

Natural Resources, Climate, and Clean Energy

Energy Resources &
Infrastructure Research

Electronic and Magnetic Properties at High Pressure

Dr. Andrew Cornelius

Department of Physics & Astronomy

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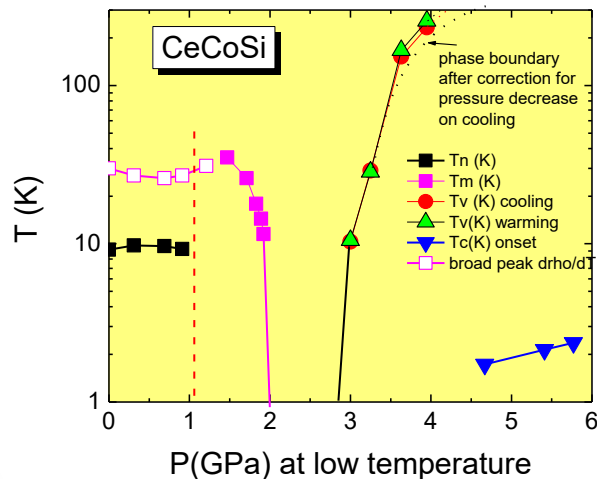
Expertise:

- Experimental high pressure measurements
- Magnetism
- Superconductivity

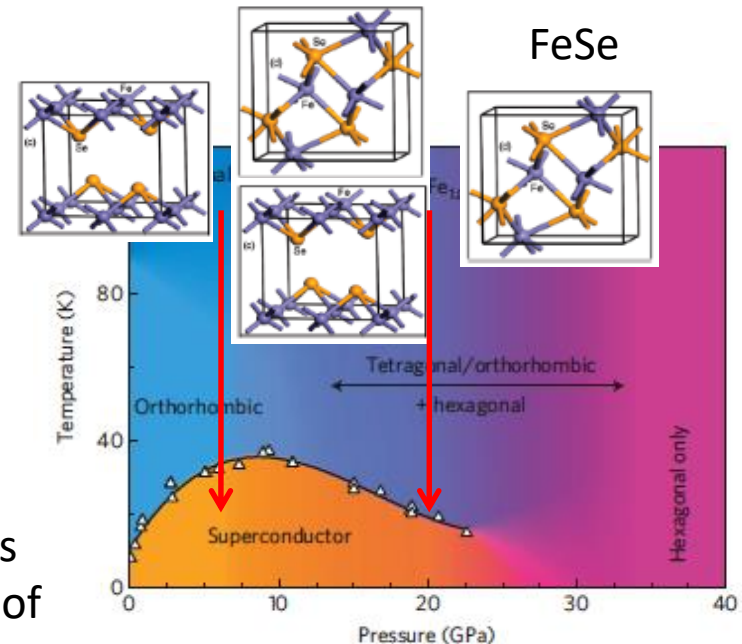
Superconductivity

Quantum Design PPMS at UNLV

- Measurements from 0.3 K to 400 K
 - Heat capacity, electric and thermal transport, and AC/DC magnetization
- Pressure cells to measure electrical properties (clamp to 3 GPa and diamond anvil cell to >100 GPa)



Addition of high pressure synchrotron experiments (diffraction and X-ray absorption) allows mapping of complex superconducting phase diagrams



Correlated-Electron Systems

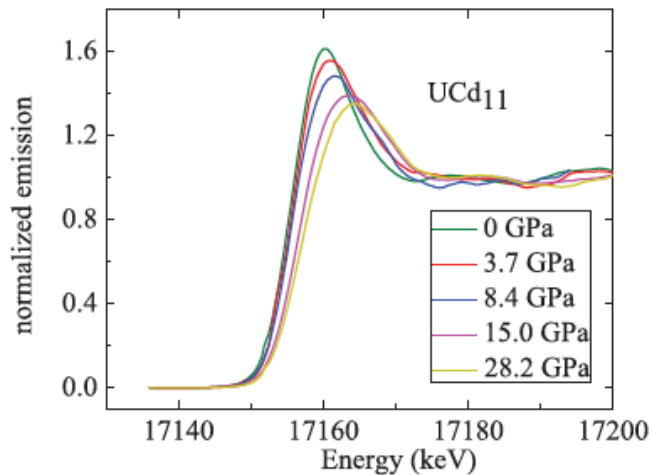
Modified periodic table

Empty Shell	Partially Filled Shell																Full Shell
4f	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
5f	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		
3d	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn						
4d	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd						
5d	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg						

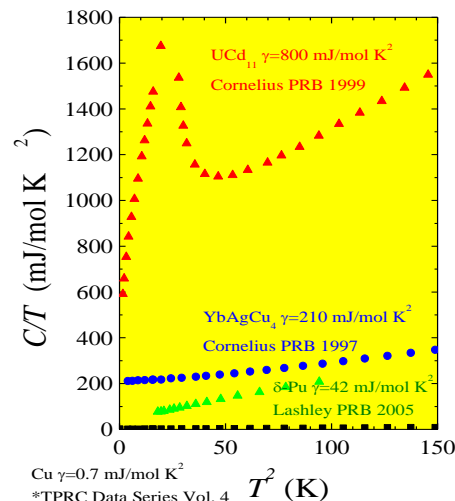
Yb³⁺

Increasing Localization

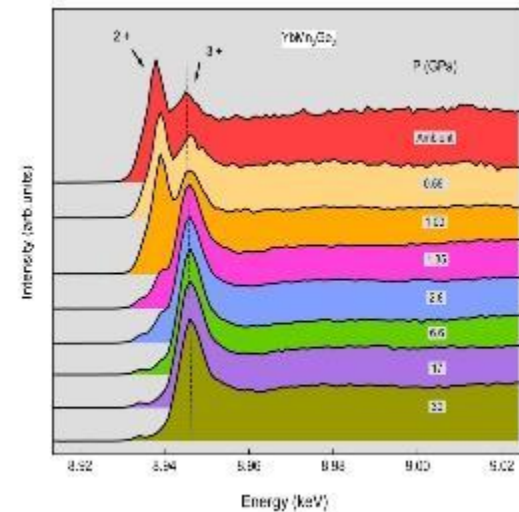
- Going from localized to delocalized electrons one often finds strong electron-electron correlations
- Correlated electron systems can yield interesting behavior: fluctuating valence, superconductivity, non-Fermi liquid, heavy fermion and many more



