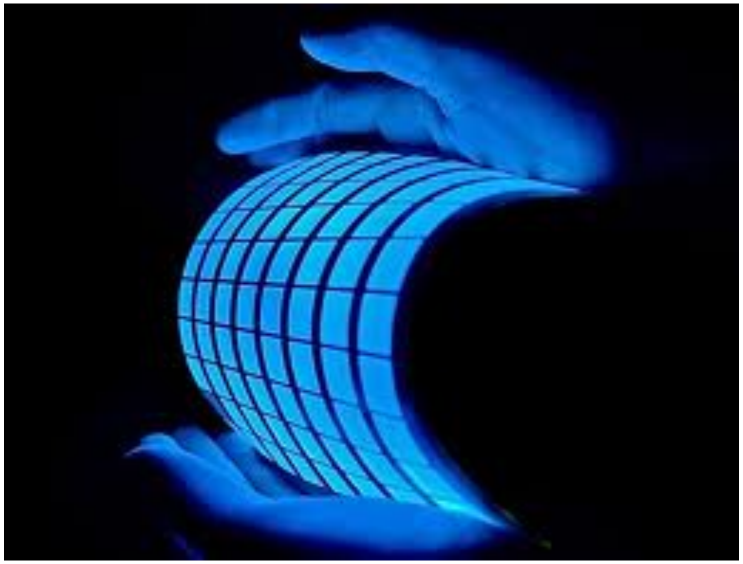
❖ Computers



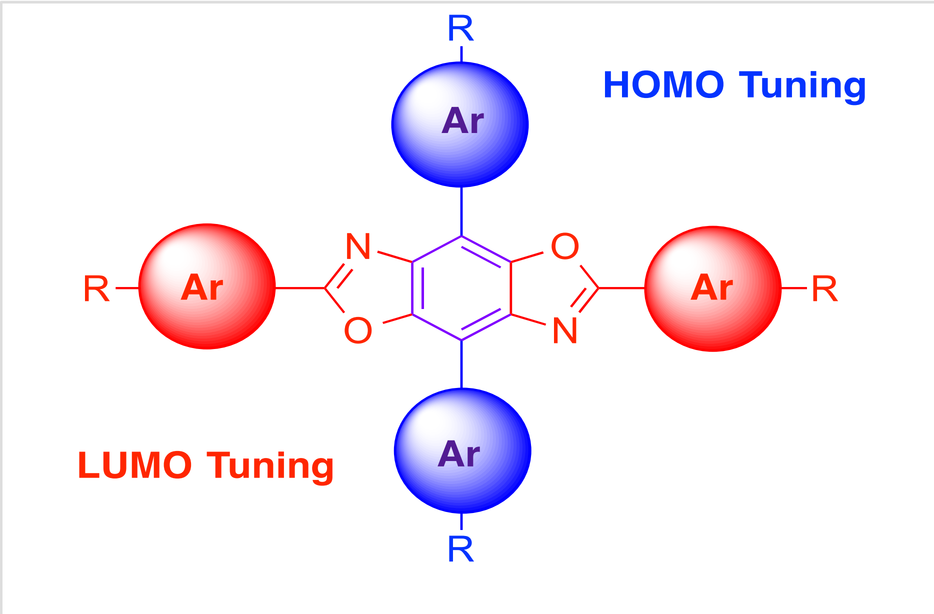
Organic electronic materials

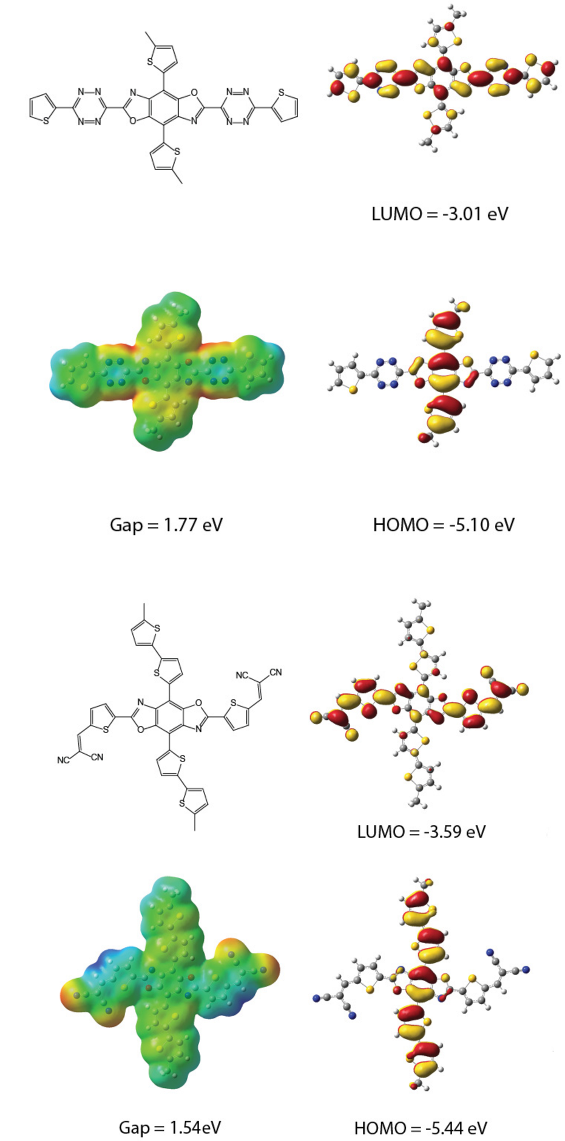






Example: Tunable Organic Semiconductors

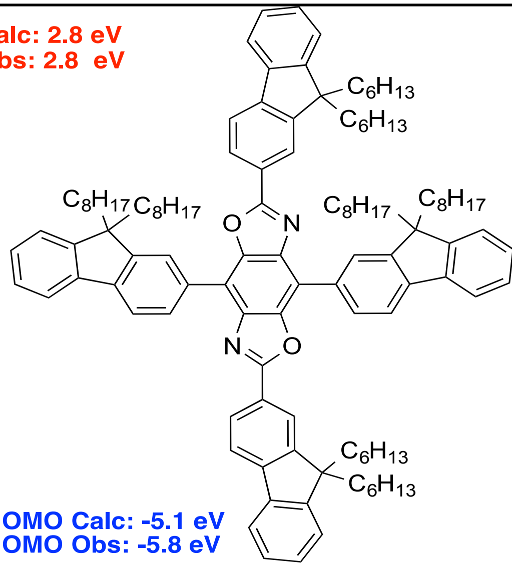




- Facilitates selective tuning of the HOMO and LUMO levels.
  - Wide band gap materials for use in OLEDS
  - Narrow band gap materials for use in OSCs

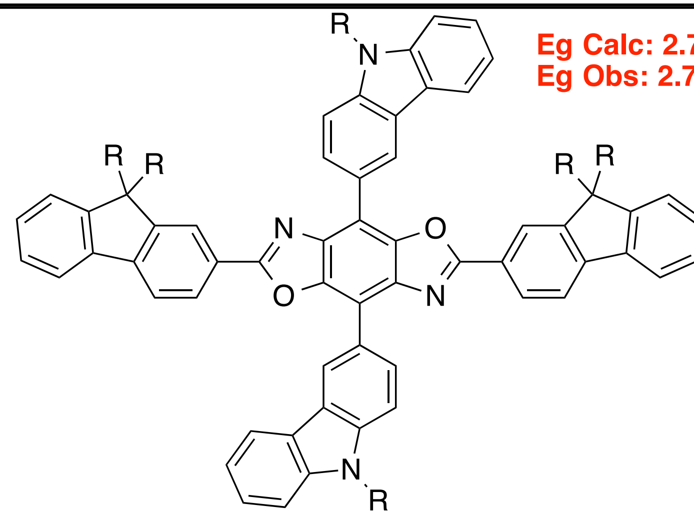
Blue light emitting diodes

Eg Calc: 2.8 eV
Eg Obs: 2.8 eV



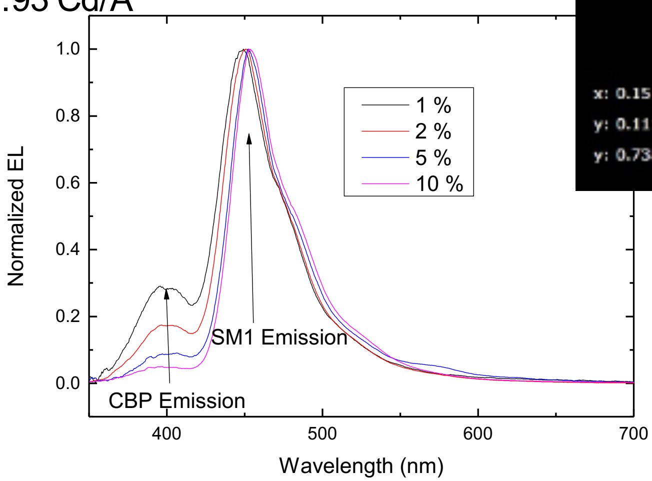
HOMO Calc: -5.1 eV
HOMO Obs: -5.8 eV

Eg Calc: 2.7 eV
Eg Obs: 2.7 eV

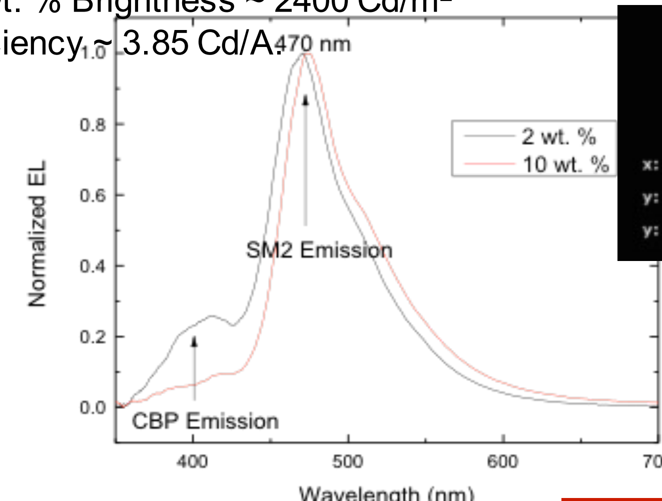


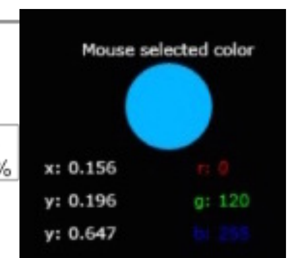
HOMO Calc: -5.3 eV
HOMO Obs: -5.6 eV

2.0 wt. %, Brightness: 1568 Cd/m^2,
EL= 1.93 Cd/A



10 wt. % Brightness ~ 2400 Cd/m^2
Efficiency ~ 3.85 Cd/A



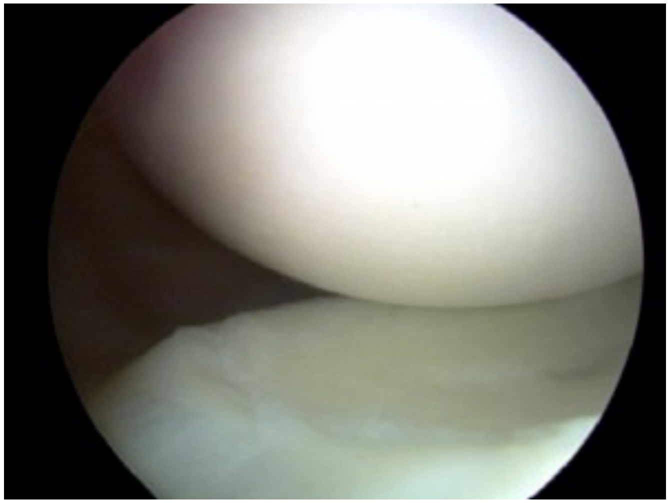


Biomimetic Growth Factor Delivery Strategies to Improve Mechanical Functionality of Engineered Cartilage

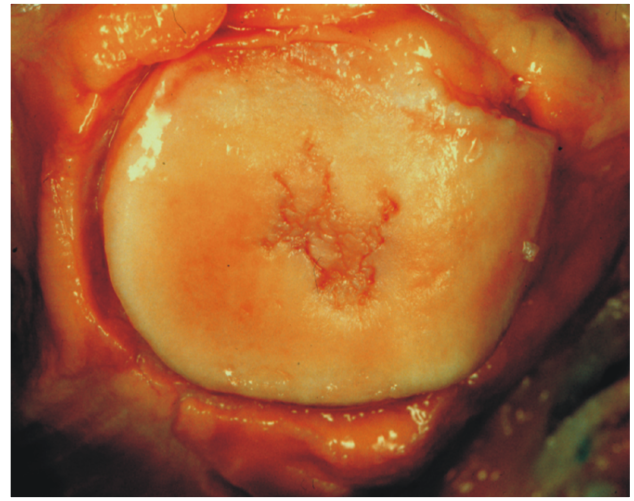
Michael Albro
Assistant Professor

Mechanical Engineering

Osteoarthritis and Cartilage Tissue Engineering

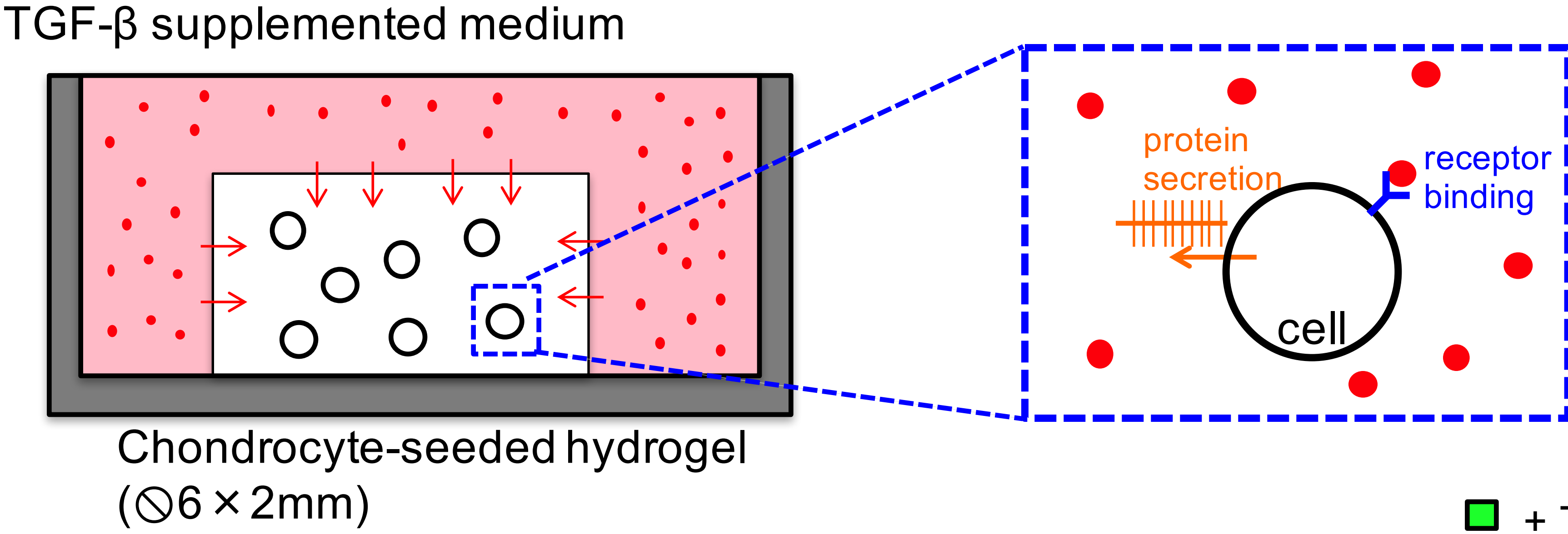


[Howardluksmd.com]



- Osteoarthritis (OA) is a debilitating condition involving the degeneration of articular cartilage.
  - 33.6% of adults of age 65+
  - Medical costs ~$180 billion per year in U.S.

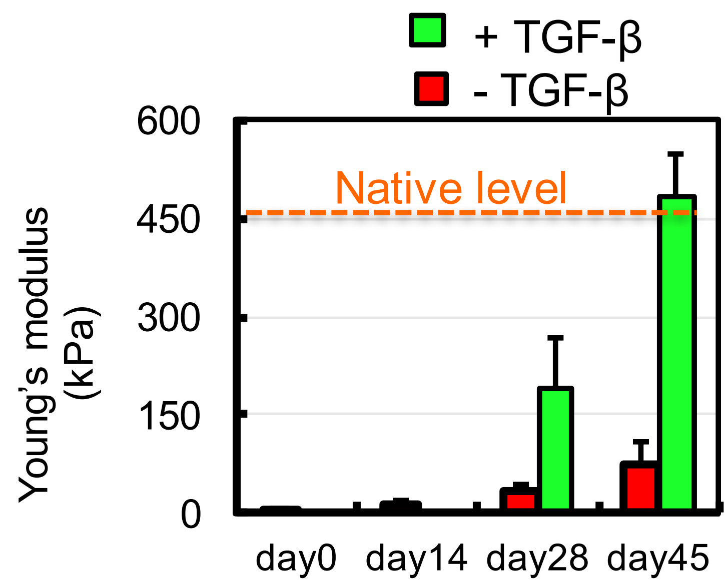
Cartilage Tissue Engineering Techniques



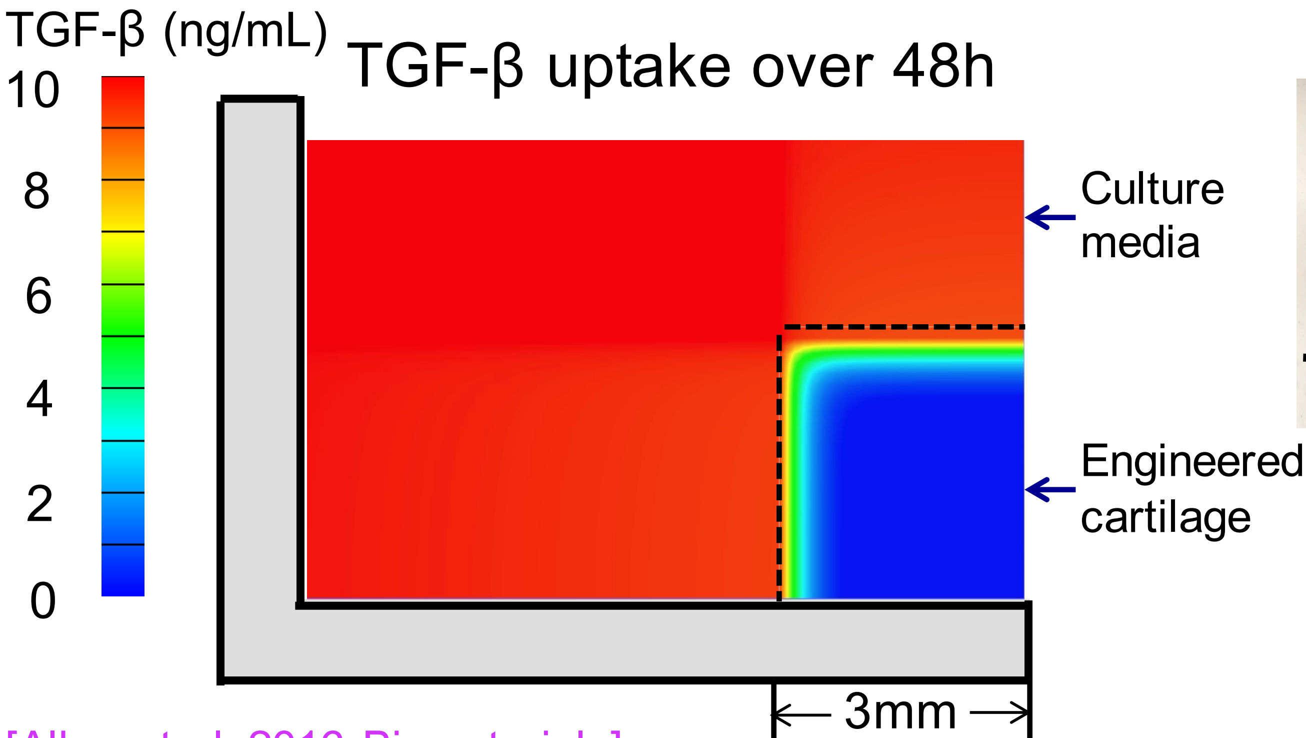
Day 0

Day 45

[Ng et al, 2009]

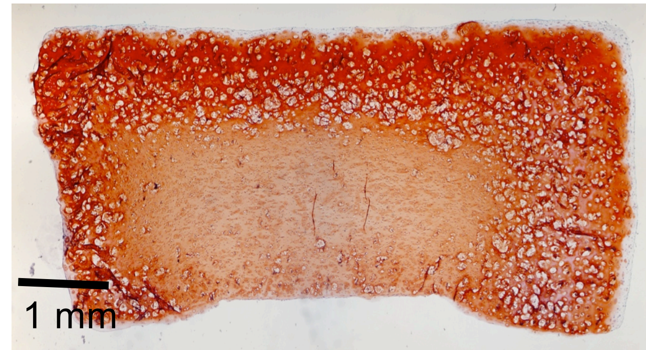


Uptake of TGF-β into Engineered Cartilage

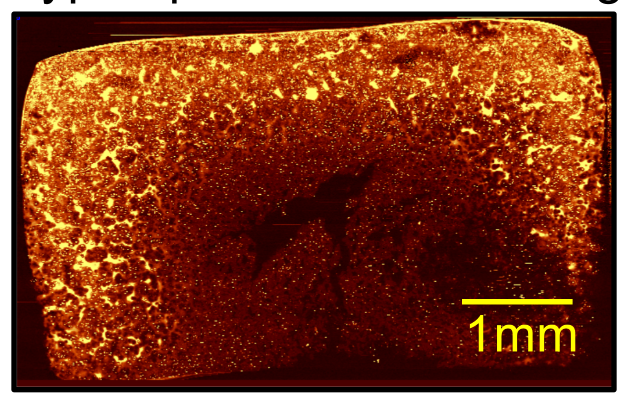


[Albro et al, 2016 Biomaterials]

Histological staining

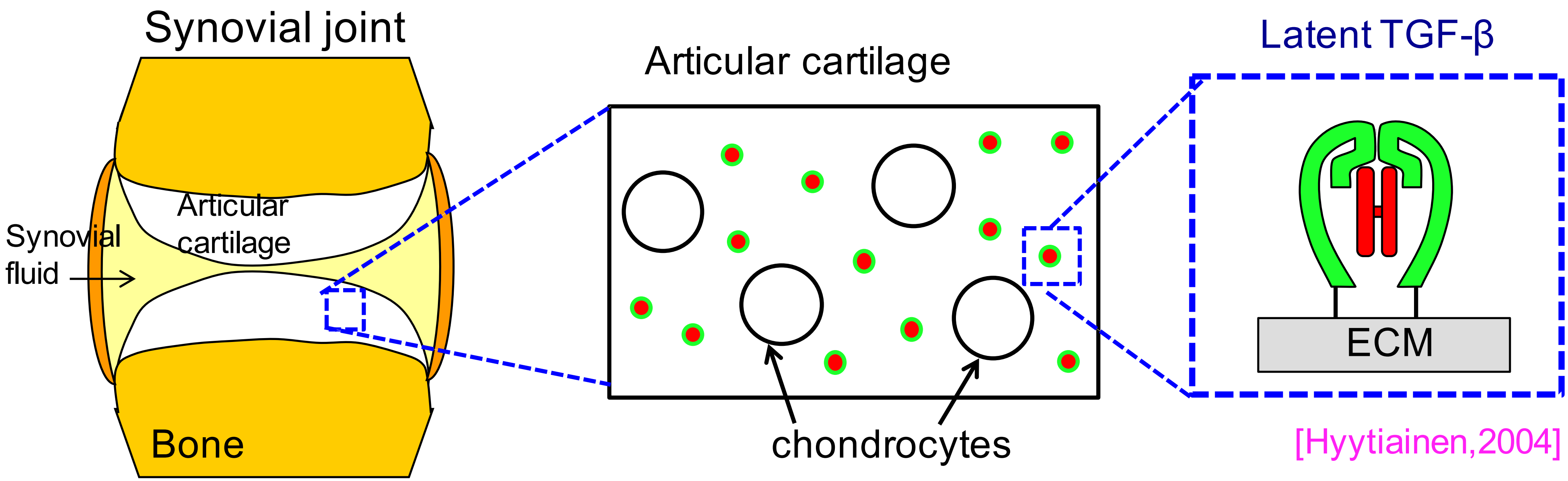


Hyperspectral Raman image

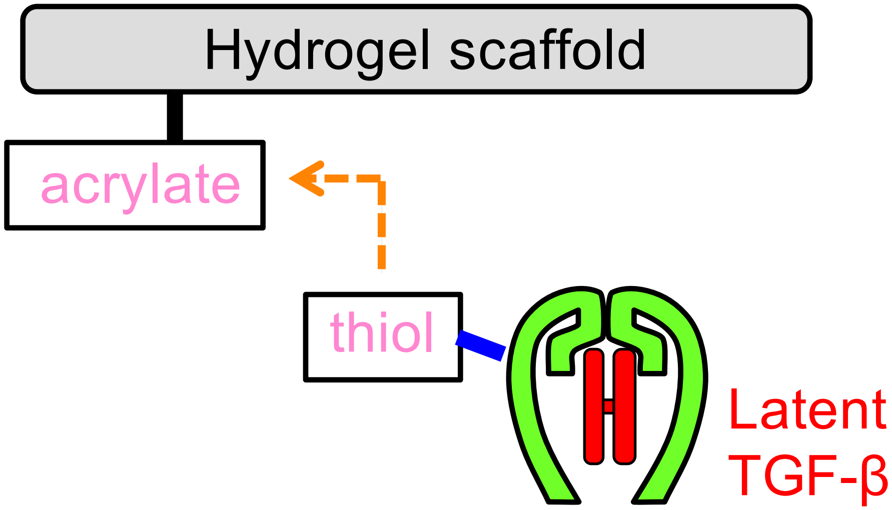


- Media supplemented TGF-β exhibits limited penetration in engineered cartilage.
- TGF-β gradients give rise to large heterogeneities in tissue growth.

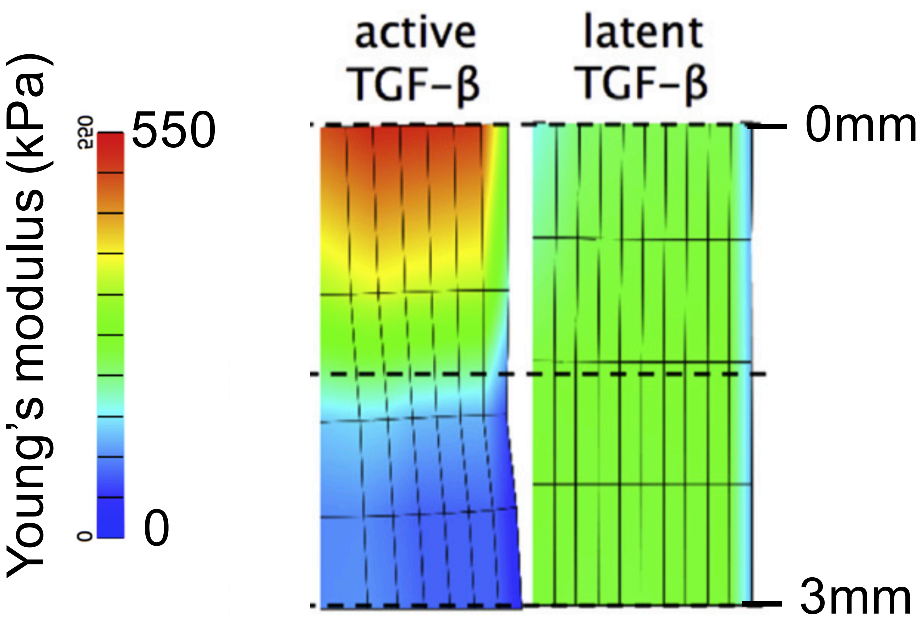
TGF-β Delivery in Native Cartilage

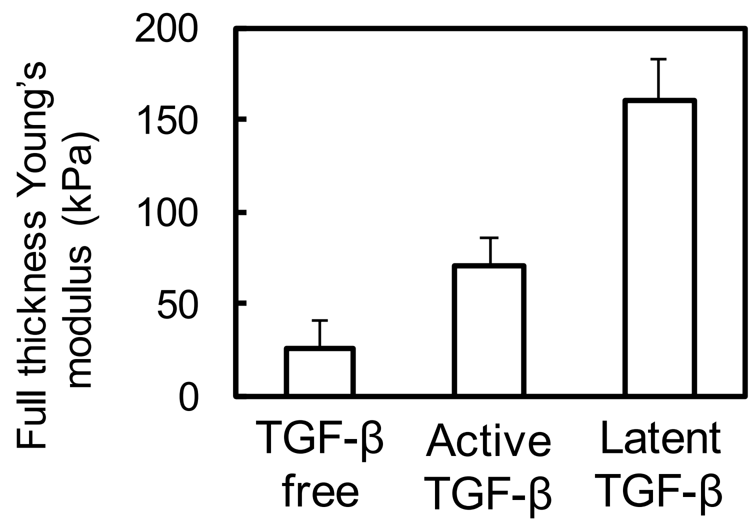


- Can biomimetic conjugation of latent TGF-β to hydrogel scaffolds improve uniformity of engineered tissue growth?
- Can we implement materials science strategies to achieve efficient growth factor conjugation?



Engineered cartilage growth with latent TGF-β





[Albro et al, 2016 Biomaterials]

Thank you

U.S. Department of Health and Human Services

NIH R01 AR46568
NIH R01 AR60361
NIH R01 AR43628

Supported by the National Institutes of Health

NIAMS
National Institute of Arthritis and Musculoskeletal and Skin Diseases

MARIE CURIE ACTIONS

SEVENTH FRAMEWORK PROGRAMME

Two-Dimensional Materials and Heterostructures

Xi Ling
Assistant Professor

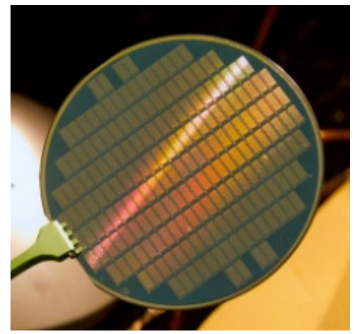
Chemistry
Materials Science & Engineering

Materials change our life

Stone Age

Iron Age

Silicon Age



Next?

?

Two-dimensional (2D) materials

(2010 Nobel Prize)

Graphene *Metal*

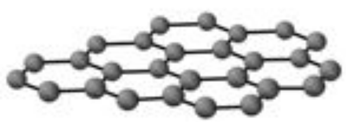
Black phosphorus

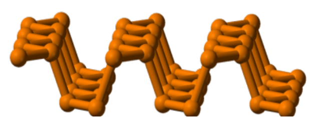
MoS_2, WS_2, $MoSe_2$….

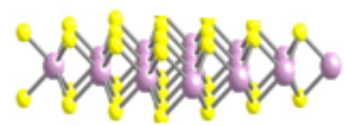
Semiconductor

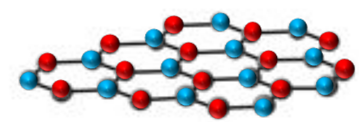
hBN *Insulator*

…





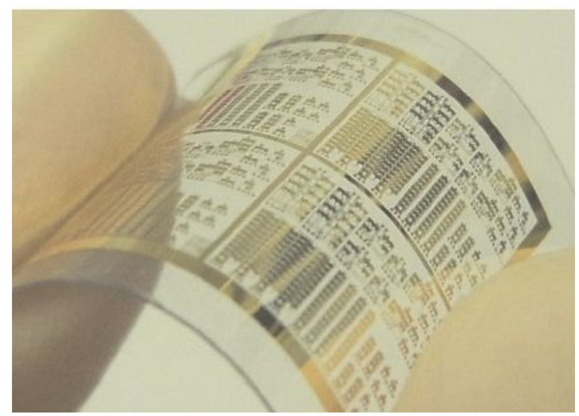




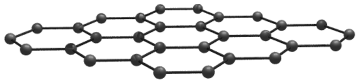
Flexible

Transparent

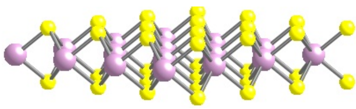
Diversely functional



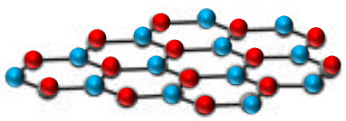
2D van der Waals heterostructures



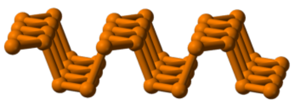
Graphene



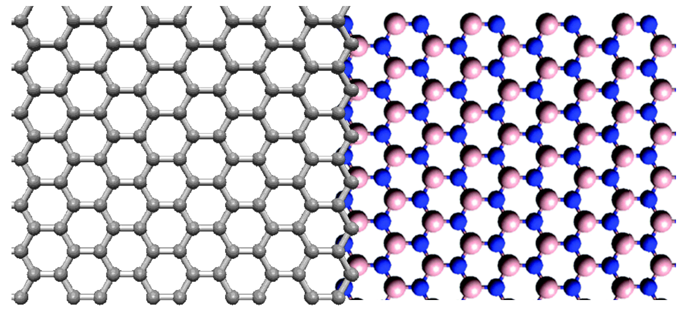
MoS_2



BN

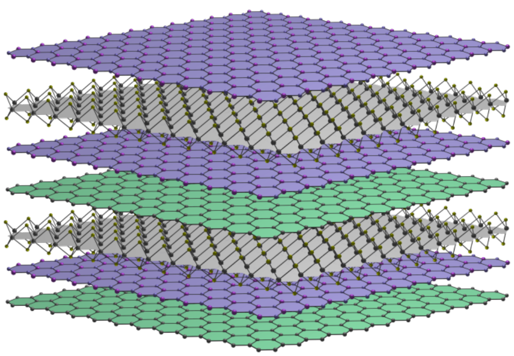


Black Phosphorous



Lateral heterostructure

Vertical heterostructure

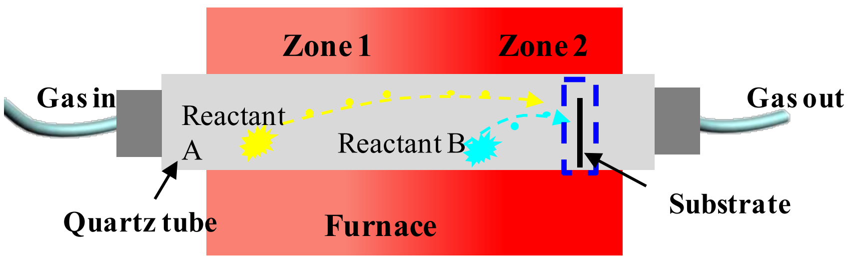


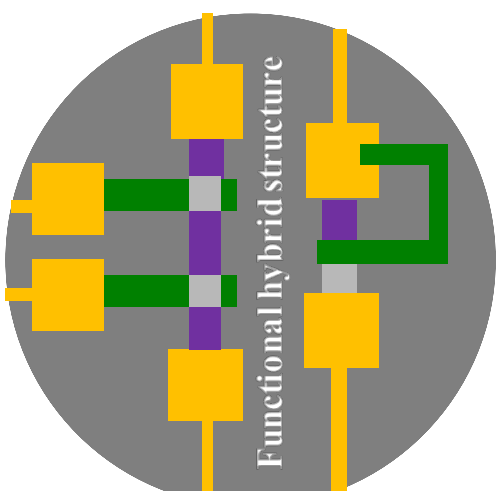
In Our Lab

Integrating 2D materials

Large-scale assembly

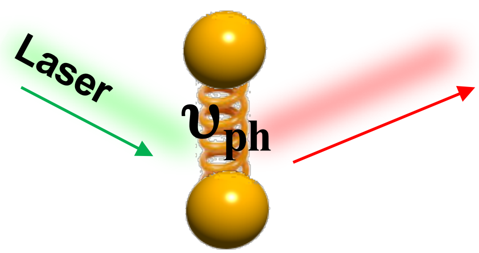
Chemical vapor deposition

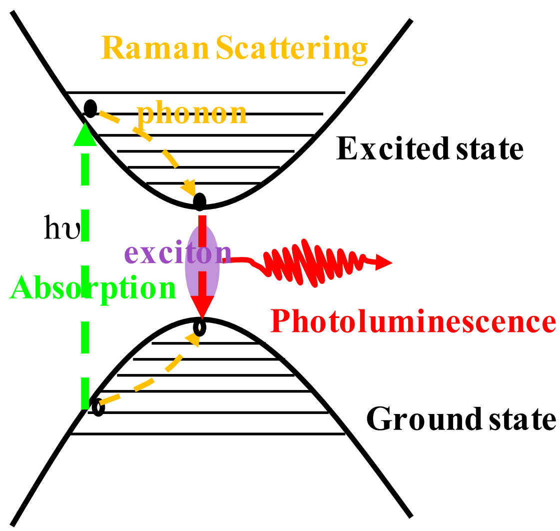




Properties

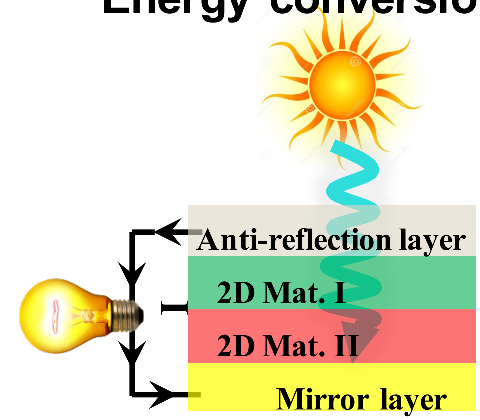
Light-matter interaction



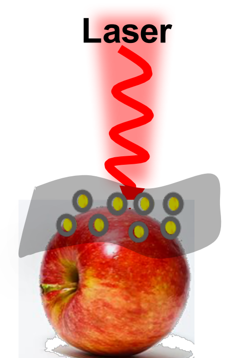


Devices

Energy conversion



Chemical Sensing



BOSTON UNIVERSITY

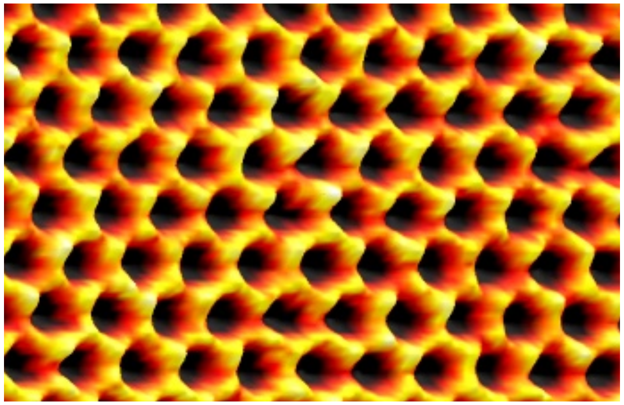
Computational Materials Science

Sahar Sharifzadeh
Assistant Professor

Electrical & Computer Engineering
Materials Science & Engineering

Why Computation?