f-electron delocalization
X-ray absorption



Heavy fermions
Heat Capacity



Fluctuating valence
X-ray fluorescence

Surface and Interface Characterization of Materials for Energy Conversion

Dr. Clemens Heske

Professor

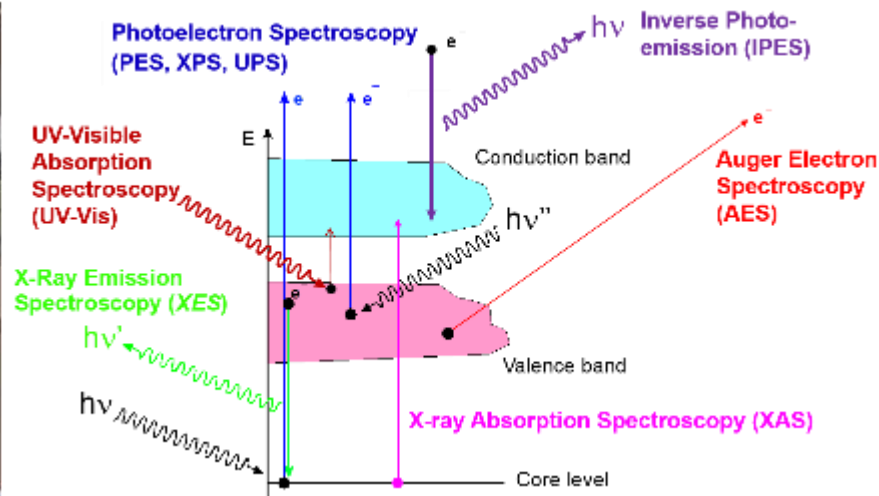
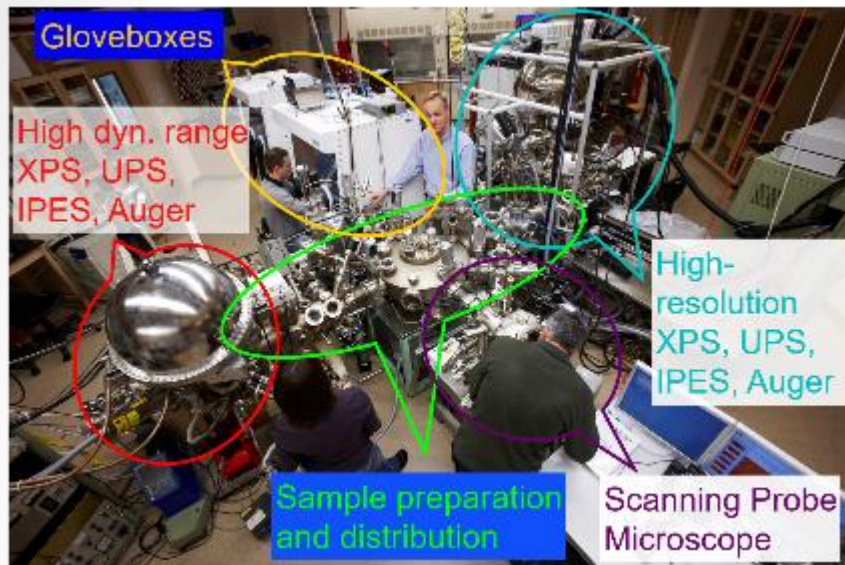
Department of Chemistry and Biochemistry

heske@unlv.nevada.edu

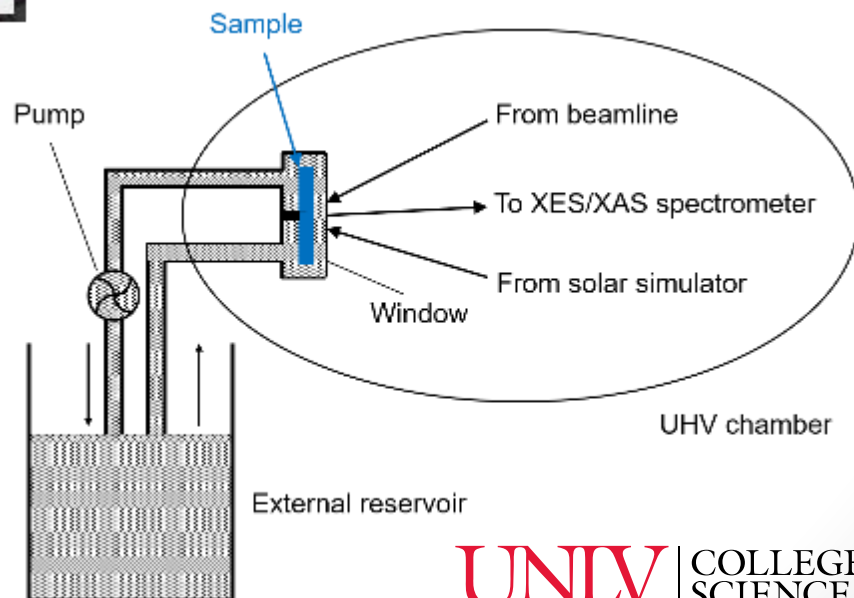
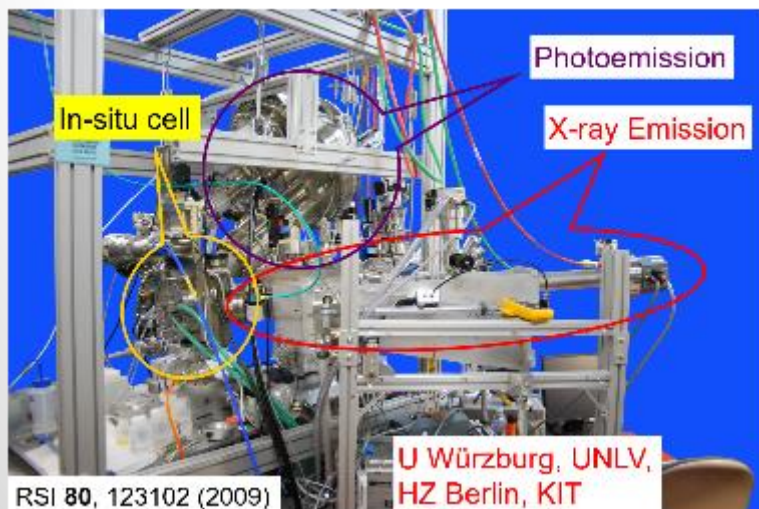
Expertise

- Electronic and Chemical Structure of Energy-Conversion Materials
- Surface and Interface Characterization
- Soft x-ray and Electron Spectroscopy
- Scanning Probe Microscopy
- Synchrotron Radiation