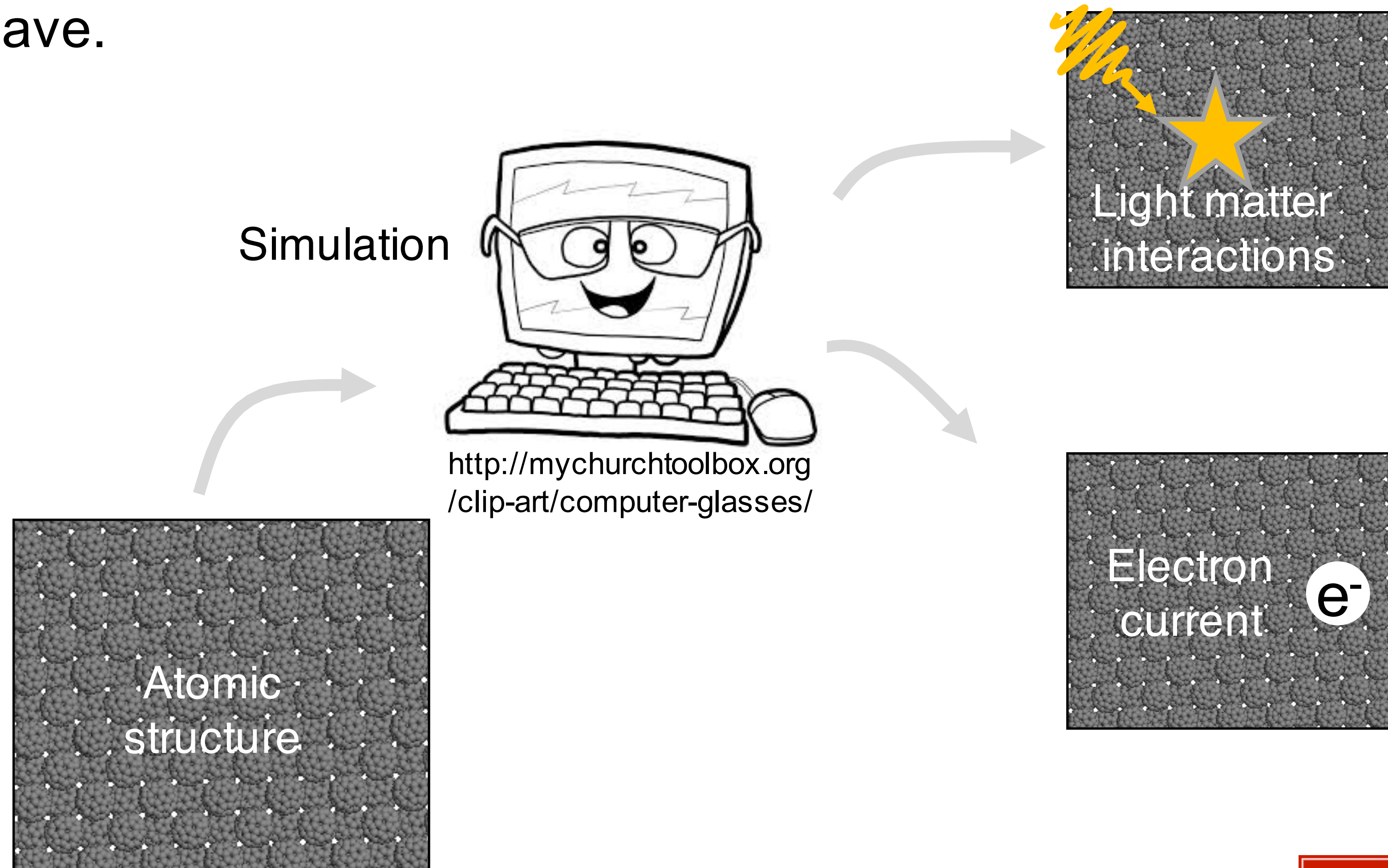
- Making materials and testing them in devices is difficult, expensive, and time-consuming
- Infinite number of possibilities as to new material chemistry



- Using computation, we can speed up the material discovery process
  - Calculate and understand material properties
  - Screen databases of materials for desired properties
  - Predict new materials with optimal or emergent properties

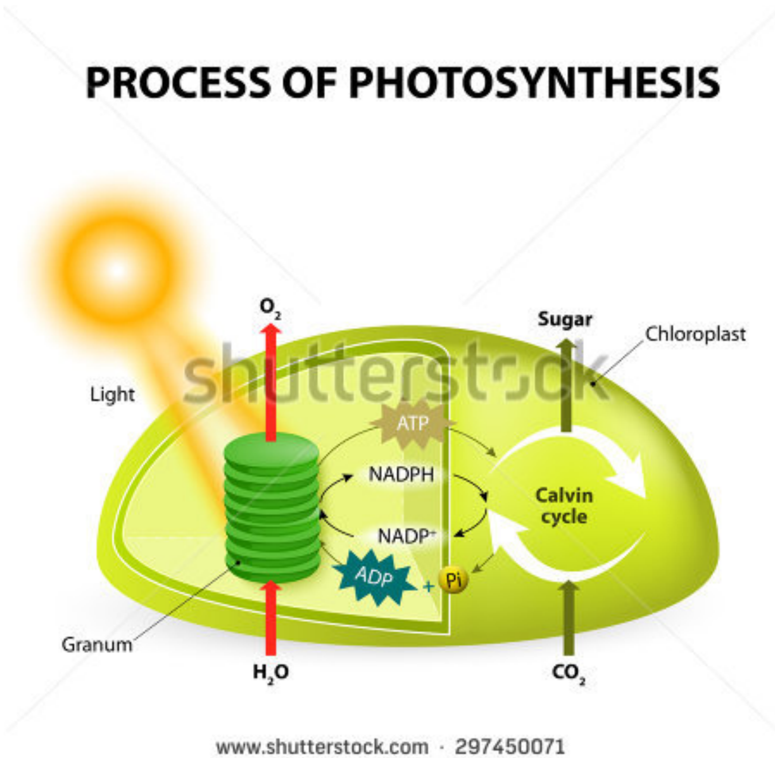
Computational Materials Science

- As we reduce the size of devices, their properties are governed by the atomic scale → need to understand how electrons and atoms behave.

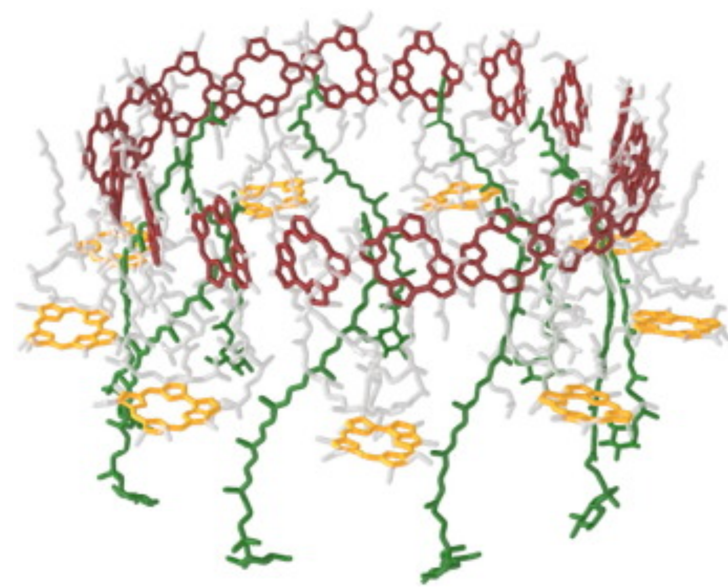


Example: New Materials for Solar Energy Conversion

- Solar energy conversion in organic materials: inspired by nature!



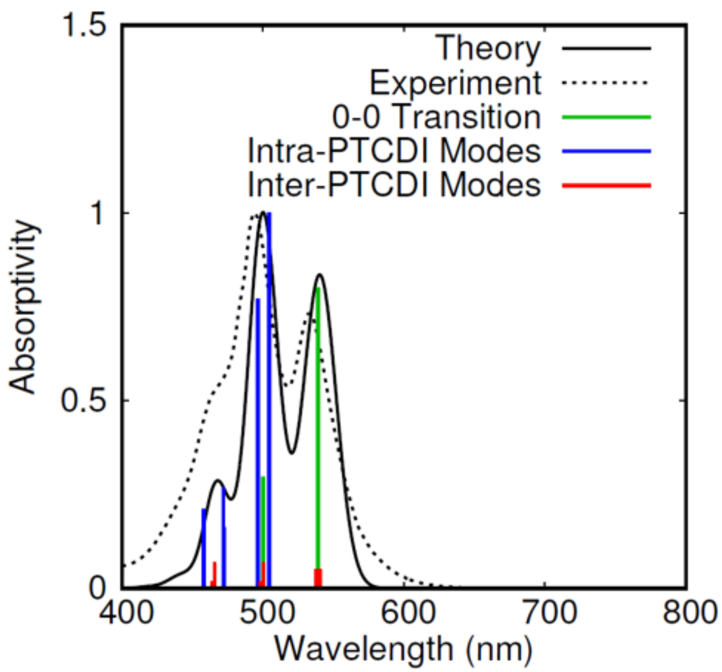
1. Light absorption
2. Energy transfer

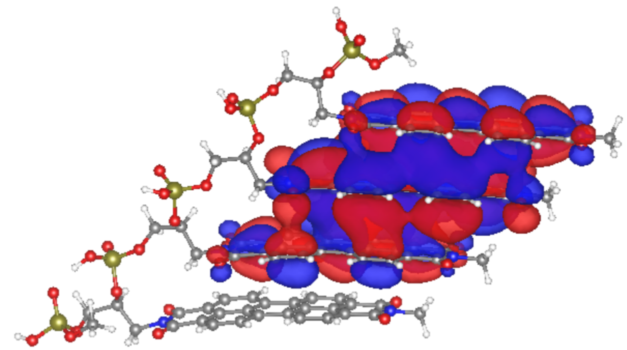


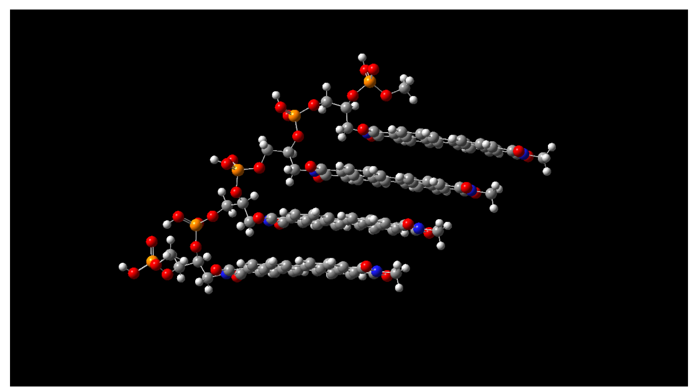
Reimers et al, BB A– Bioenergetics (2016)

First-Principles Computation to Understand Energy Transfer

- How does an electron behave after light absorption?
- How do atomic vibrations (due to finite temperature) influence energy transfer







With new understanding gained, we can design new organic materials

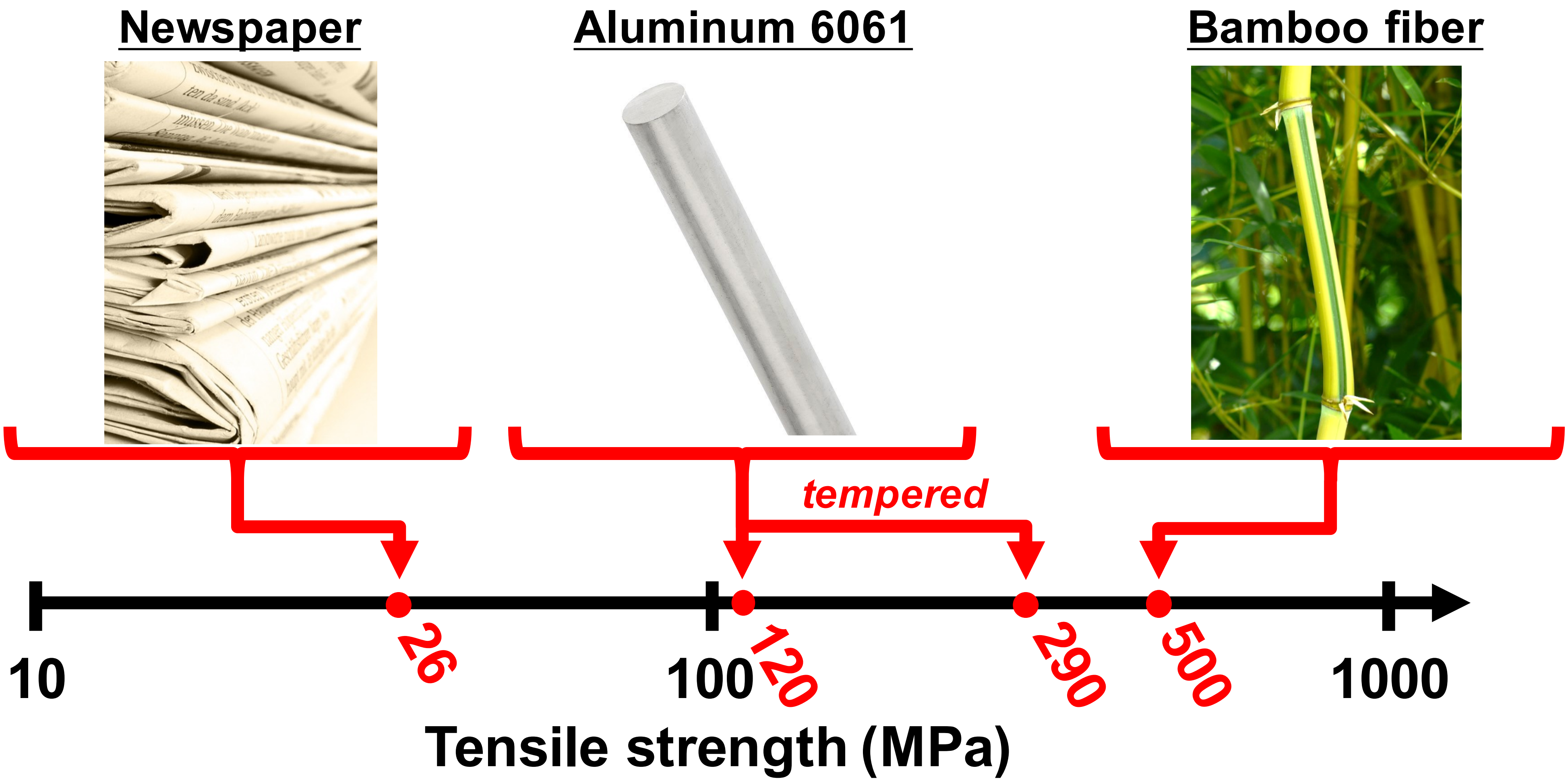
Nanomanufacturing where Top-Down Meets Bottom-Up

Keith A. Brown

Assistant Professor

Mechanical Engineering
Materials Science & Engineering
Physics
Moorman-Simon Interdisciplinary Career Development Professor

What Makes a Material Strong?

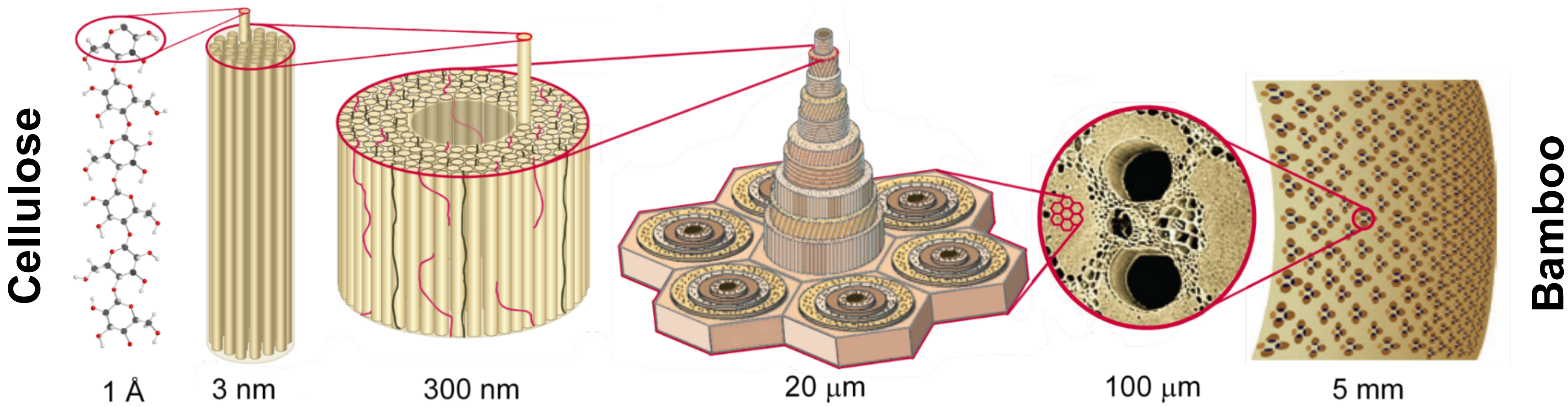


Rao, *et al. Composite Structures* **2007**, 77, 288.

Technical Association of the Pulp and Paper Industry

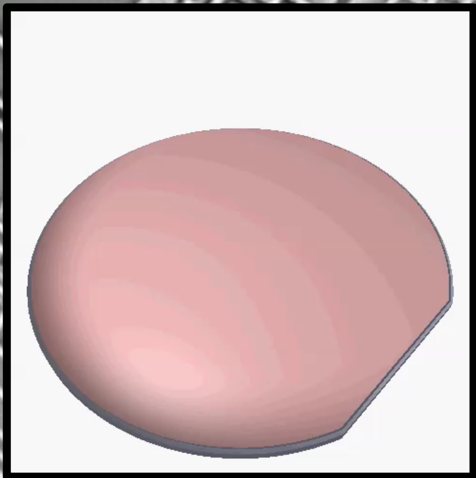
Aluminum Standards and Data 2006 Metric SI, The Aluminum Association

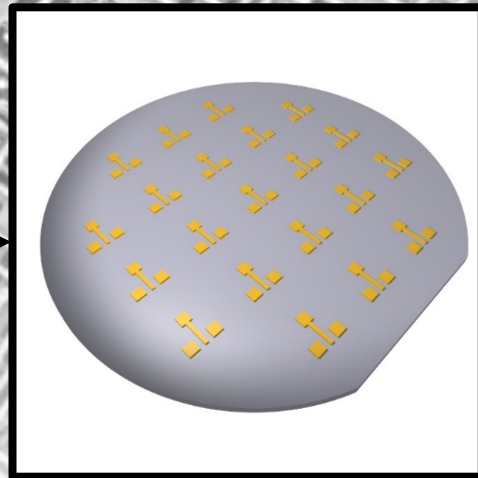
Natural Materials Derive Performance from Hierarchical Structure from Molecules to Millimeters



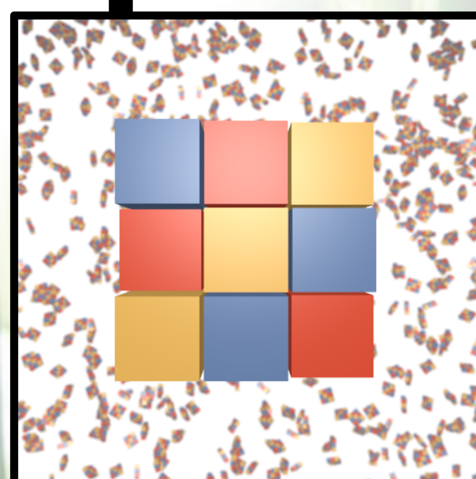
Motivating question:
Can we artificially structure materials from molecules to millimeters?

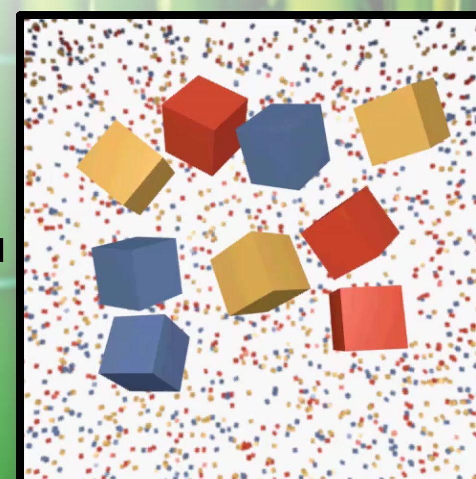
Wegst, *et al., Nature Mater.* **2015**, 14, 23.