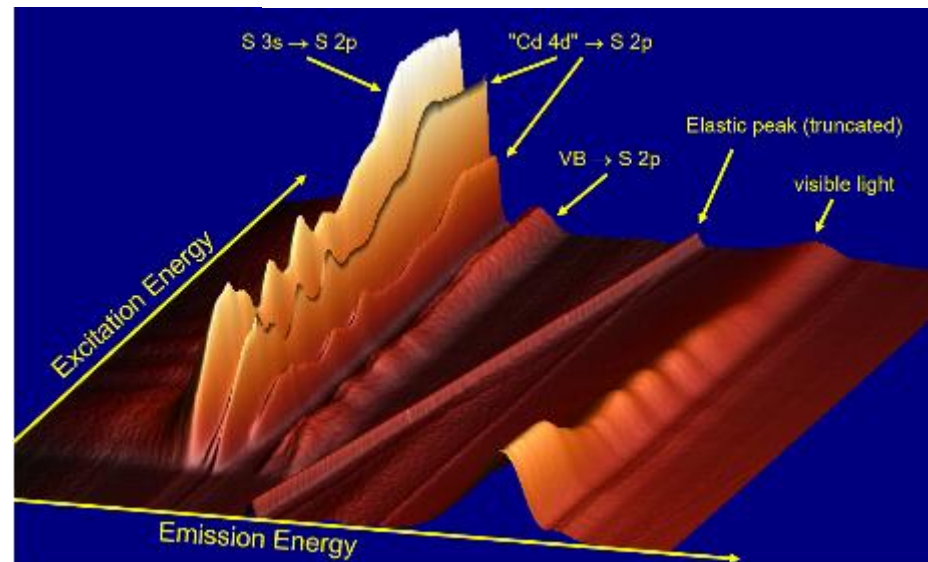
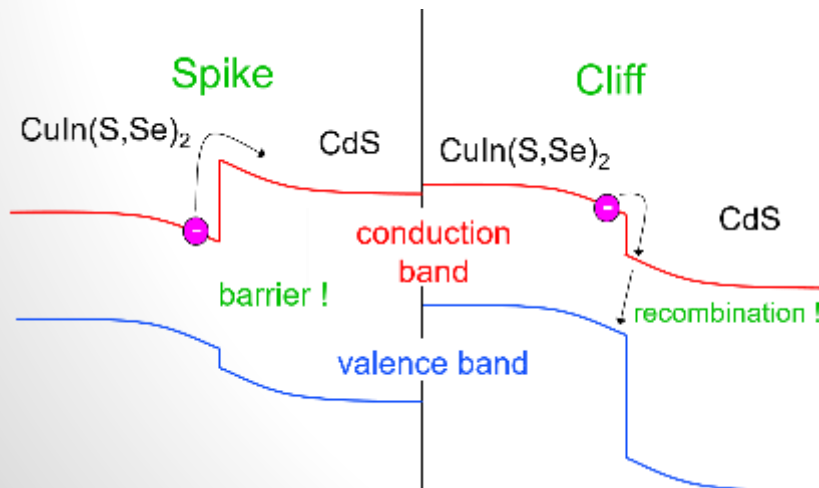
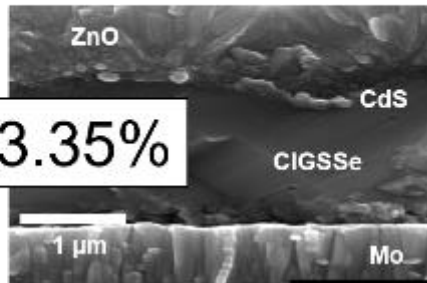
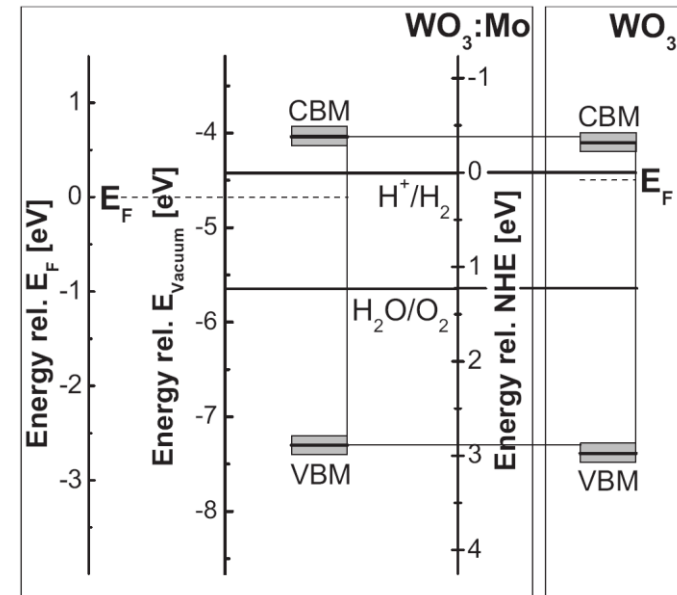
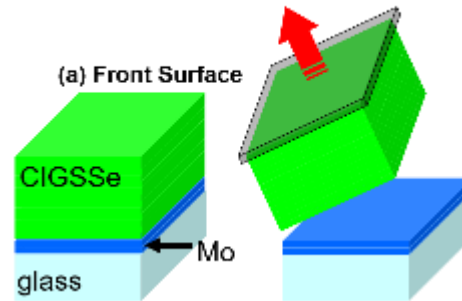
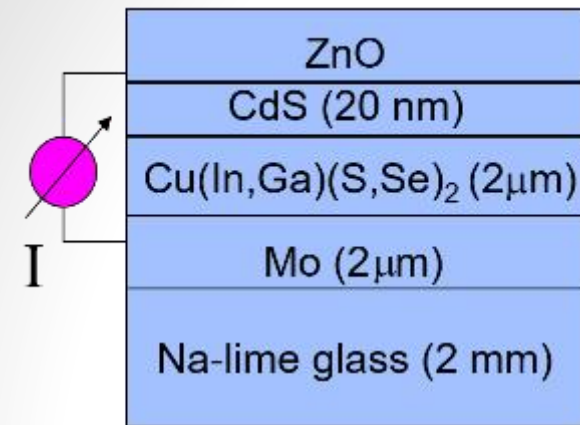
Surface and Interface Characterization



SALSA: Solid And Liquid Spectroscopic Analysis



Materials for Energy Conversion

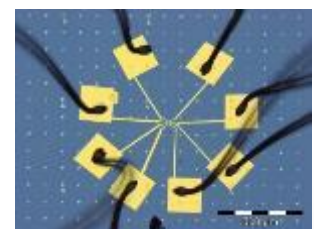
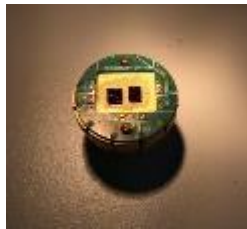
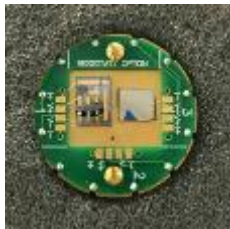
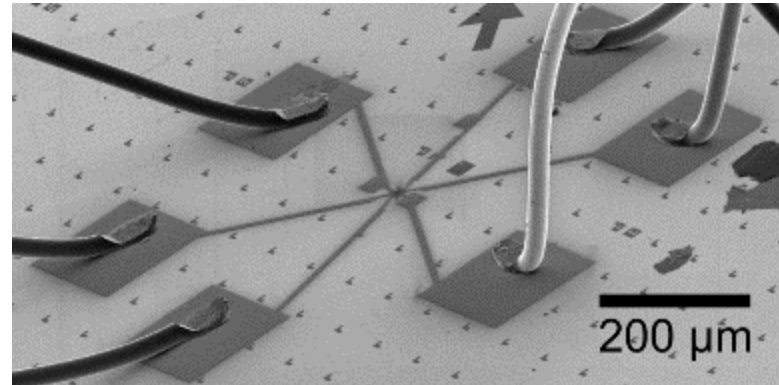


Island – Quantum computing, quantum sensing



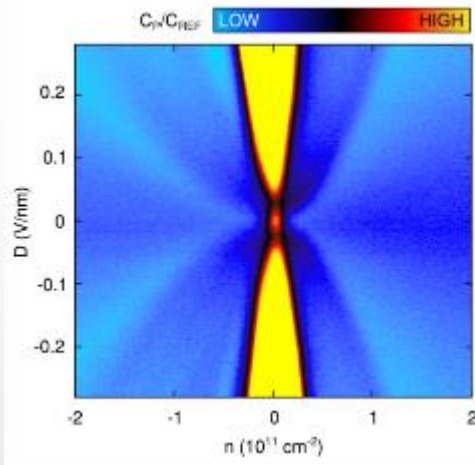
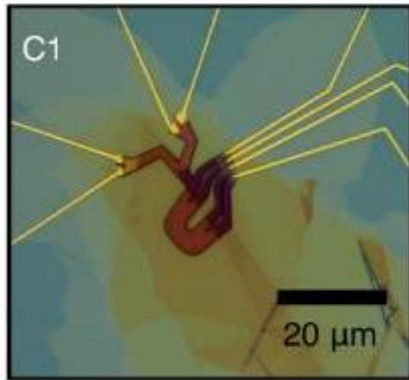
Areas of Research

- Nanotechnology, device physics
- Photodetection and quantum sensing
- Quantum computing, topological qubits
- Non-equilibrium, driven systems
- Superconductivity, proximity effects
- Low dimensional materials

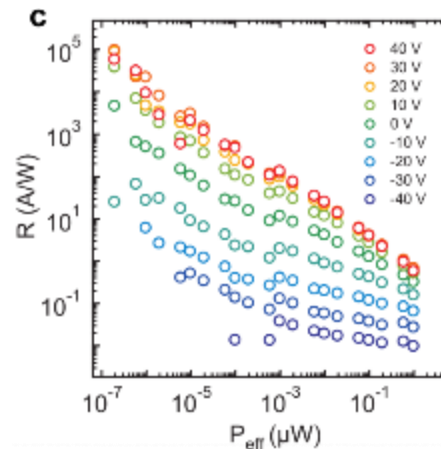
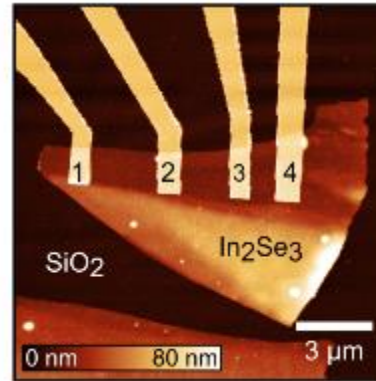