Nanomanufacturing where Top-Down meets Bottom-Up





Integrated circuit: www.nisenet.org

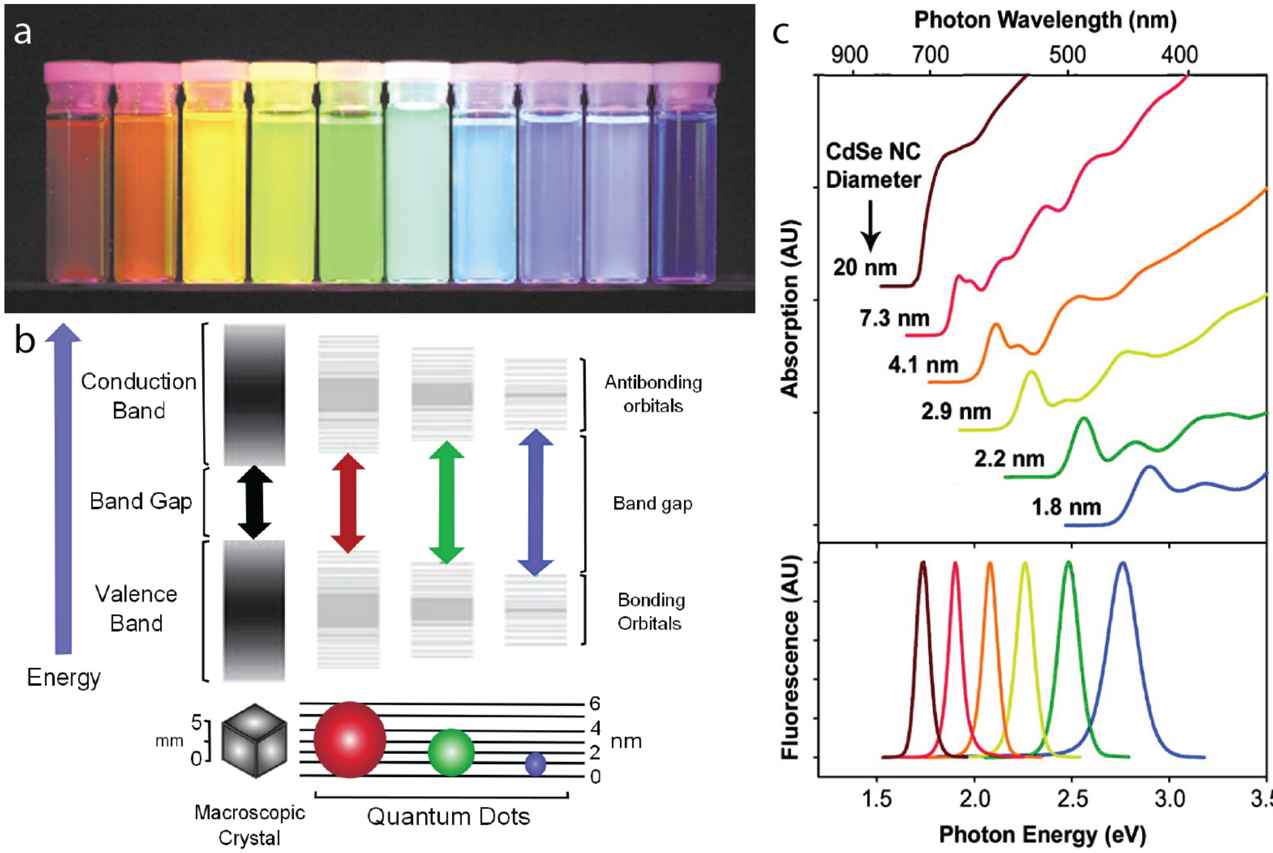
Bamboo: Matt Gibson

Advanced Quantum Dot Synthesis for Biosensing and Biomedical Imaging

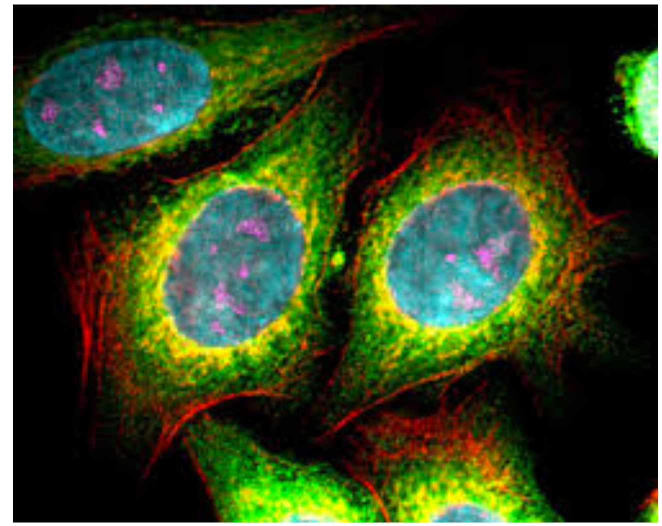
Allison Dennis
Assistant Professor

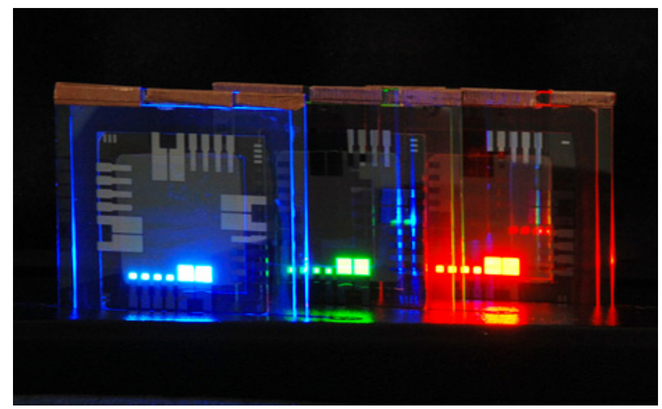
Biomedical Engineering

Semiconductor Nanocrystal Quantum Dots



Chou and Dennis, *Sensors*, 2015, 13(6), 13288 – 13325.



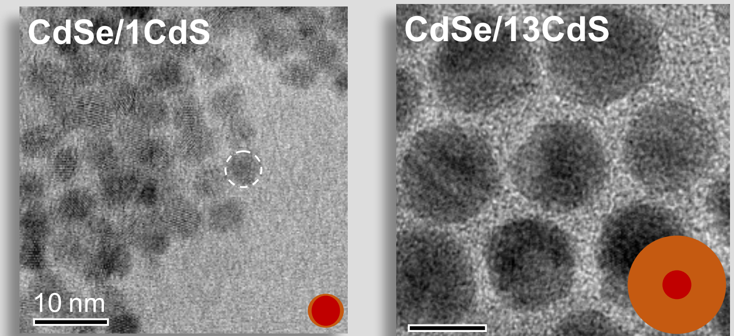


5 color multiplexed cell image and QD LEDs

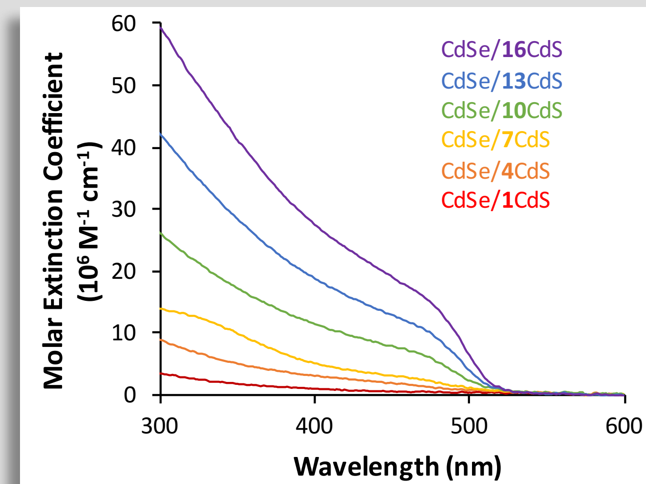
courtesy of Invitrogen and IEEE

BOSTON UNIVERSITY

‘Giant’ Nanocrystal Quantum Dots (g-NQDs)



Thick, epitaxial shells enable bandgap tuning and tailoring of the absorption cross-section.

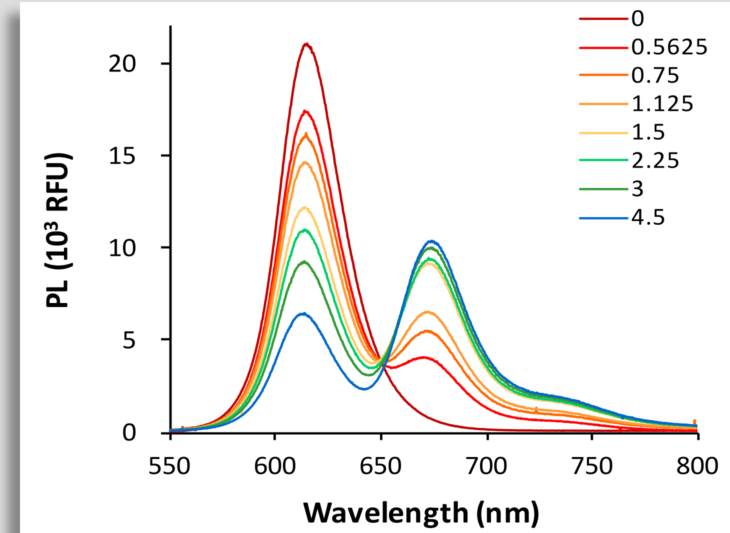


Composition	Emission range	Bandgap alignment
CdSe/ZnS	500 – 600 nm	Type I
CdSe/CdS*	550 – 650 nm	Quasi Type II
ZnSe/InP*	**500 – 900 nm**	**Inverted Type I**
InP/ZnS	**500 – 700 nm**	**Type I**
InP/ZnSe*	**500 – 700 nm**	**Type I**
InP/CdS*	650 – 1000 nm	Type II
InP/CdSe*	650 – 1100 nm	Type II

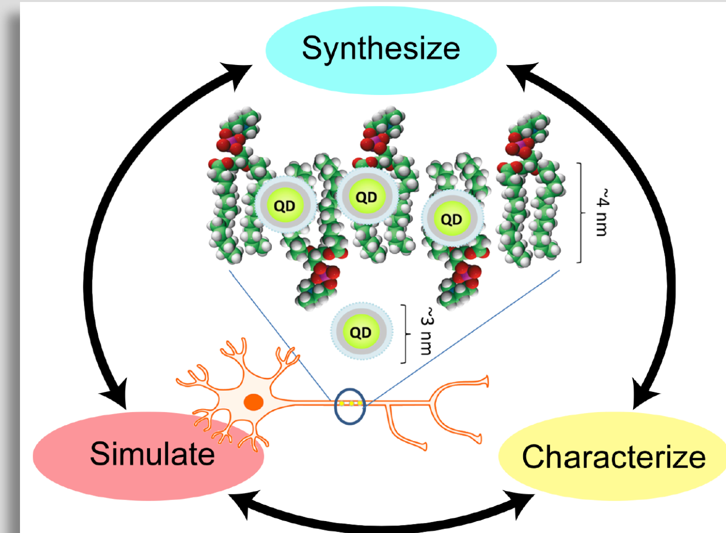
*QDs can be capped with ZnS as appropriate to enhance brightness, stability, and biocompatibility for bioimaging.

Different core and shell semiconductor compositions for different applications– tailoring optoelectronic properties and reducing cadmium-based nanotoxicity.

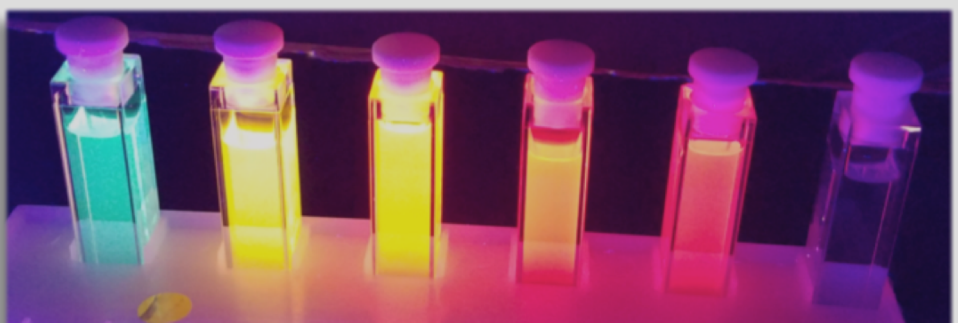
Research on Tap: Materials Science and Engineering: The Science of Stuff



Ratiometric Biosensors for Label-Free Detection of Hormones



Optimizing Voltage Response for Imaging Action Potentials in Neurons



Molecular Phenotyping of Breast Cancers Using Cadmium-Free NIR Emitters

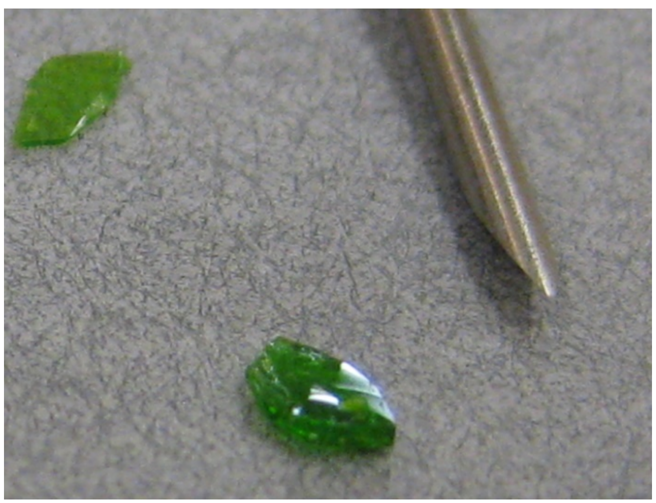
Boston University Office of the Vice President and Associate Provost for Research

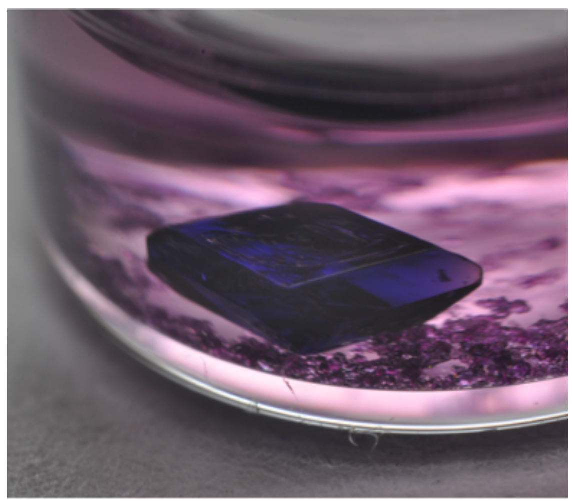
BOSTON UNIVERSITY

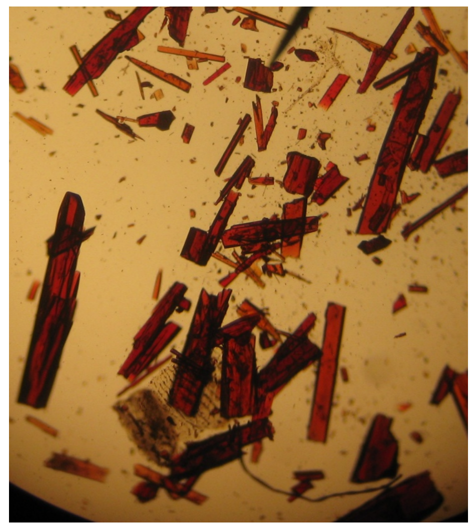
Single Molecule Magnets

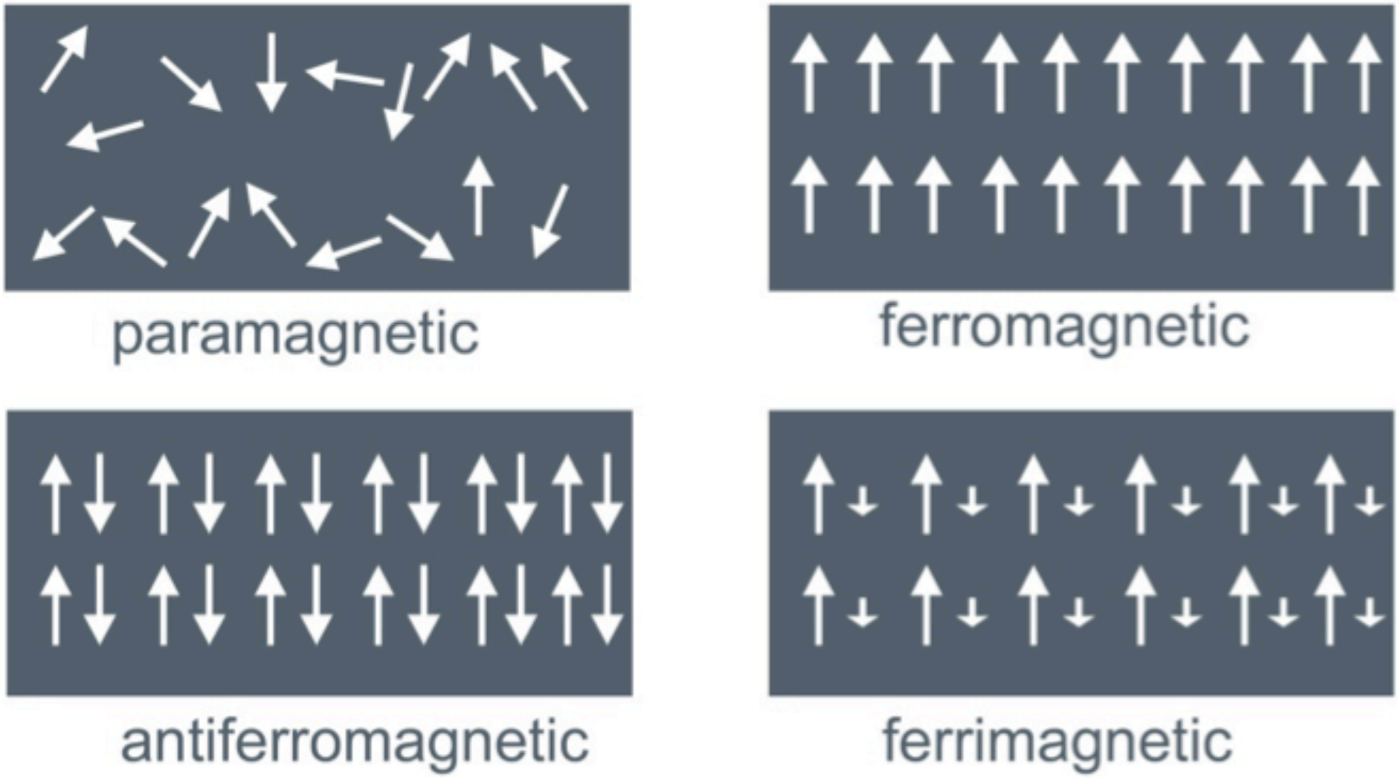
Linda H. Doerrer
Associate Professor

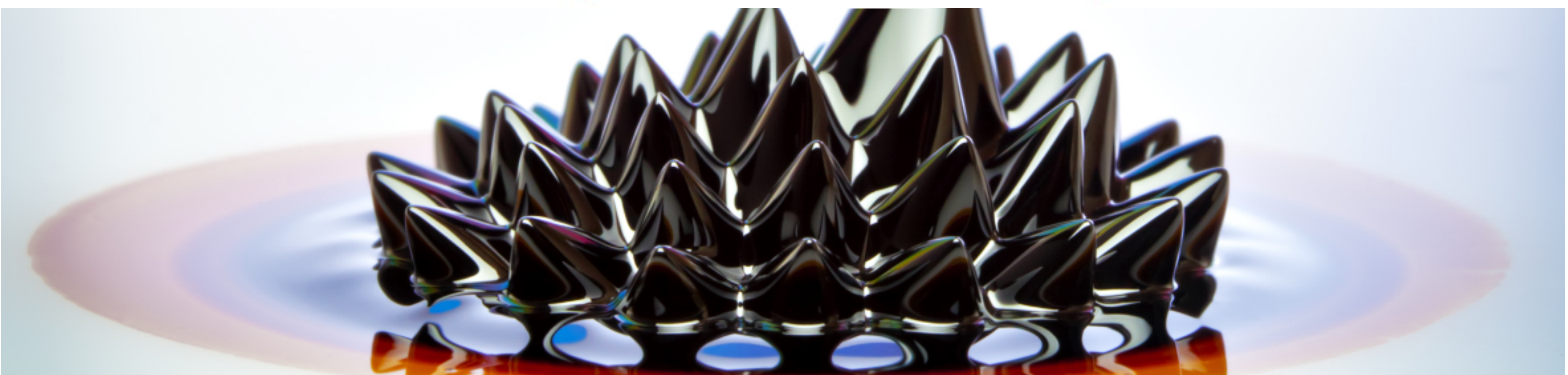
Chemistry





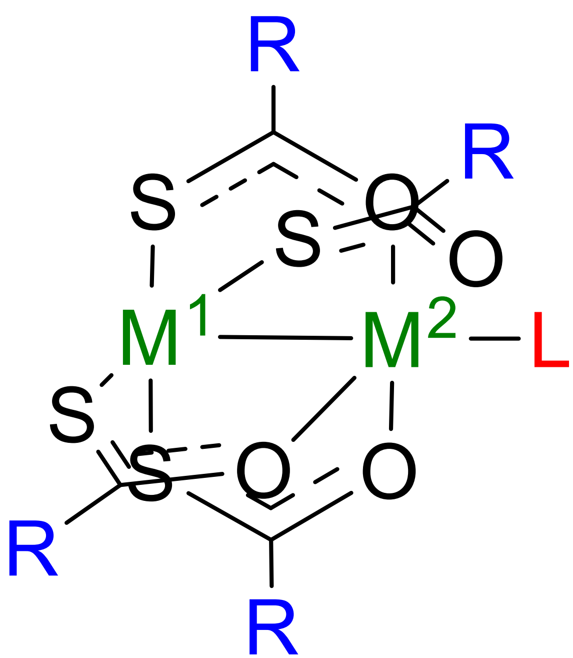



paramagnetic
ferromagnetic
antiferromagnetic
ferrimagnetic



Requirements in Single Chain Magnet Design

- Magnetically Isolated Chain
- Paramagnetic Ground State
- Axial Magnetic Anisotropy

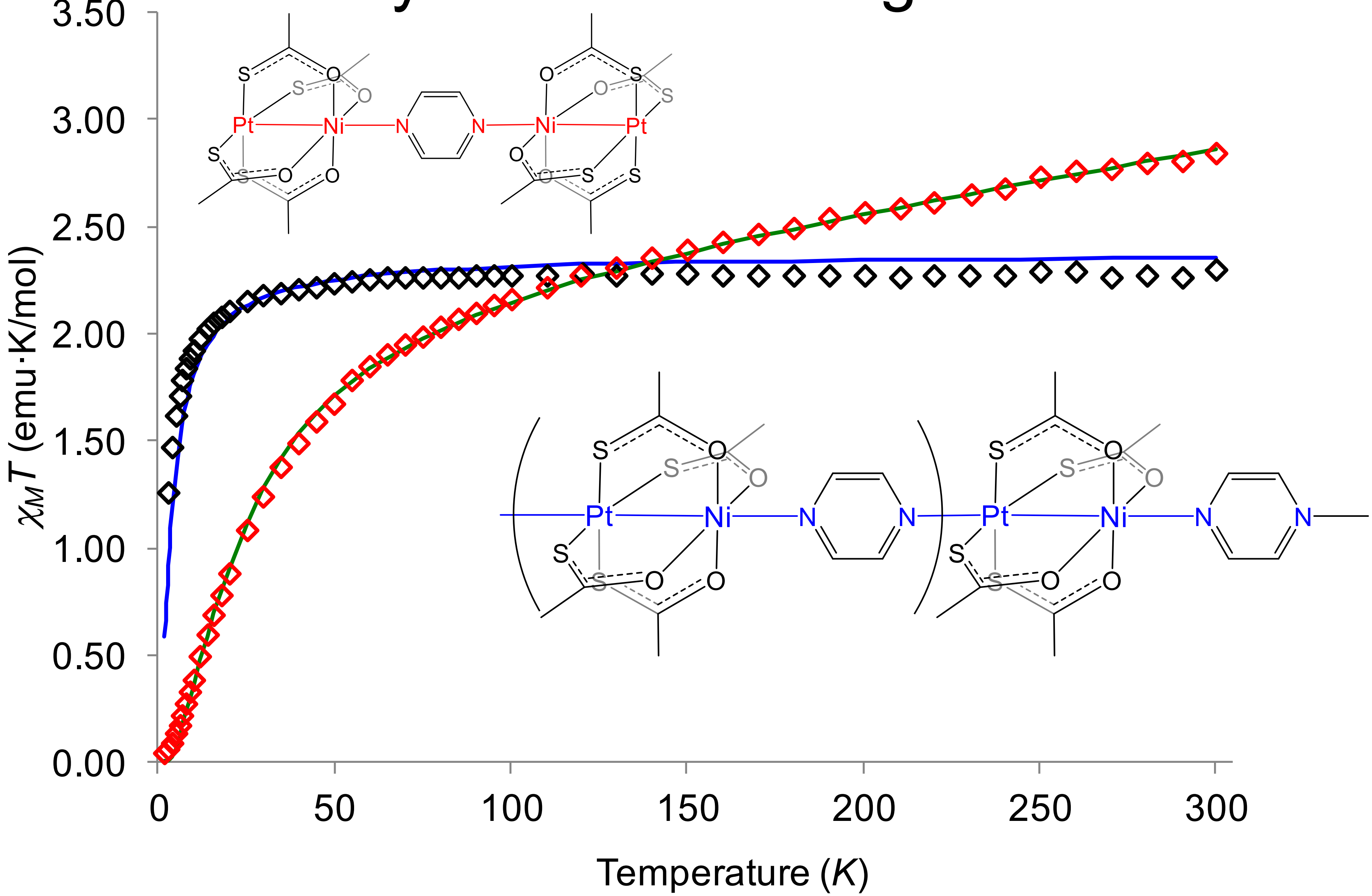


Modification of Backbone

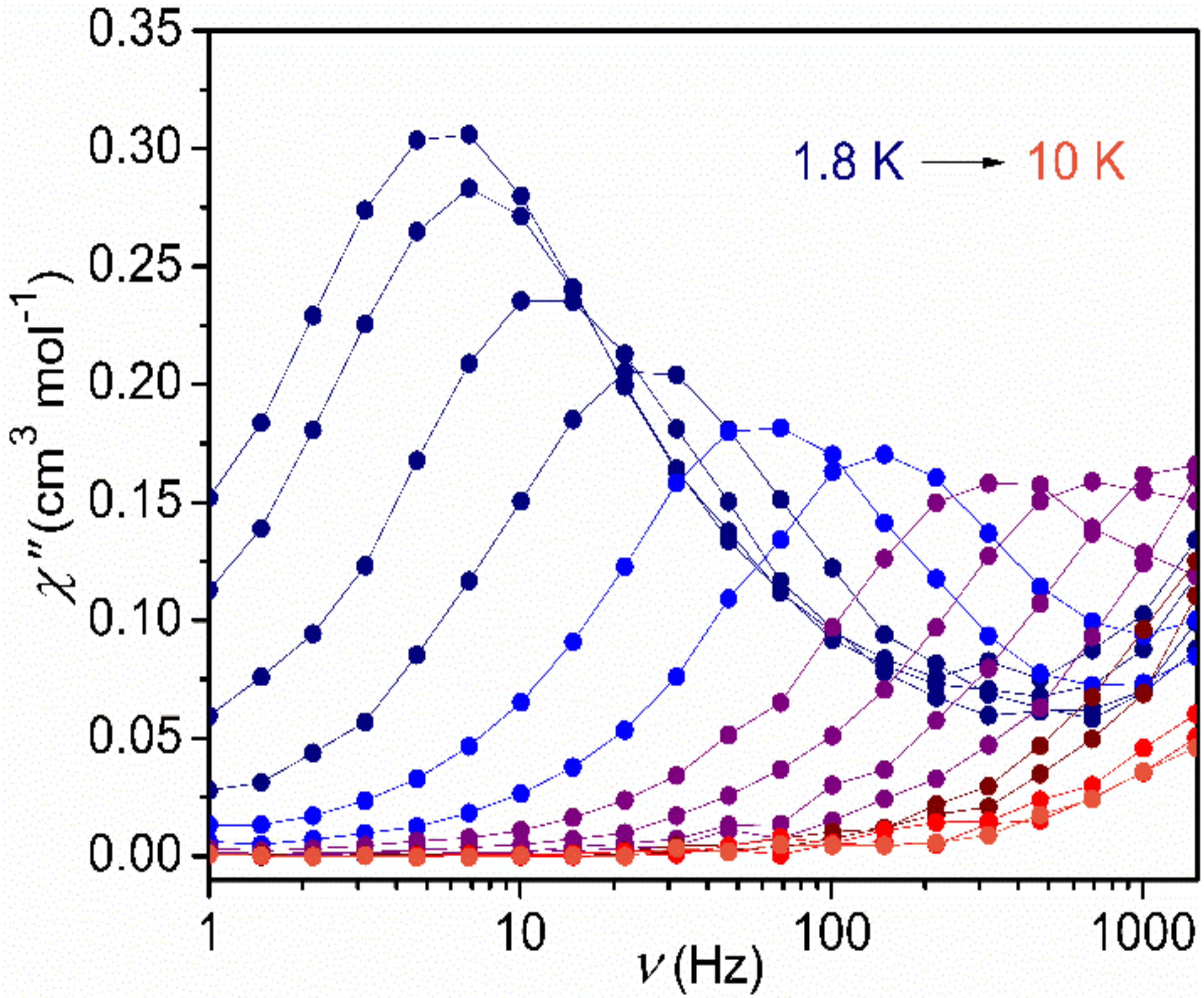
Incorporating Different Metals

Bridges to form chains

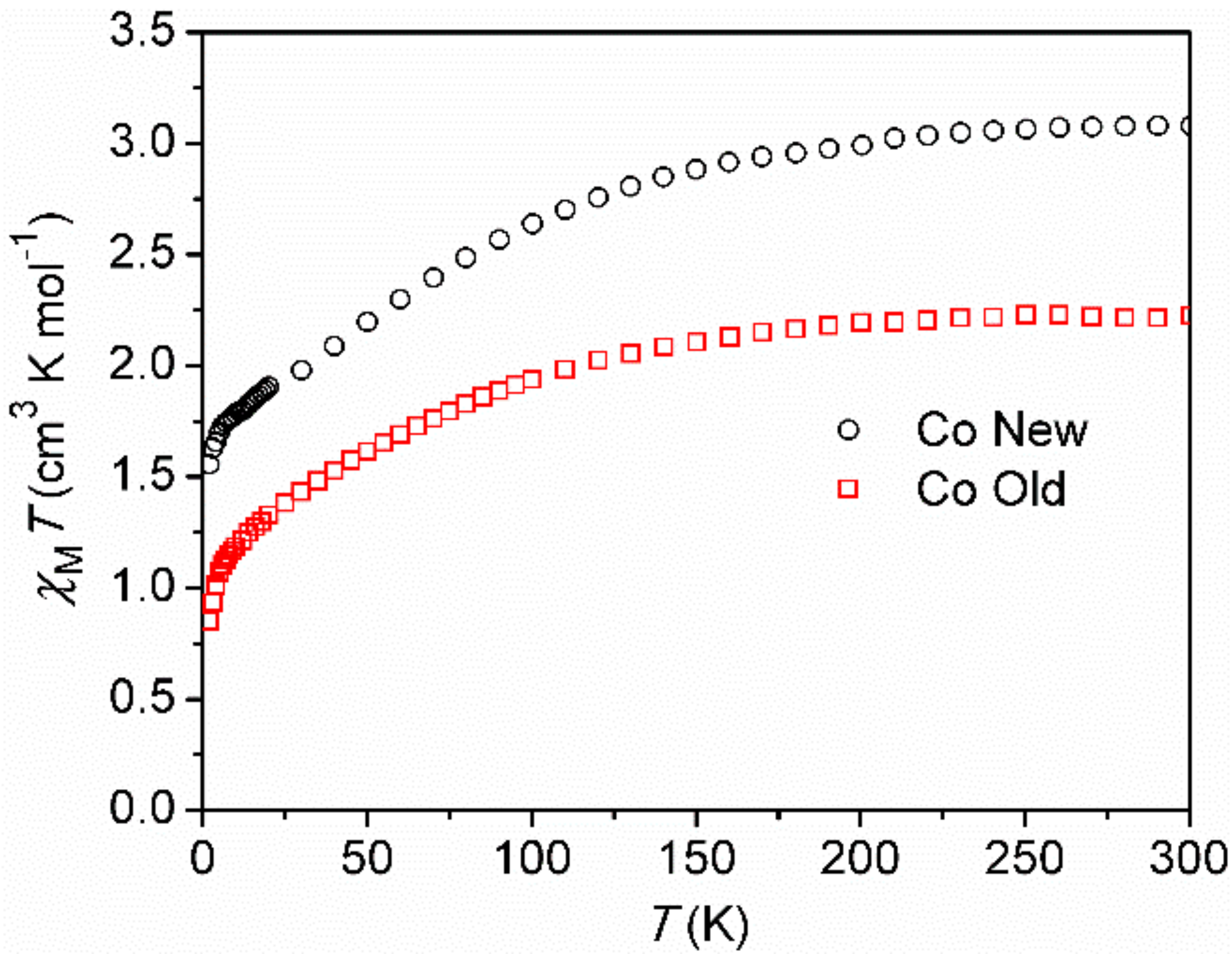
Asymmetric building blocks in chains

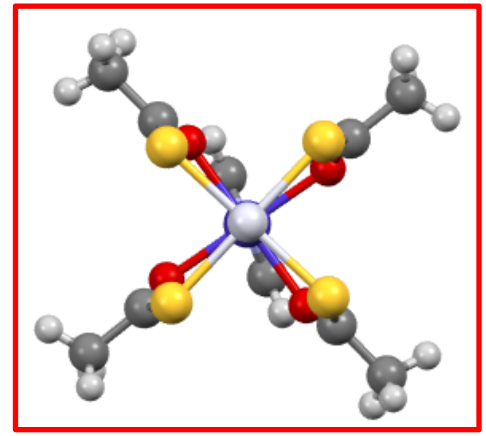


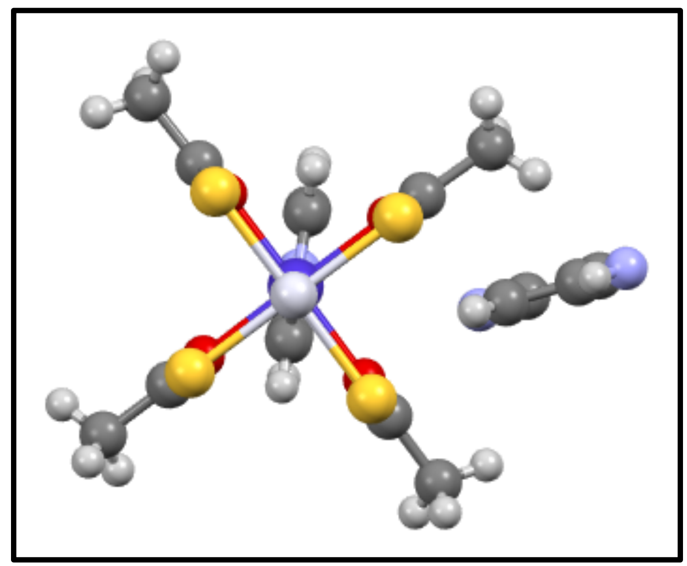
Single Chain Magnet Behavior



Separating the Chains *Changes* the Magnetism !