Island – Quantum computing, quantum sensing

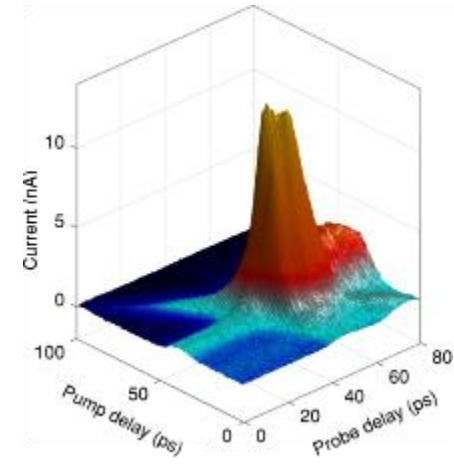
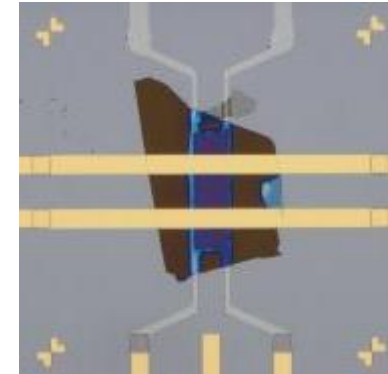
Quantum computing:
Topological phases for fault-tolerant, universal quantum computing.



Industry-disruptive photodetectors: Ultra-sensitive phototransistors designed with 2D materials and heterostructures.



Transient phases of driven systems: Non-equilibrium response of pumped nanomaterials below the diffraction limit.



Island, J. O., et al. *Nature* **571** (2019): 85–89.

Island, J. O., et al. *Nano Letters* **15** (2015): 7853-7858.

Island – Quantum computing, quantum sensing

Journal publications

Spin-orbit-driven band inversion in bilayer graphene by van der Waals proximity effect

J. O. Island, X. Cui, C. Lewandowski, J. Y. Khoo, E. M. Spanton, H. Zhou, D. Rhodes, J. C. Hone, T. Taniguchi, K. Watanabe, L. S. Levitov, M. P. Zaletel, A. F. Young, *Nature* **571**, 85-89 (2019). (arXiv)



Enhanced superconductivity in atomically thin TaS₂

E. Navarro-Moratalla*, J. O. Island*, S. Manas-Valero, E. Pinilla-Cienfuegos, A. Castellanos- Gomez, J. Quereda, G. Rubio-Bollinger, L. Chirolli, J. A. Silva-Guilln, N. Agrat, G.A. Steele, F. Guinea, H.S.J. van der Zant, E. Coronado, *Nature Communications* **15**, 7853 (2016). (arXiv)



Proximity-induced Shiba states in a molecular junction

J. O. Island, R. Gaudenzi, J. de Bruijckere, E. Burzuri, C. Franco, M. Mas-Torrent, C. Rovira, J. Veciana, T. M. Klapwijk, R. Aguado, H. S. J. van der Zant, *Physical Review Letters* **118**, 117001 (2017). (arXiv)



TiS₃ transistors with tailored morphology and electrical properties

J. O. Island, M. Barawi, R. Biele, A. Almazan, J.M. Clamagirand, J.R. Ares, C. Sanchez, H.S.J. van der Zant, J.V. Alvarez, R. D'Agosta, I. J. Ferrer, A. Castellanos-Gomez, *Advanced Materials* **27**, 2595 (2015). (arXiv)



Environmental instability of few-layer black phosphorus

J. O. Island, G.A. Steele, H.S.J. van der Zant, and A. Castellanos-Gomez, *2D Materials* **2**, 011002 (2015). (arXiv)



Ultrahigh photoresponse of few-layer TiS₃ nanoribbon transistors

J. O. Island, M. Buscema, M. Barawi, J.M. Clamagirand, J.R. Ares, C. Sanchez, I.J. Ferrer, G.A. Steele, H.S.J. van der Zant, and A. Castellanos-Gomez, *Advanced Optical Materials* **2**, 641 (2014). (arXiv)



Gate controlled photocurrent generation mechanisms in high-gain In₂Se₃ phototransistors

J. O. Island*, S.I. Blanter*, M. Buscema, H.S.J. van der Zant, and A. Castellanos-Gomez, *Nano Letters* **15**, 7853 (2015). (arXiv)



Precise and reversible band gap tuning in single-layer MoSe₂ by uniaxial strain

J. O. Island, A. Kuc, E.H. Diependaal, H.S.J. van der Zant, T. Heine, and A. Castellanos- Gomez, *Nanoscale* **8**, 2589 (2016). (arXiv)



Economic Geology

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Department of Geoscience

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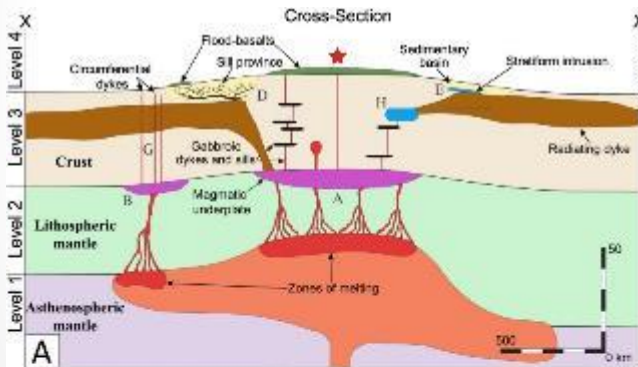
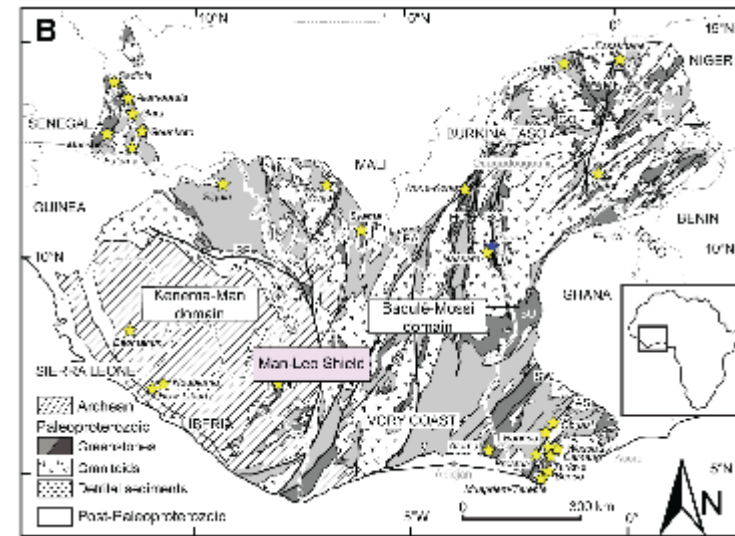
Expertise:

Geochemistry, mineral exploration, ore deposit geology, mineral economics, mineral exploration technique development, igneous petrology, environmental impact of mining

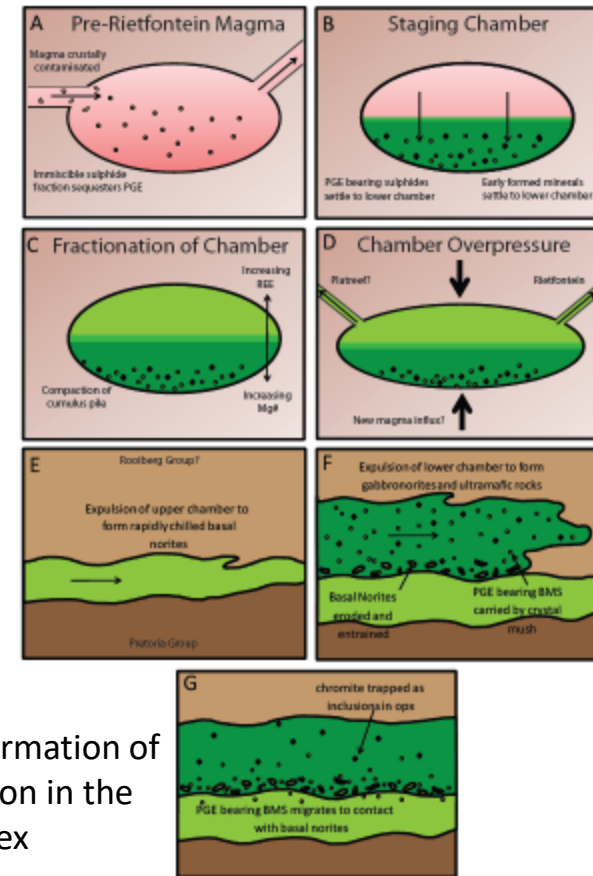
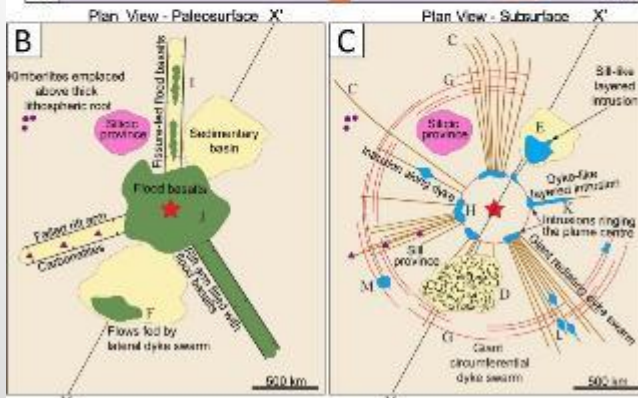
Geochemistry

- Understanding mineralizing systems
- Links between tectonic and magmatic events and mineral systems
- Development of mineral exploration tools

Distribution of Orogenic Au deposits within West Africa



Links between Large Igneous Province plumbing systems and mineralization

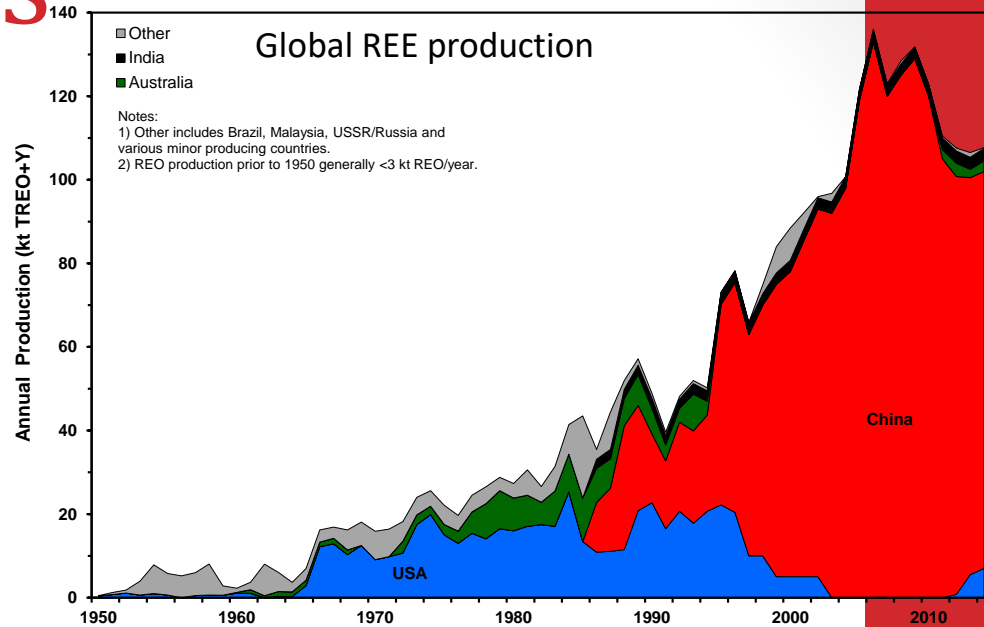
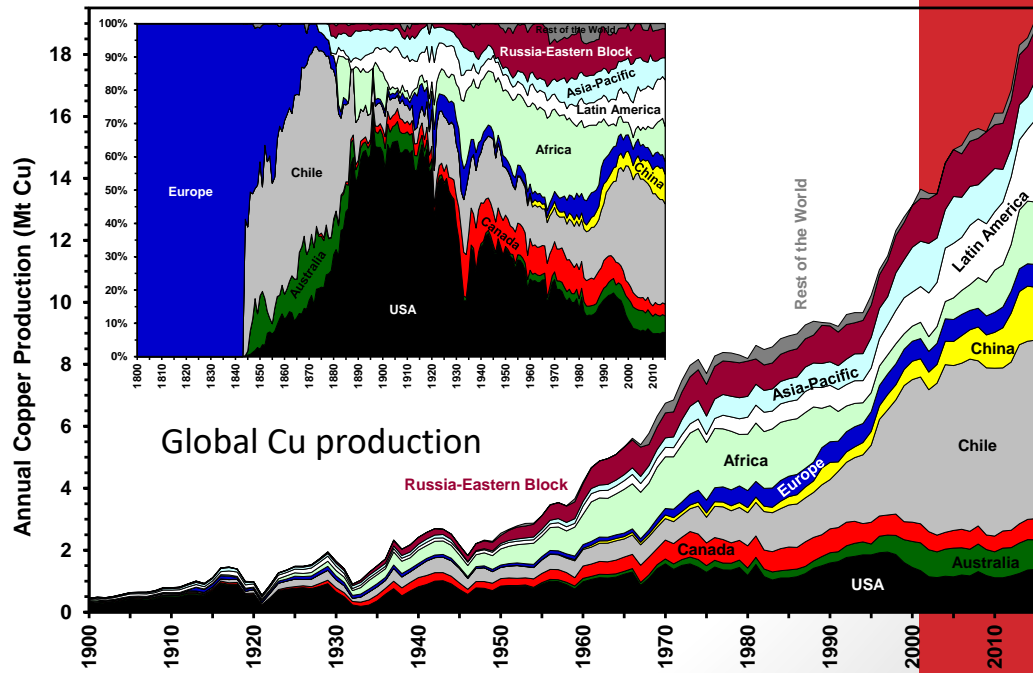
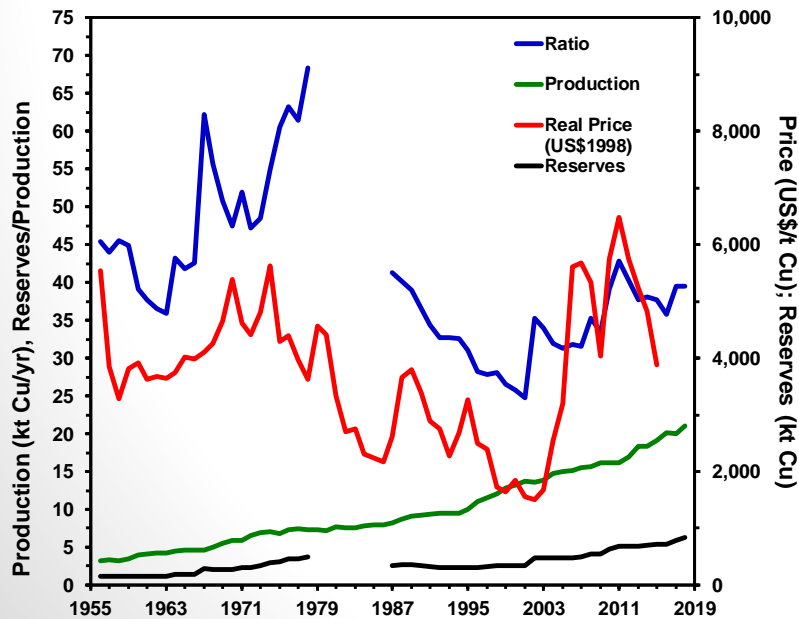