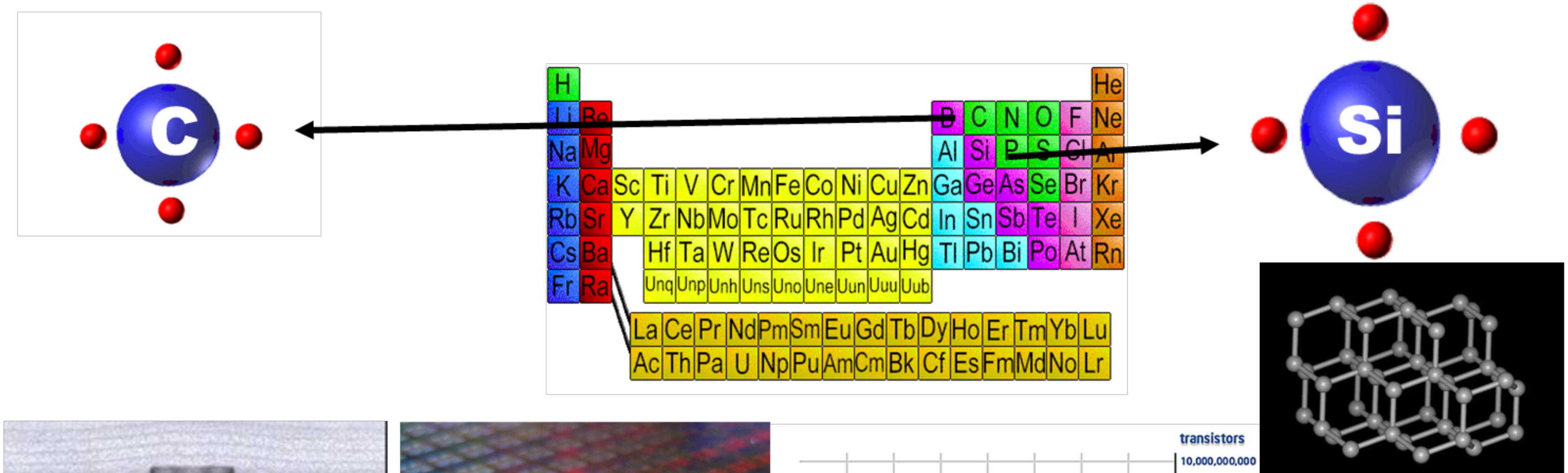


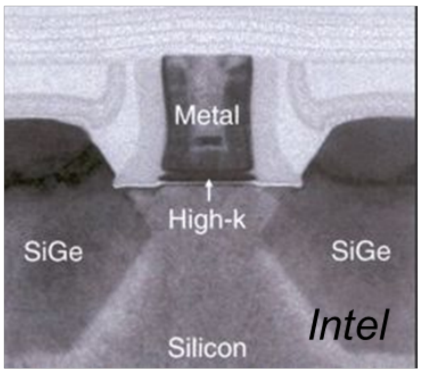


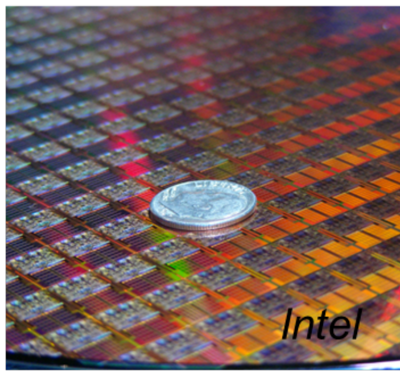
Atomic Membranes

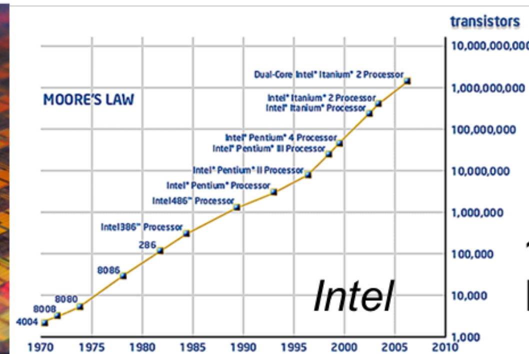
Scott Bunch
Assistant Professor

Mechanical Engineering



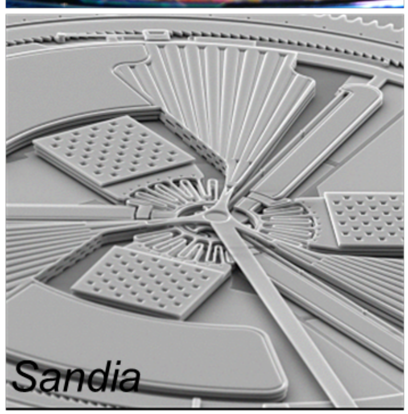






Electrical

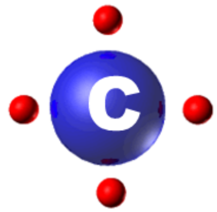
~ $1 Trillion business

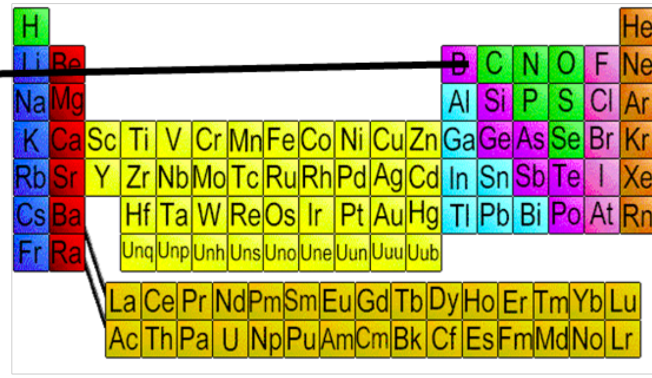


1. Accelerometers
2. Pressure Sensors
3. Ink Jet Printer Nozzles
4. Displays
5. RF MEMS

Mechanical

$10 Billion business
14% annual growth



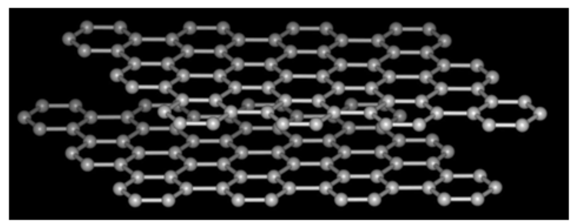


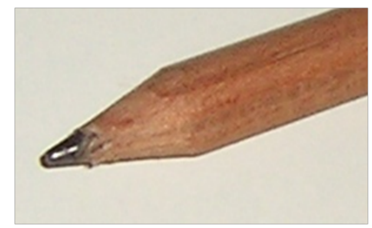
Superior Properties

Electrical
Mechanical
Thermal

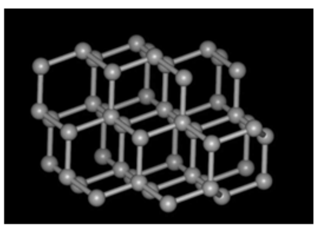
Different Bonding

Graphite





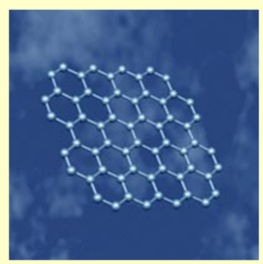
Diamond

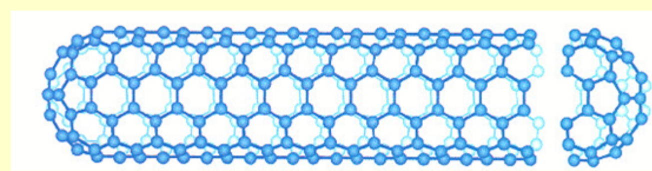


Hope Diamond

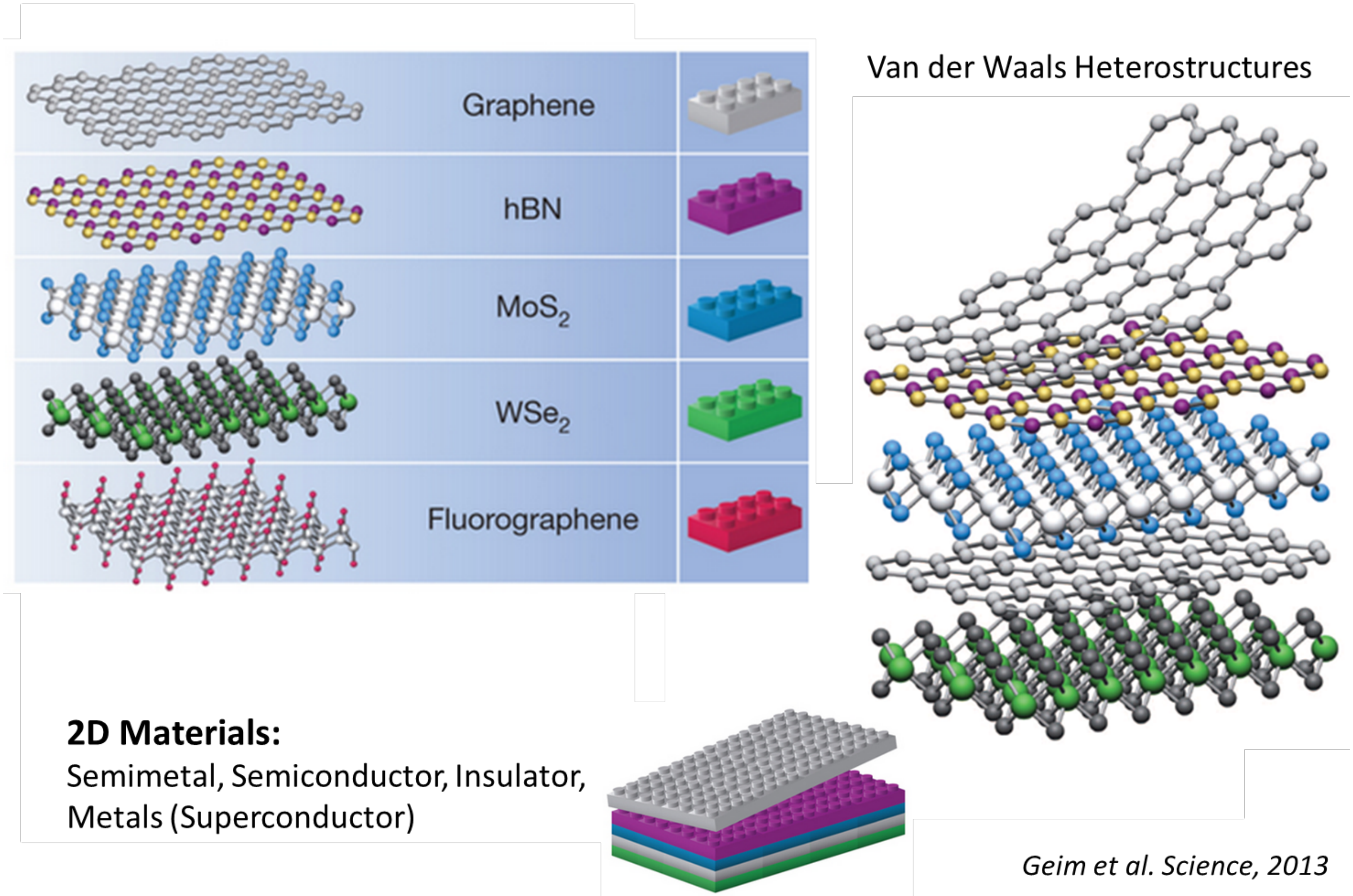
Apollo Diamonds

Graphene/Nanotubes





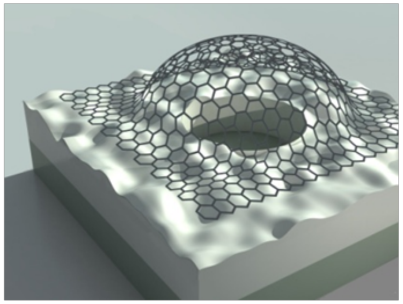
2D Materials beyond Graphene



2D Materials:
Semimetal, Semiconductor, Insulator, Metals (Superconductor)

Geim et al. Science, 2013

Atomic Membrane Nanomechanics



Theme 1:

Graphene and MoS_2
Mechanics and Adhesion

S.P. Koenig et al. Nature Nanotechnology, **6**, 543–546 (2011)

J.S. Bunch and Martin L. Dunn Solid State Communications (review article), **152**, 1359–1364 (2012)

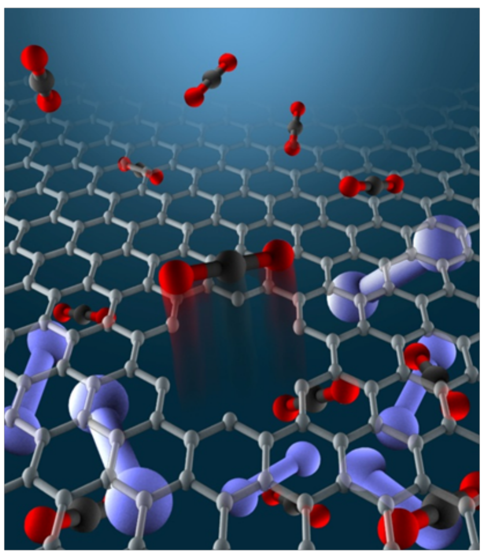
X. Liu et al. Nano Letters, **13**, 2309-2313 (2013)

N. Boddeti et al. Journal of Applied Mechanics, **80**, 040909 (2013)

N. Boddeti et al. Nano Letters, **13,** 6216-6221 (2013)

X. Liu et al. in preparation. (2016)

D. Lloyd et al. Nano Letters, **16** (9), 5836-5841 (2016)



Theme 2:

Gas and Ion Transport through Porous Graphene

S.P. Koenig et al., Nature Nanotechnology, **7**, 728-732 (2012)

L. Drahushuk et al., ACS Nano **10**, *786-795, (2015)*

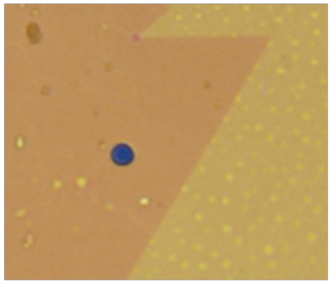
L. Wang et al., Nature Nanotechnology, **10**, 785-790 (2015)

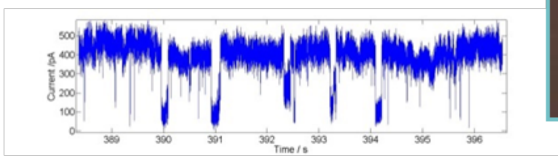
L. Cantley et al., Science, **under consideration** (2016)

Research on Tap: Materials Science and Engineering: The Science of Stuff

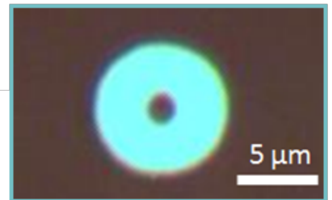


MoS_2 ion transport

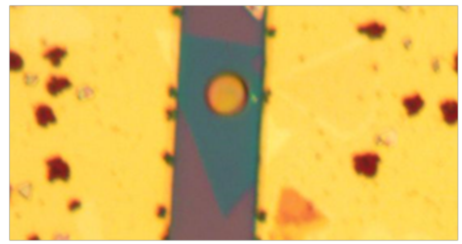




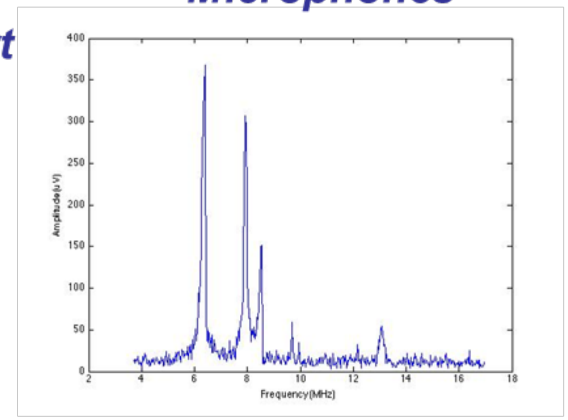
High Strain MoS_2



Electrical Transport MoS_2



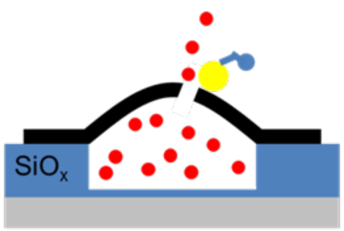
Mechanical Resonance MoS_2 and Graphene Pressure Sensors and Microphones

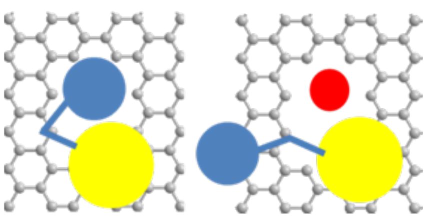


Harold Park
David Campbell

Anna Swan
Bennet Goldberg

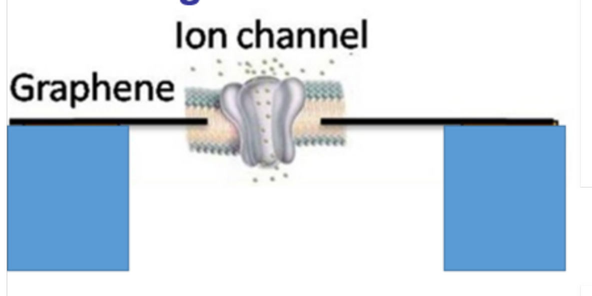
Functionalizing the Pore site





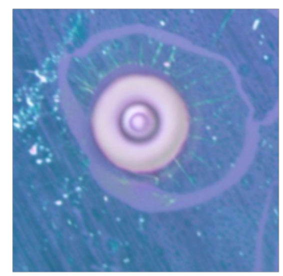
Michael Strano (MIT)

Biological Ion Channels



Kenneth Rothschild

Bowls for Bacteria




Alice White
Kamil Ekinci
Shyamsunder Erramilli

Boston University Office of the Vice President and Associate Provost for Research

BOSTON UNIVERSITY

Lanthanide Binding Tags (LBTs): New Chemical Tools for Molecular Visualization

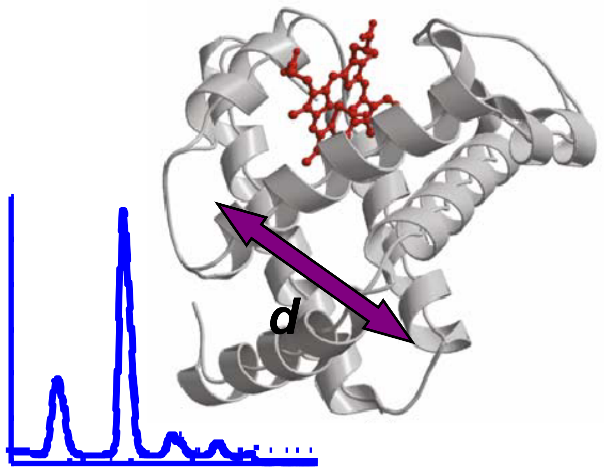
Karen Allen

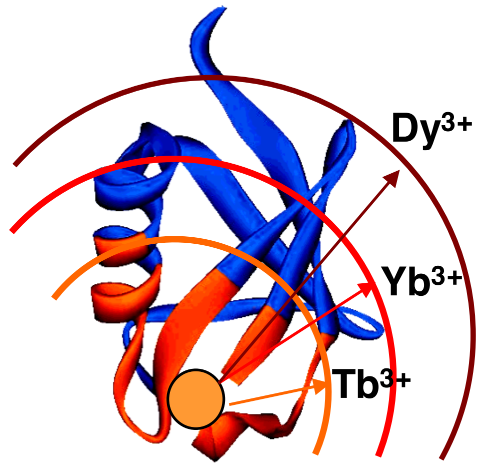
Professor

Chemistry

Allen Lab: Lanthanide Binding Tags (LBTs): New Chemical Tools for Molecular Visualization

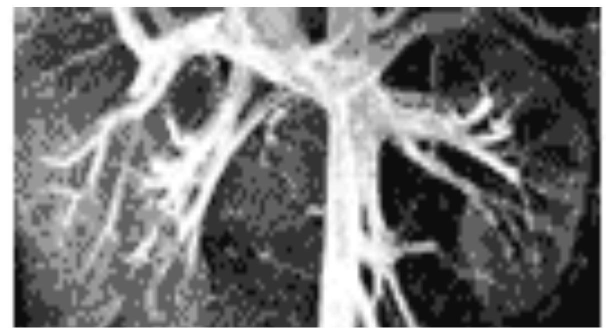
Luminescence probes for tagging and LRET

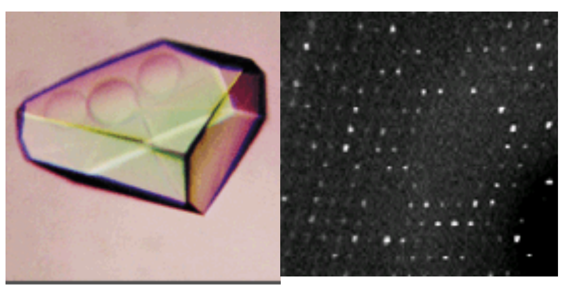




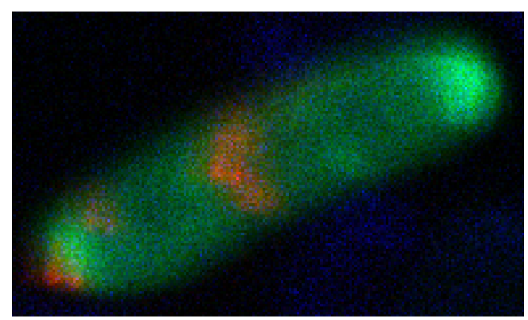
Paramagnetic NMR probes

MRI Contrast Agents



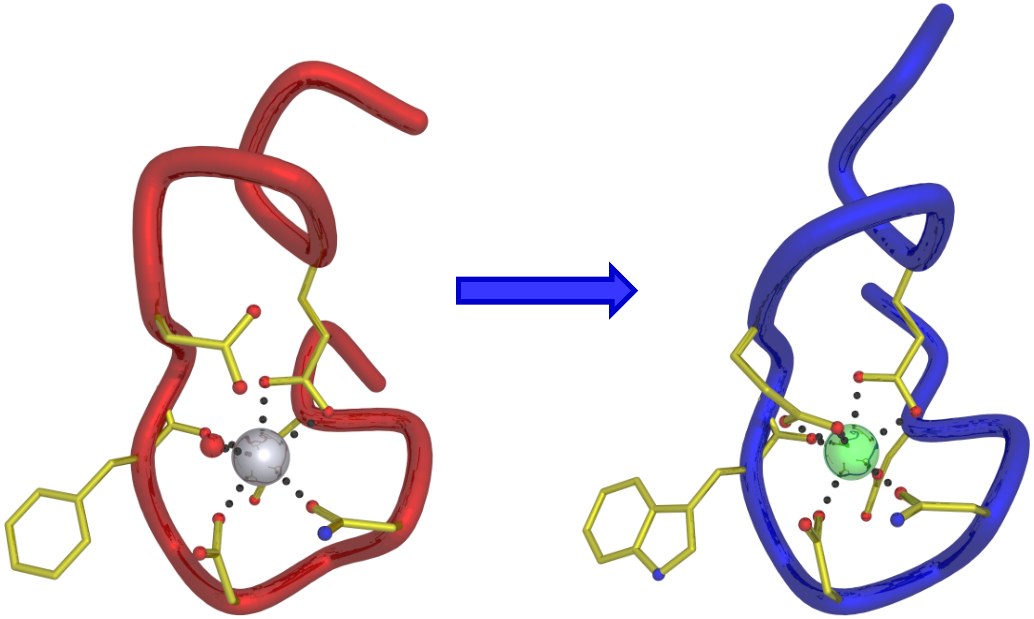


Heavy atom for X-ray diffraction



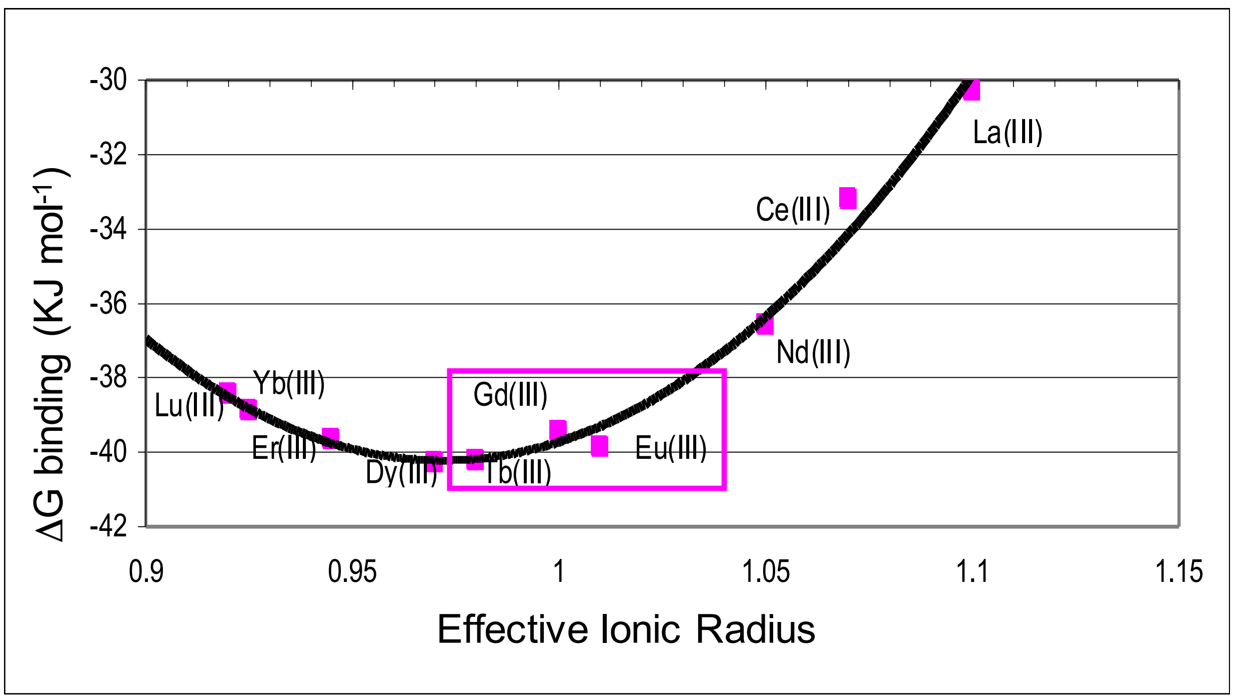
X-ray Fluorescence Tags

57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu

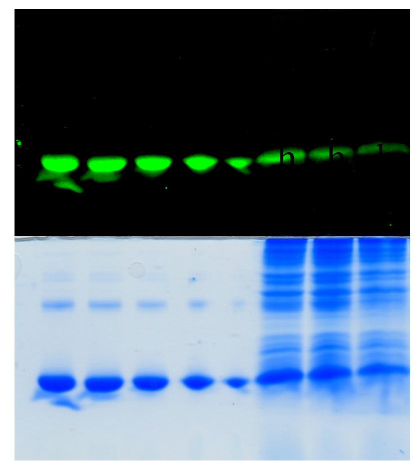


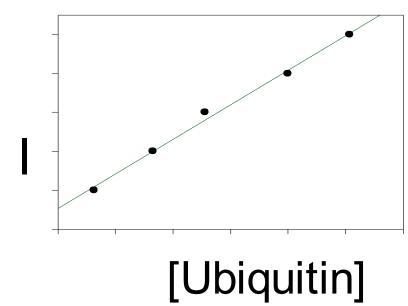
Affinities for lanthanides

Lanthanide (selected)	Radius (A)	K_D (nM)
La	1.1	4000
Ce	1.07	1200
Nd	1.05	300
Eu	1.01	78
Gd	1	93
Tb	0.98	57
Dy	0.97	66
Er	0.945	85
Yb	0.925	117
Lu	0.92	140