Model for the formation of PGE mineralization in the Bushveld Complex

Mineral economics

- Understanding global metal resources
- Assessing future demand and supply
- Materials for green technology and critical metals

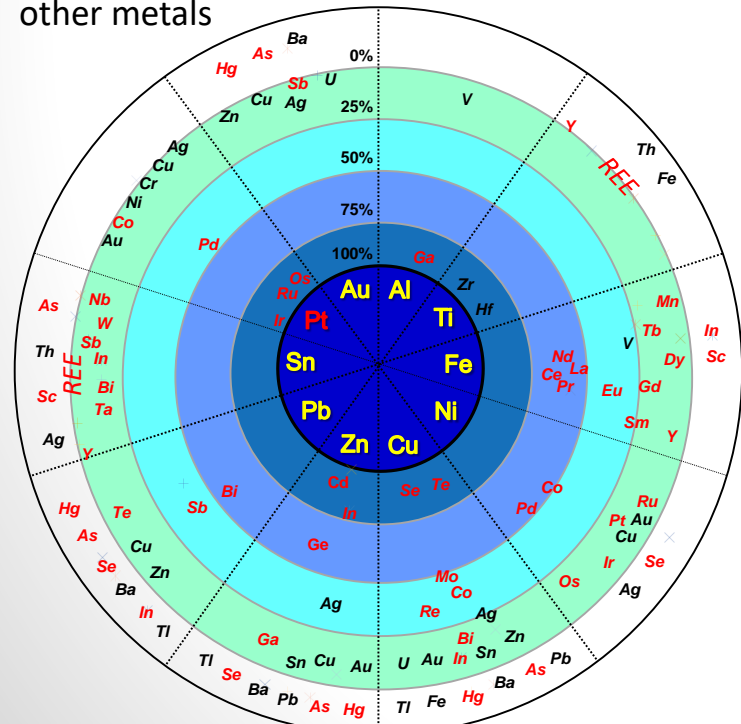
Understanding global metal reserves and production



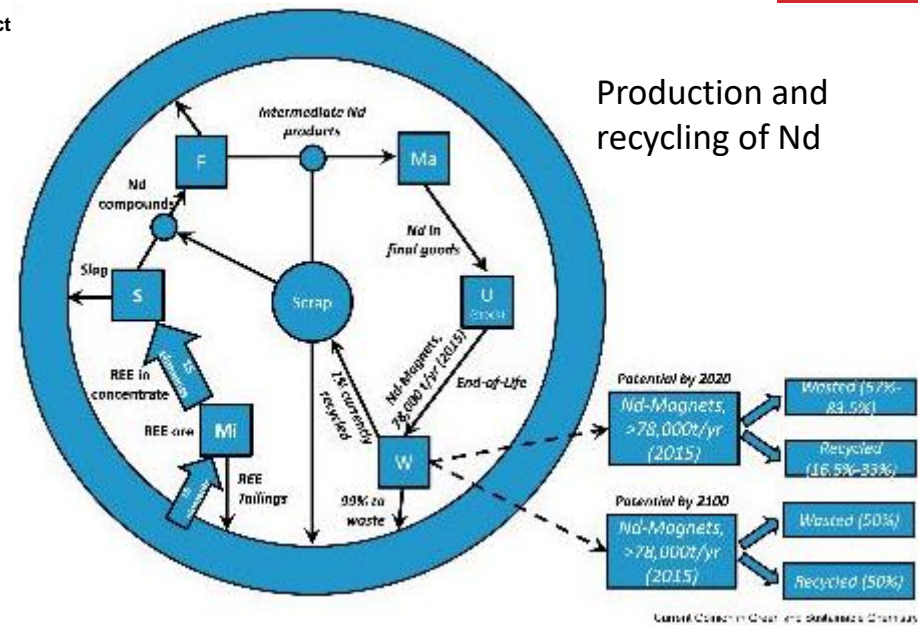
Critical metals

- Identification of potential sources of the critical metals
- Determining the processes that concentrate critical elements and development of associated exploration tools

Metal companionship;
understanding how critical
metal production is reliant on
other metals

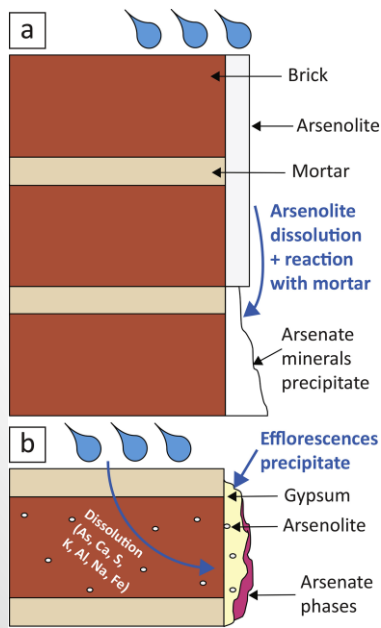
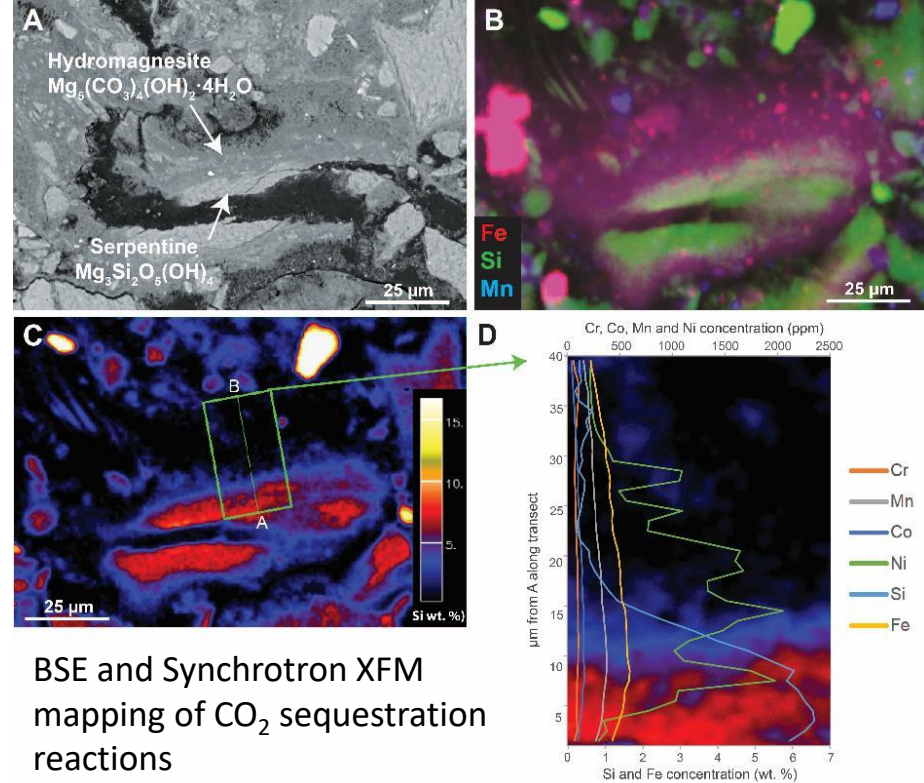


Be-bearing rare metal pegmatite, southern Nevada



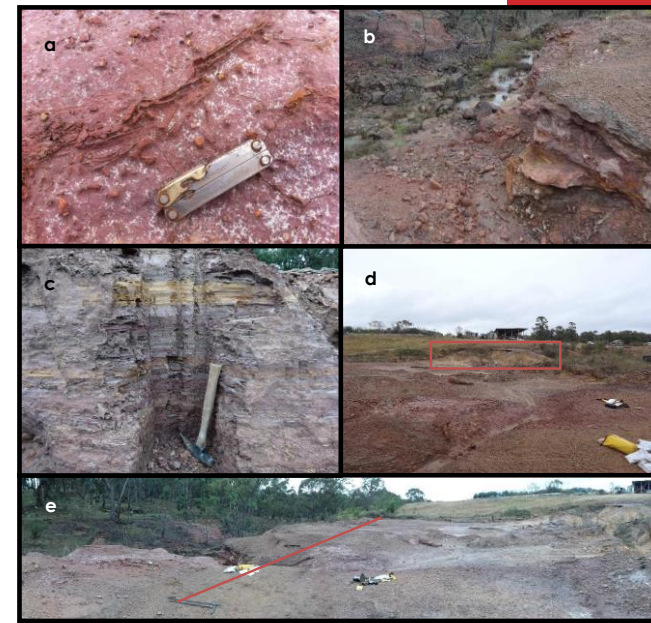
Environmental impact of mining

- Assessing environmental impacts
- Potential of wealth from waste; assessing mining waste metal production and CO₂ sequestration potential



Understanding arsenic mobility in mining and mineral processing environments

Assessing the environmental impact and critical metal potential of mineral processing waste and tailings



Other research areas

- GIS-based mineral prospectivity modeling in 2D and 3D space
- Machine learning approaches to exploration targeting
- Igneous petrology and the formation of Large Igneous Provinces
- Pegmatites and highly evolved rhyolites as sources of critical metals
- I run a well-equipped fluid inclusion lab that allows the determination of the composition and the temperature and pressure of trapping of hydrothermal fluids associated with mineral deposit formation. I also have a wide range of expertise in other analytical fields, including SIMS, ICP-MS, LA-ICP-MS, ICP-OES and XRF, stable and radiogenic isotopes, XRD, EPMA, SEM, and synchrotron beam analytical approaches.

Organic Materials Chemistry

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Expertise

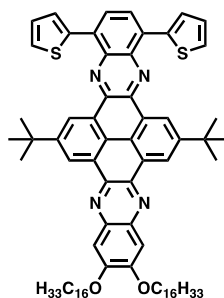
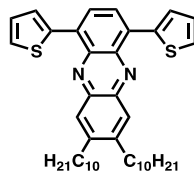
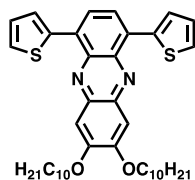
- Organic semiconductors with tunable electronic properties
- Self-assembly (nanomaterials, organogels, etc.)
- All organic room-temperature phosphors
- Materials development for solid-state emission with high quantum yield

Electronic-Property Tuning with Smart Molecular Design

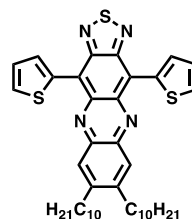
E_{LUMO} -3.16 eV

-3.26 eV

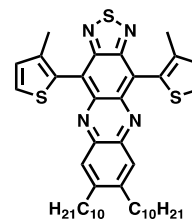
-3.22 eV



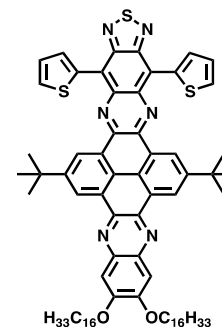
-3.89 eV



-3.80 eV



-3.84 eV



E_{HOMO} -5.43 eV

-5.45 eV

-5.49 eV

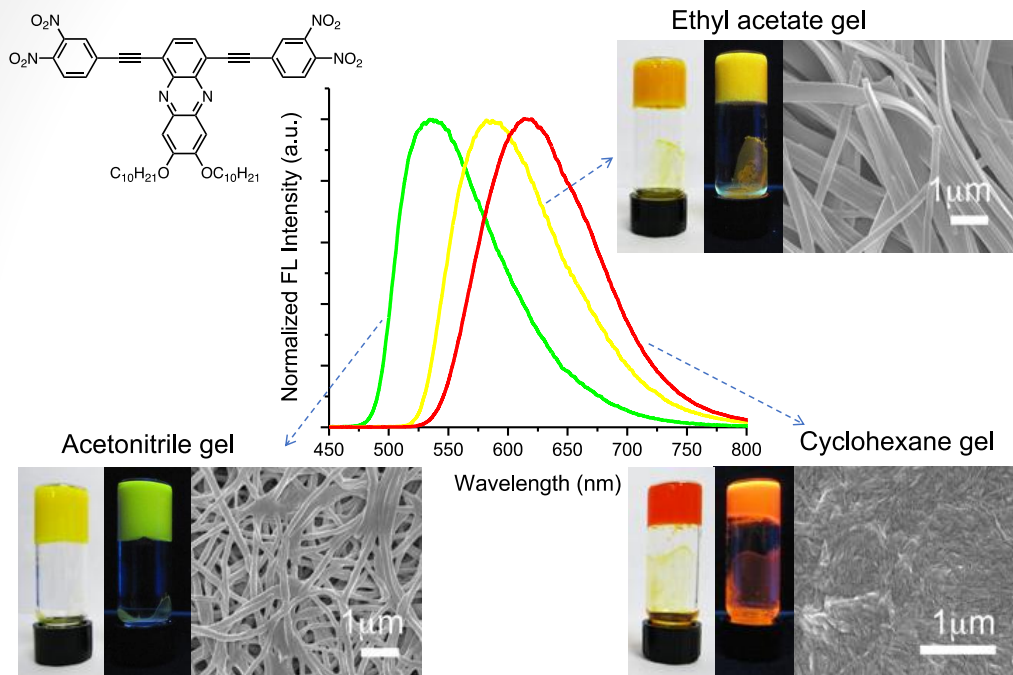
-5.32 eV

-5.51 eV

-5.40 eV



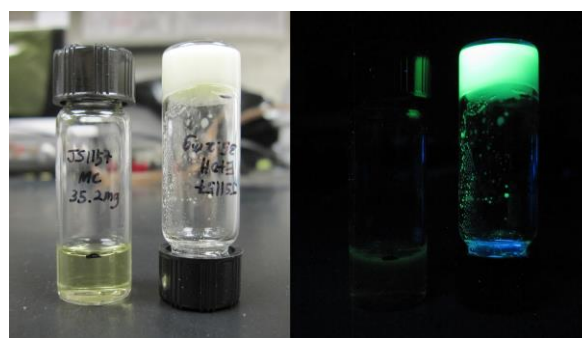
Solvent-Dependent Morphology Control through Organogelation