Angew. Chem. Int. Ed. 2004, 43, 3682 –3685

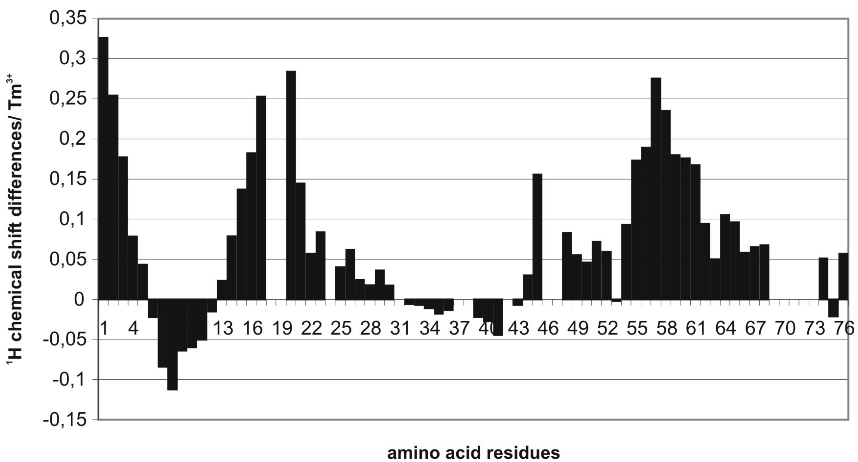


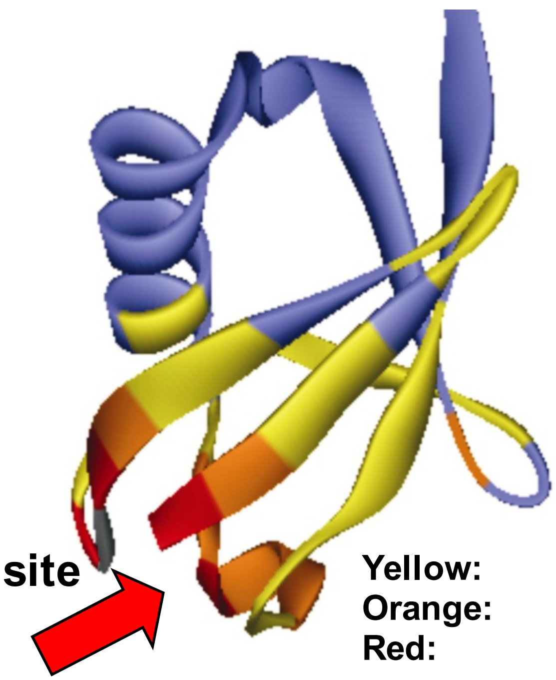


NMR

Crystallography

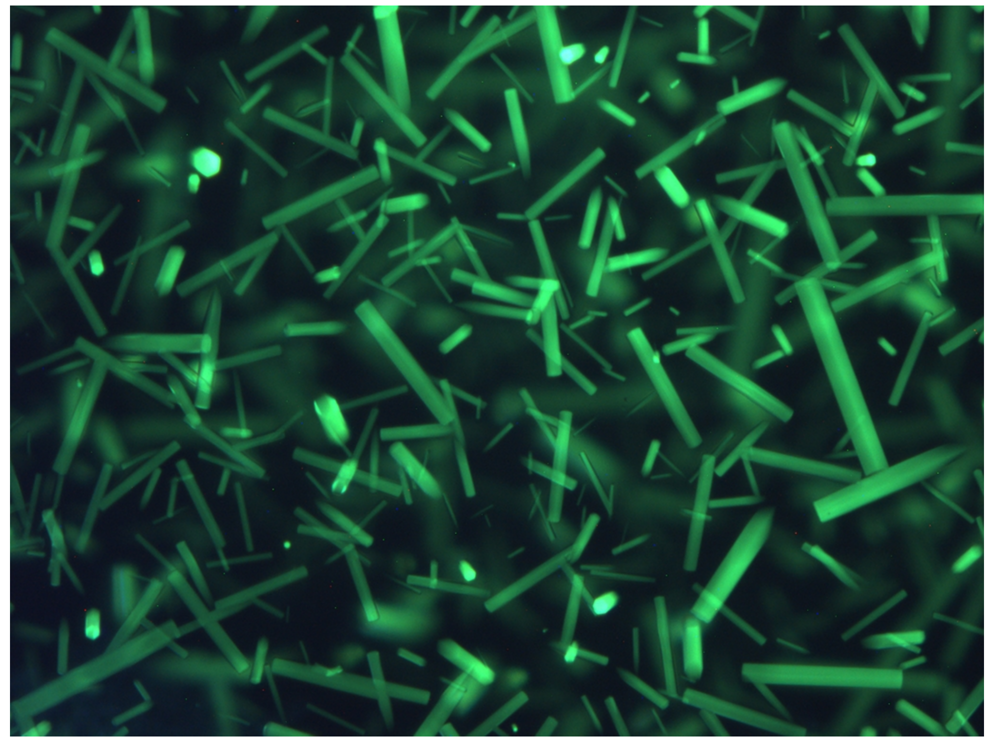
Bound Ln can provide pseudo contact shifts and dipolar couplings (sufficient order in probe)

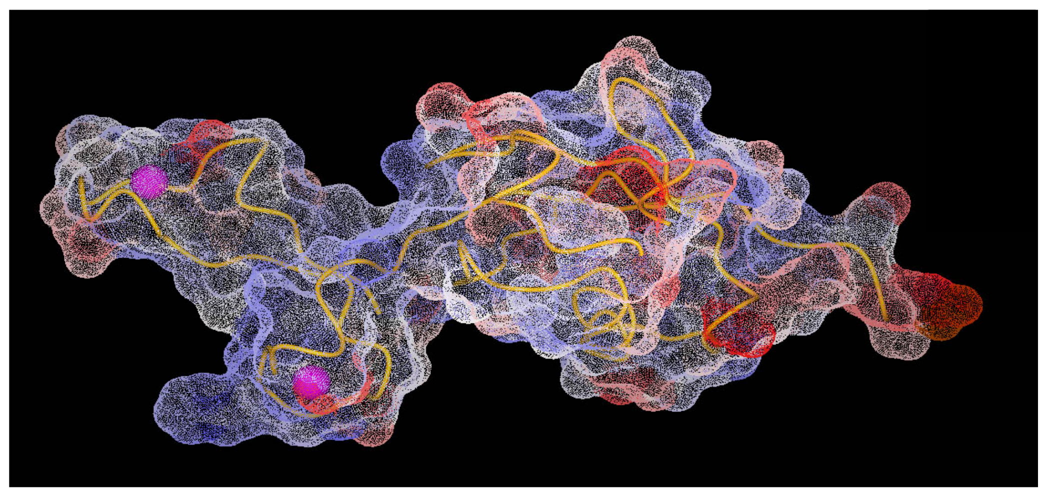




Yellow:	Δppm > 0.05 ppm
Orange:	Δppm > 0.15 ppm
Red:	Δppm > 0.25 ppm

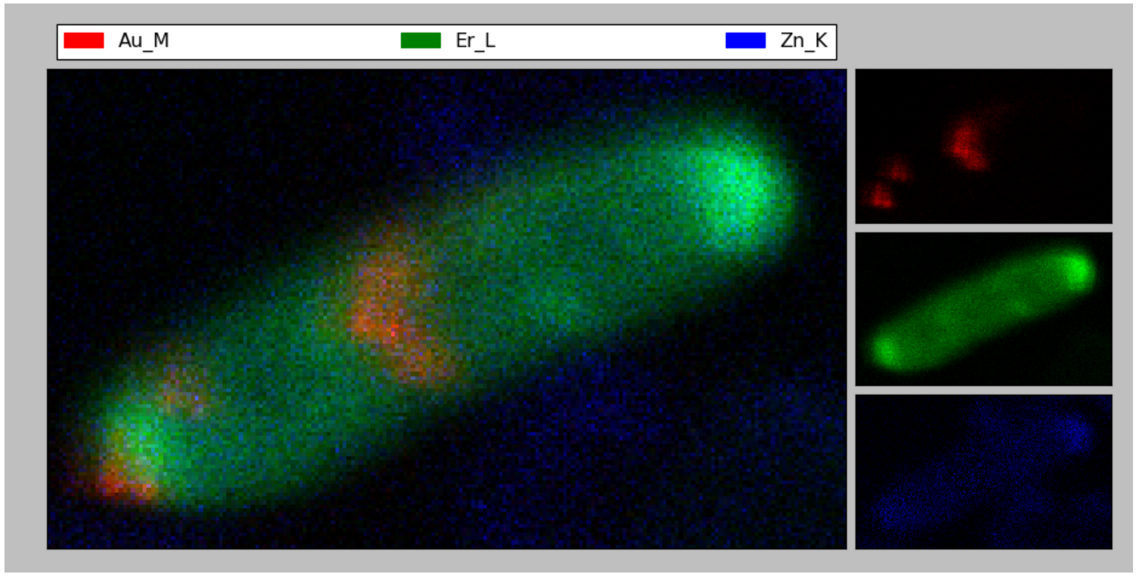
J Biomol NMR. 2015 , 63, 275-82



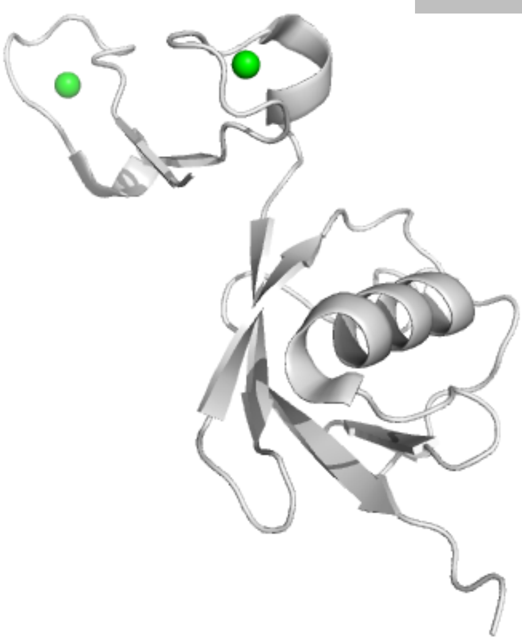


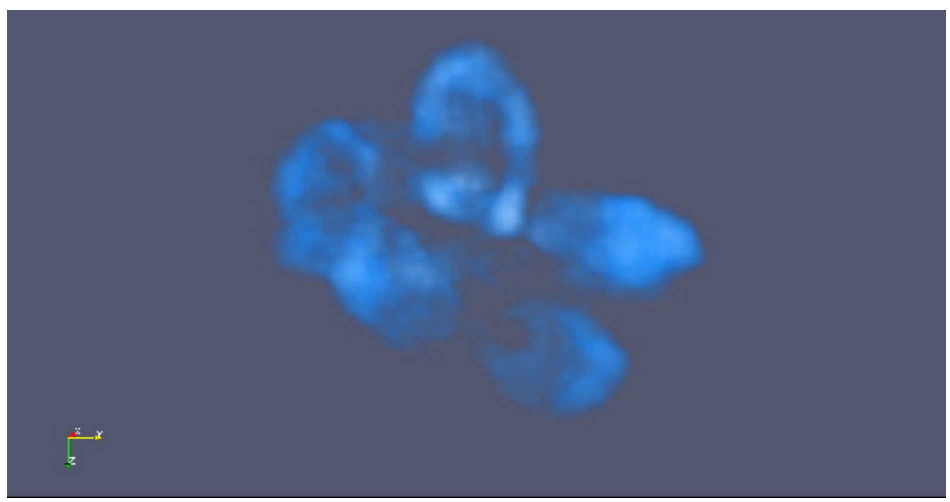
J. Am. Chem. Soc. 2007, 129, 7114-7120

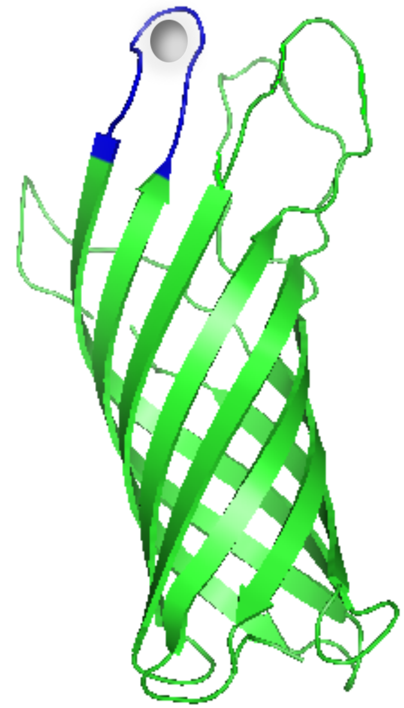
New Applications in X-ray Fluorescence Microscopy



15 nm resolution!







L. Easthon & K. O'Toole, unpublished

Materials for Electrochemical Energy Conversion

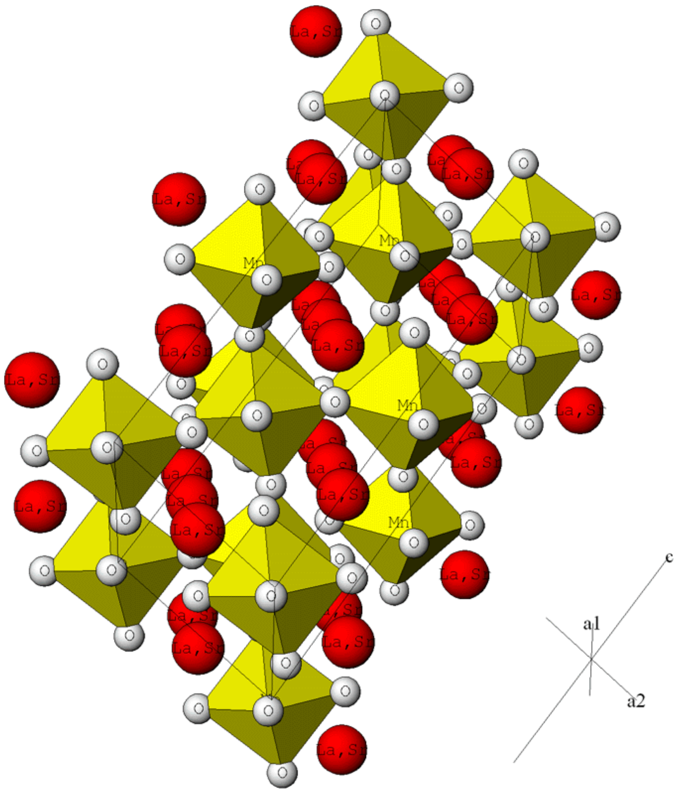
Srikanth Gopalan
Associate Professor

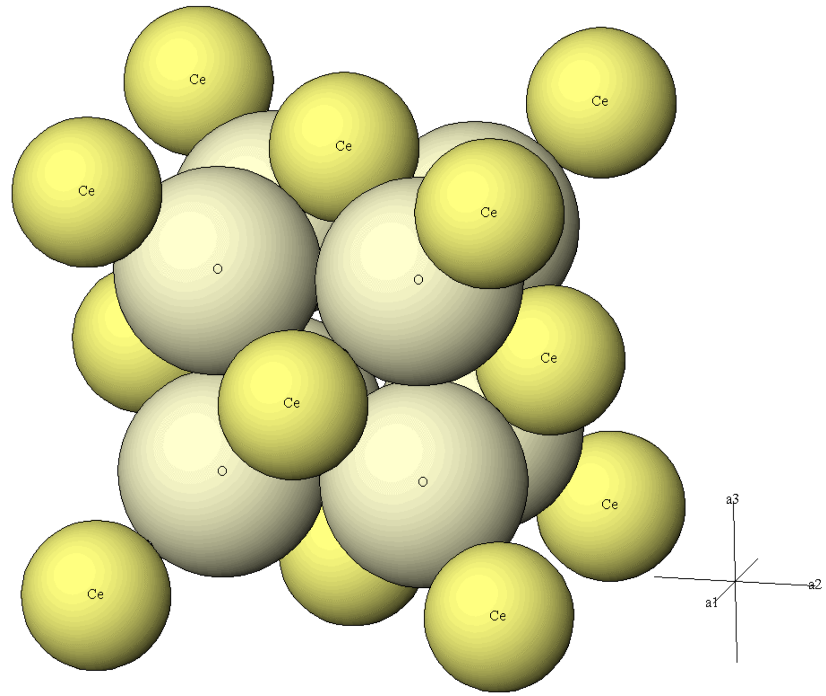
Mechanical Engineering
Materials Science & Engineering

Overarching Themes

- Materials: Conducting Oxides – Ionic and Electronic Transport
- Experimental – Materials synthesis, design and fabrication of devices – fuel cells, membrane-based reactive separation of gases, sensors etc.
- Modeling/Theory – Materials thermodynamics and kinetics, transport phenomena

Conducting Ceramics: Complex Oxides

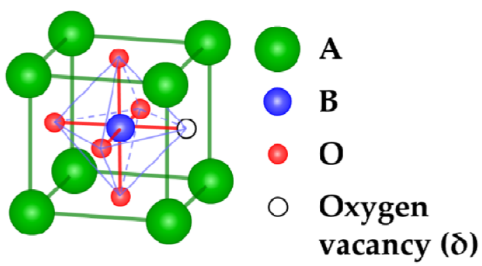


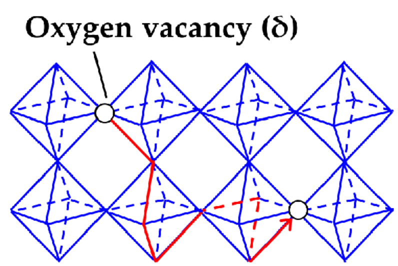


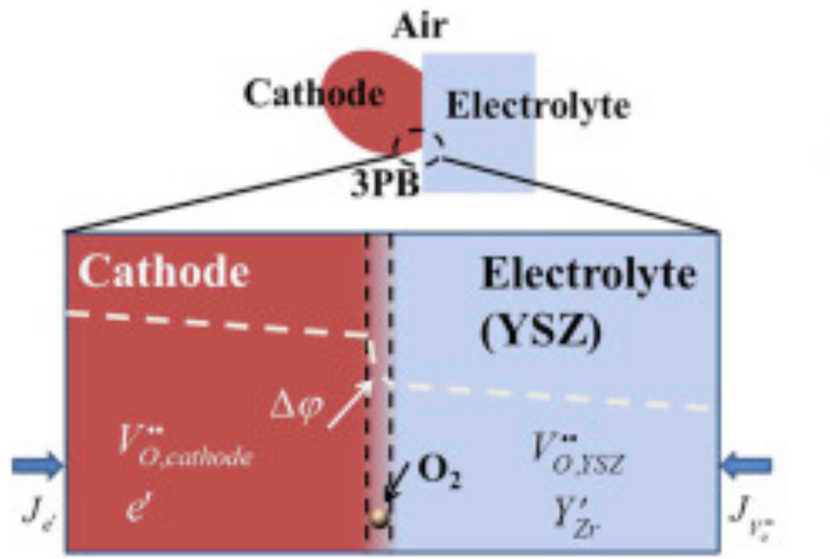
Manipulating Transport by Point Defect Chemistry

Point defects in materials are central to mass and charge transport

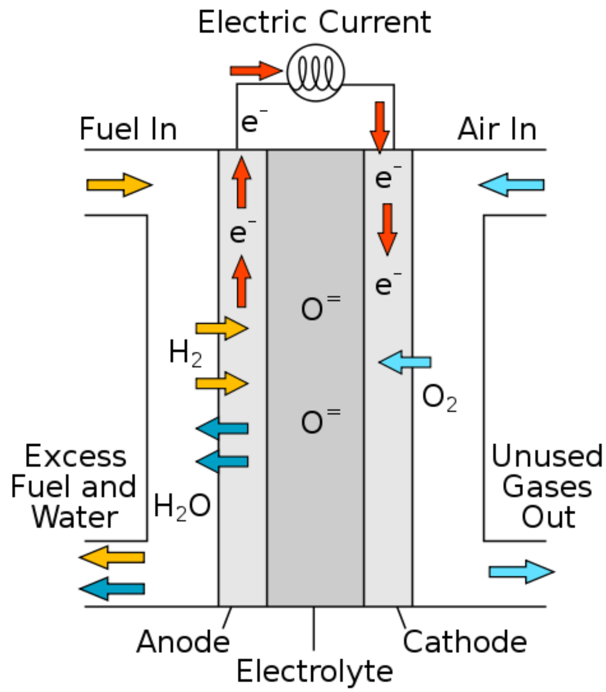
Unlike electronic, magnetic, and optical applications where the goal is to minimize point defects, in solid state ionics, presence of point defects are critical to transport of ions

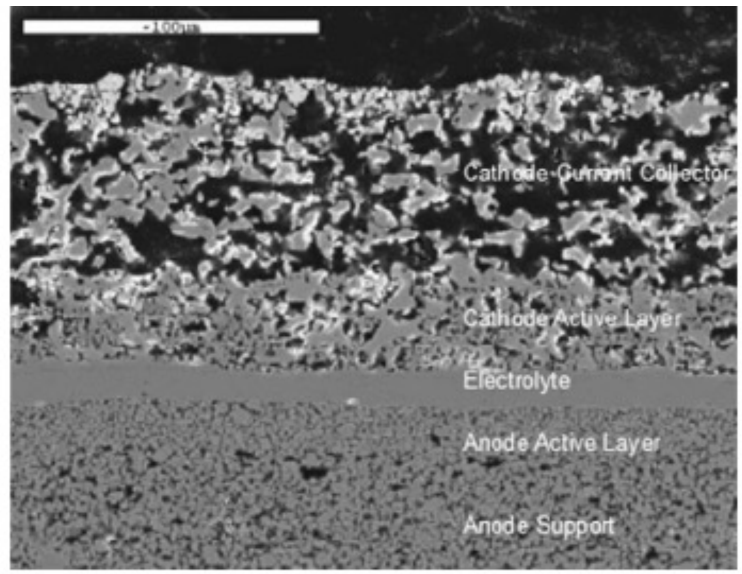


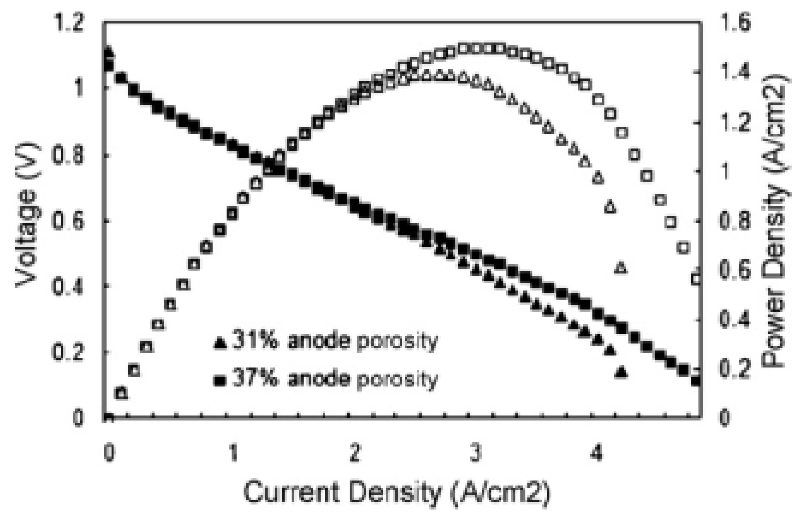




Devices: Solid Oxide Fuel Cells (SOFCs)



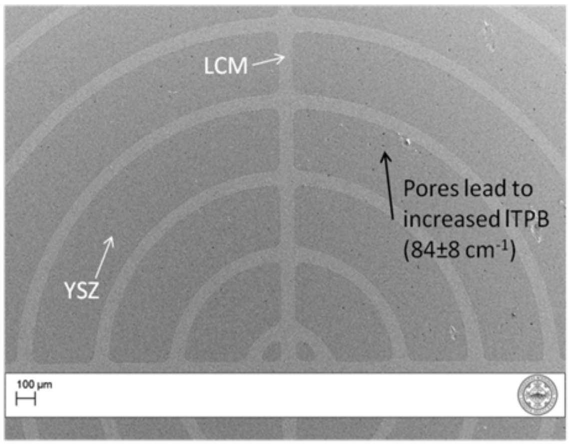


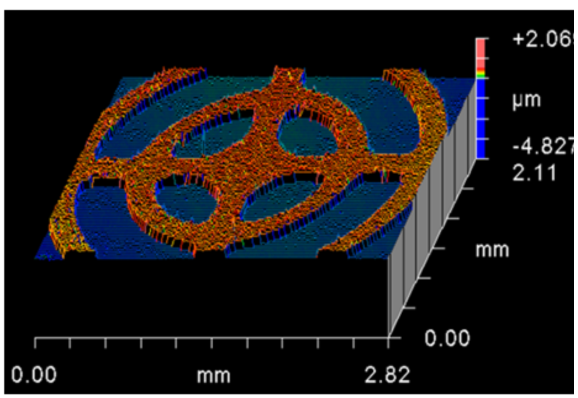


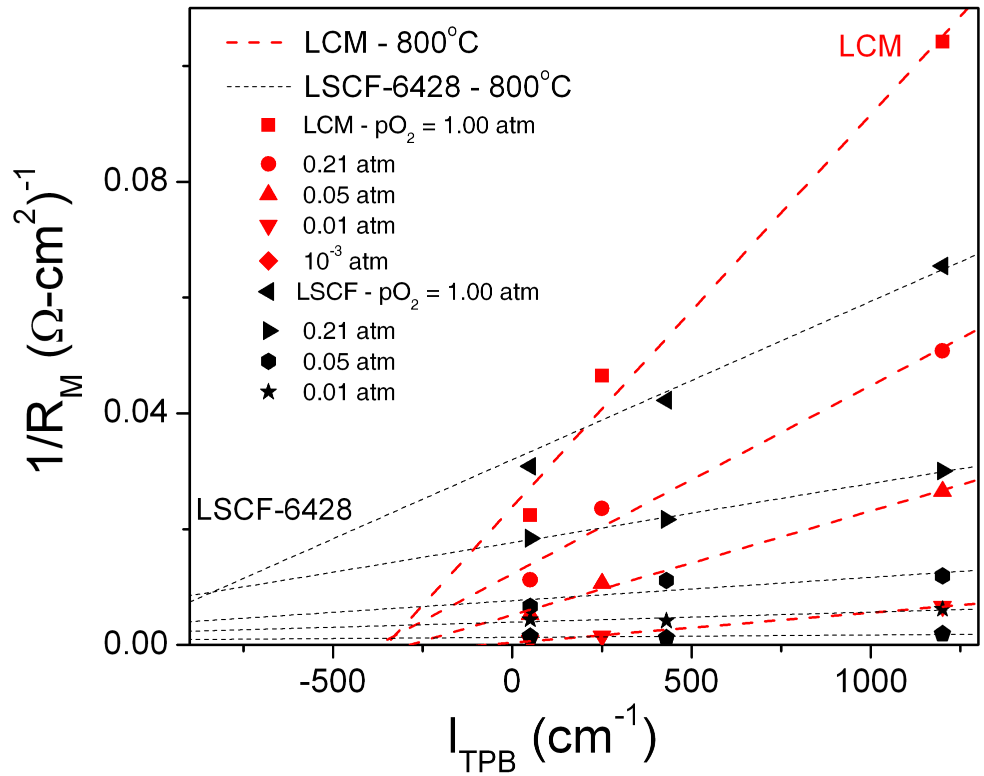
KJ Yoon, P Zink, S Gopalan, UB Pal,
Journal of power Sources 172 (1), 39-49

SOFCs: Transport and Electrode Reaction Kinetics

Patterned Electrodes:

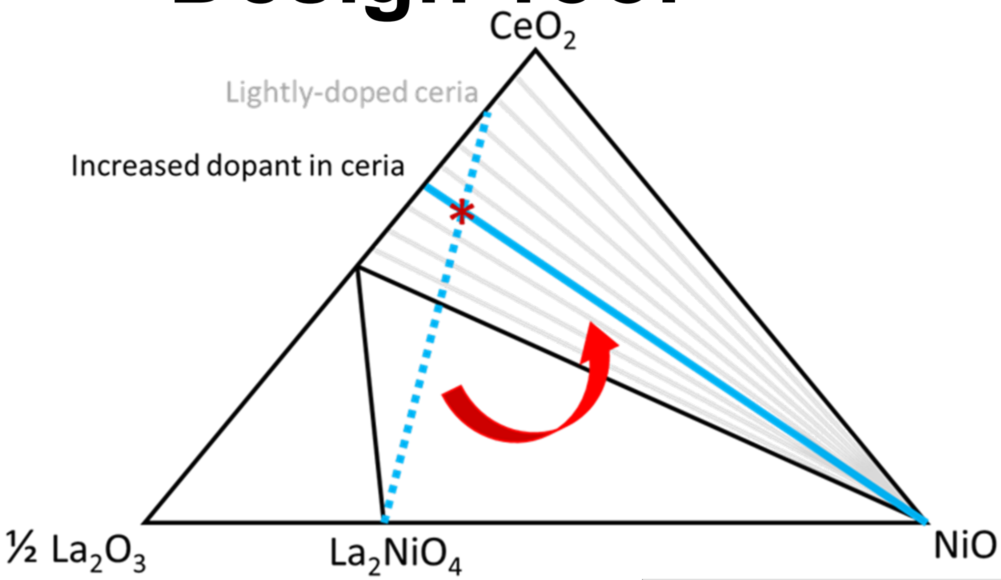


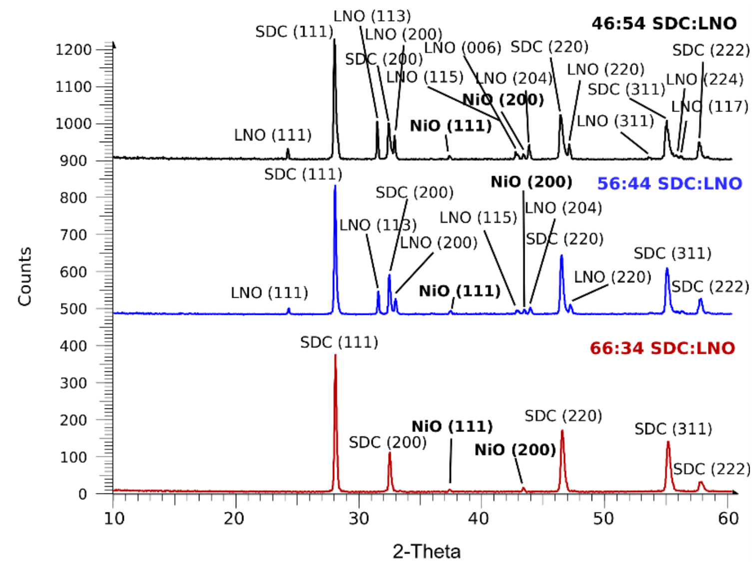


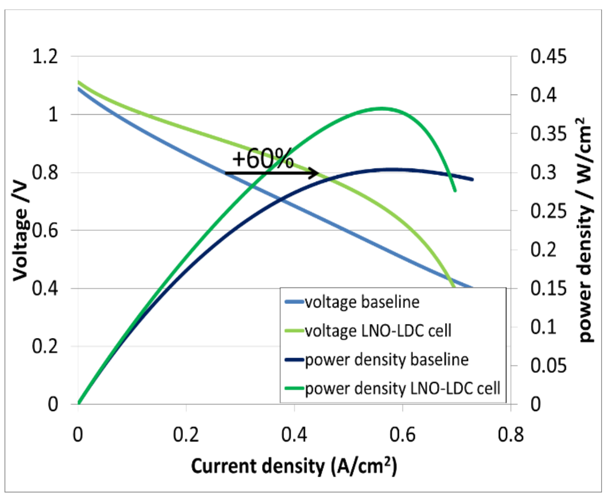


Miara, SN Basu, UB Pal, S Gopalan
Journal of The Electrochemical Society 159 (8), F419-F425

SOFCs: Thermodynamics as a Material Design Tool

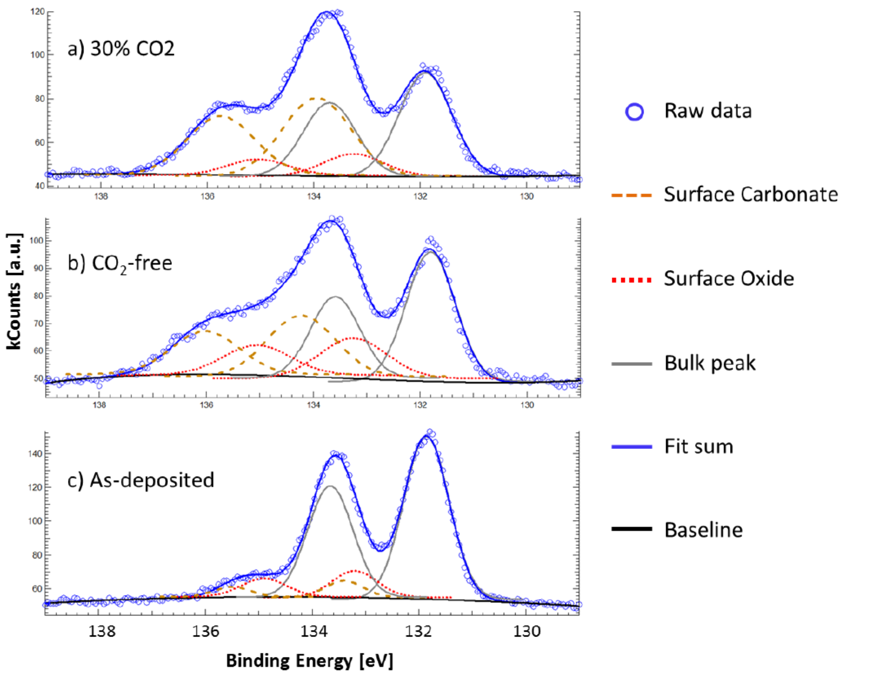




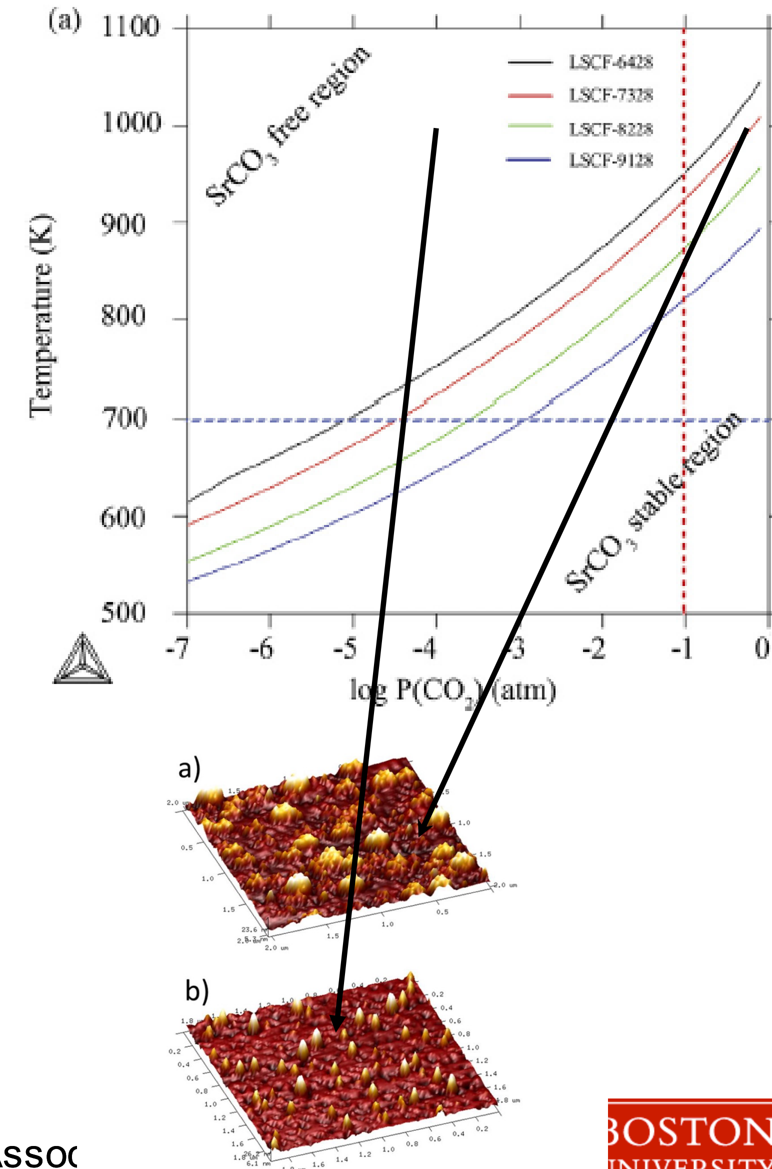


D Cetin, S Poizeau, J Pietras, S Gopalan
Solid State Ionics 300, 91-96

SOFCs: Computational Thermodynamics

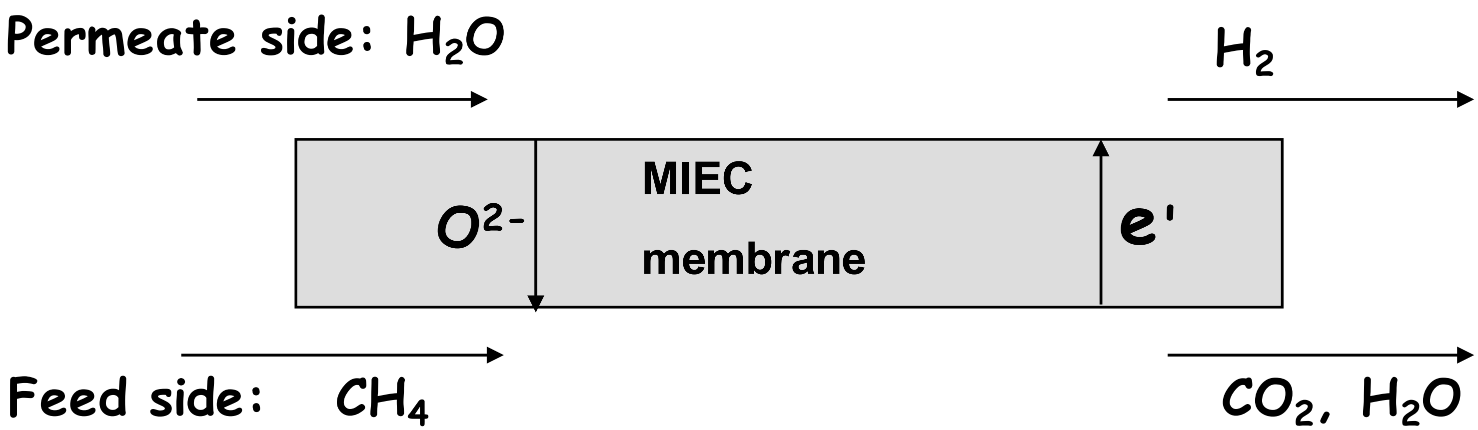


S Darvish, S Gopalan, Y Zhong
Journal of Power Sources 336, 351-359



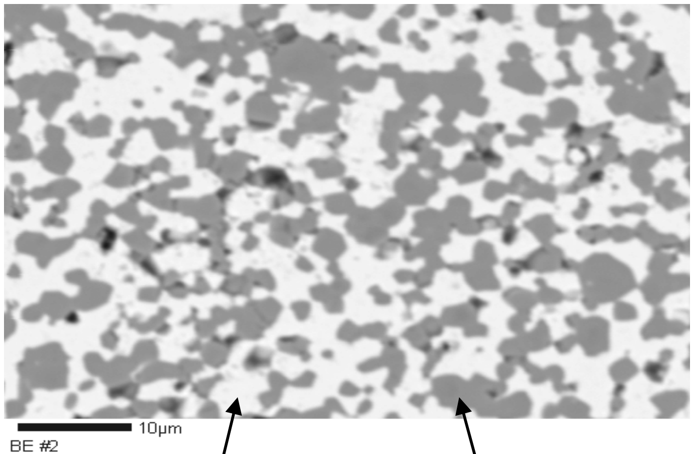
MIEC Membranes: Hydrogen Generation and CO_2 Segregation

$H_2O + 2e' = O^{2-} + H_2$



$CH_4 + 4O^{2-} = CO_2 + 2H_2O + 8e'$

MIEC Membranes: Hydrogen Generation and CO_2 Segregation

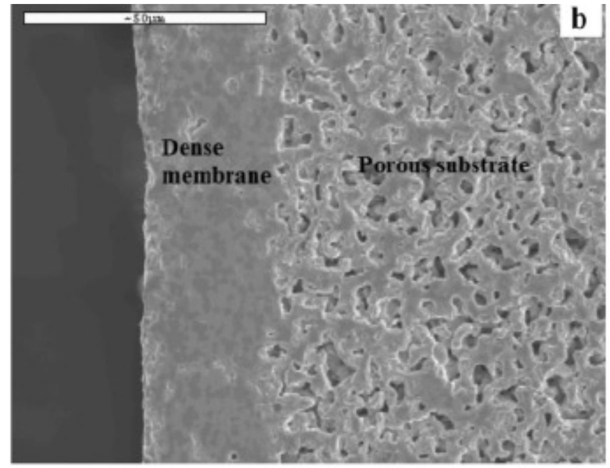


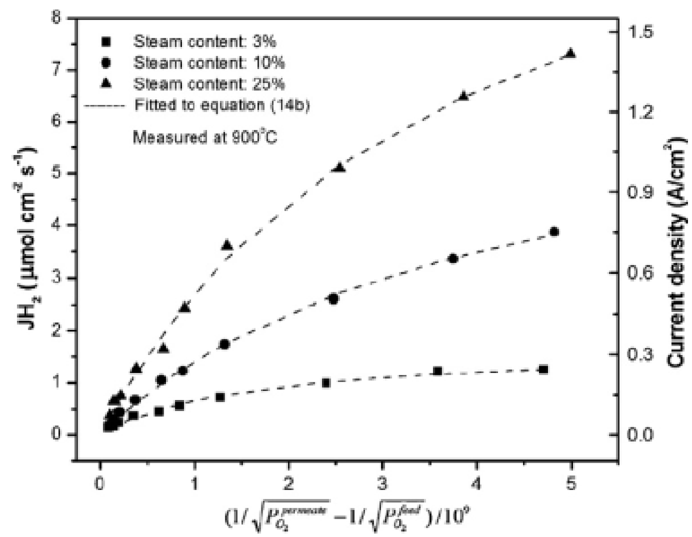
O^{2-} conductor

GDC

e′ conductor

YSTA





Electrochimica Acta 56 (20), 6989-6996

Acknowledgments

Boston University Office of the Vice President and Associate Provost for Research