Journal of Materials Chemistry



Solid-State
Emission with
High
Quantum
Yield



Gel-Induced
Room
Temperature
Phospho-
rescence

Hydrology

Dr. Michael Nicholl

Department of Geoscience

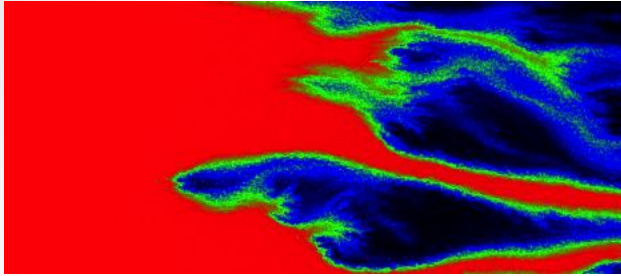
Phone: (702) 895-4616

Email: michael.nicholl@unlv.edu

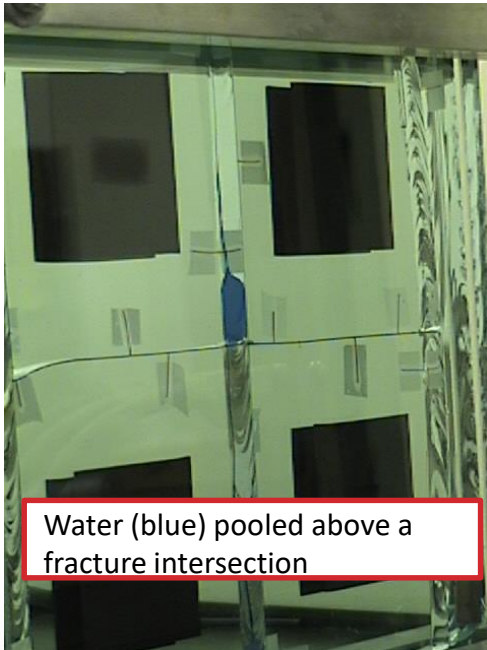
Expertise:

- Unsaturated zone hydrology
- Fractured rock hydrology
- Environmental fluid mechanics

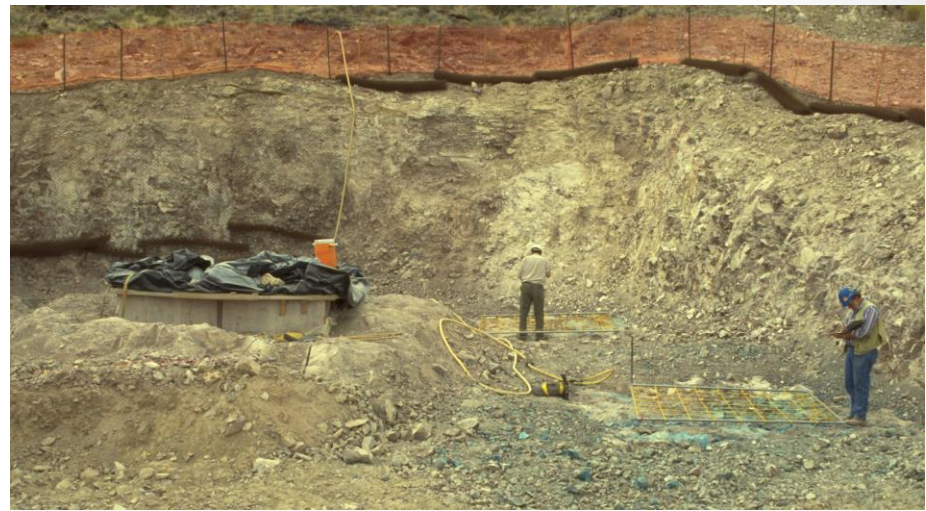
Fractured Rock Hydrology



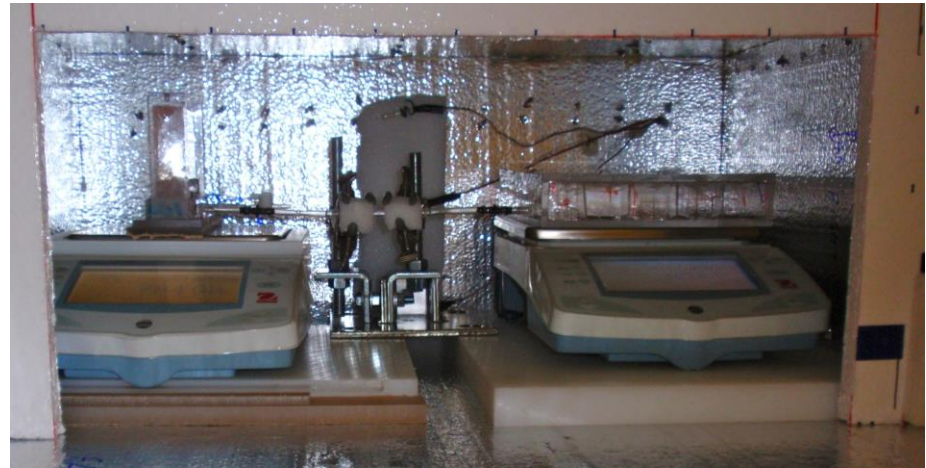
False color image of a miscible displacement experiment in a single fracture



Water (blue) pooled above a fracture intersection



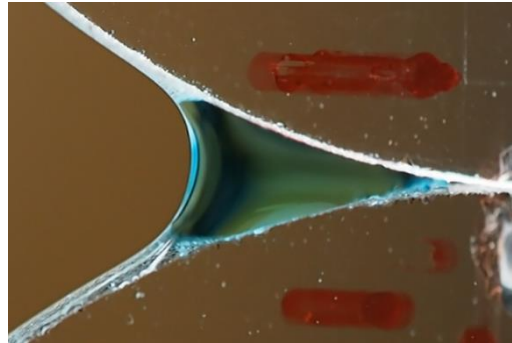
Field mapping of fracture networks
blue dye (right foreground) is from an infiltration test



Isothermal flow across a single rock fracture (matrix-to-matrix flow)

- ❑ Two-phase flow and transport in fractured rock
- ❑ Laboratory experimentation, field mapping, numerical simulations
- ❑ Contaminant transport, geothermal energy, enhanced petroleum recovery

Unsaturated Porous Media



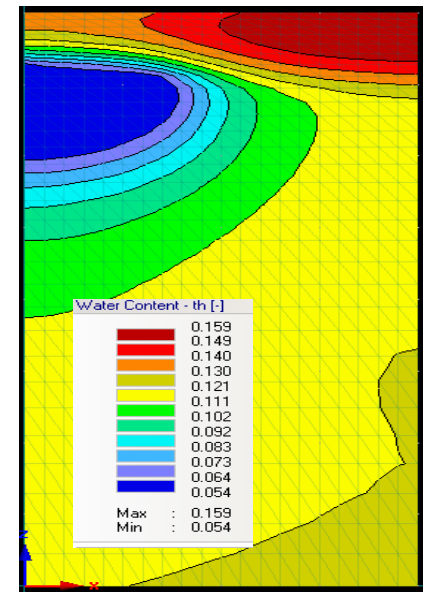
Millimeter-scale transport experiment



Hydraulic conductivity of a rock slab



Sampling Chloride as a proxy for root-driven horizontal flow



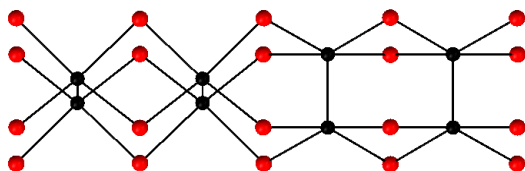
2D simulation of root-driven transport

- ❑ Challenging existing conceptual models for unsaturated and two-phase flow
- ❑ Design and execution of critical laboratory/field/numerical experiments

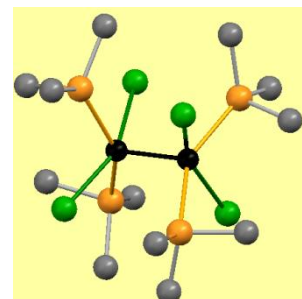
→ Synthetic and coordination chemistry

Technetium binary and ternary halide compounds

Compounds with multiple metal-metal bonds



TcCl_2 : a unique structure-type



$\text{Tc}_2\text{Cl}_4(\text{PMe}_3)_4$

→ Chemistry relevant to remediation and fuel cycle applications

Separation, vitrification, and waste forms (alloys)



Demonstration of the separation of
uranium from technetium for fuel cycle application

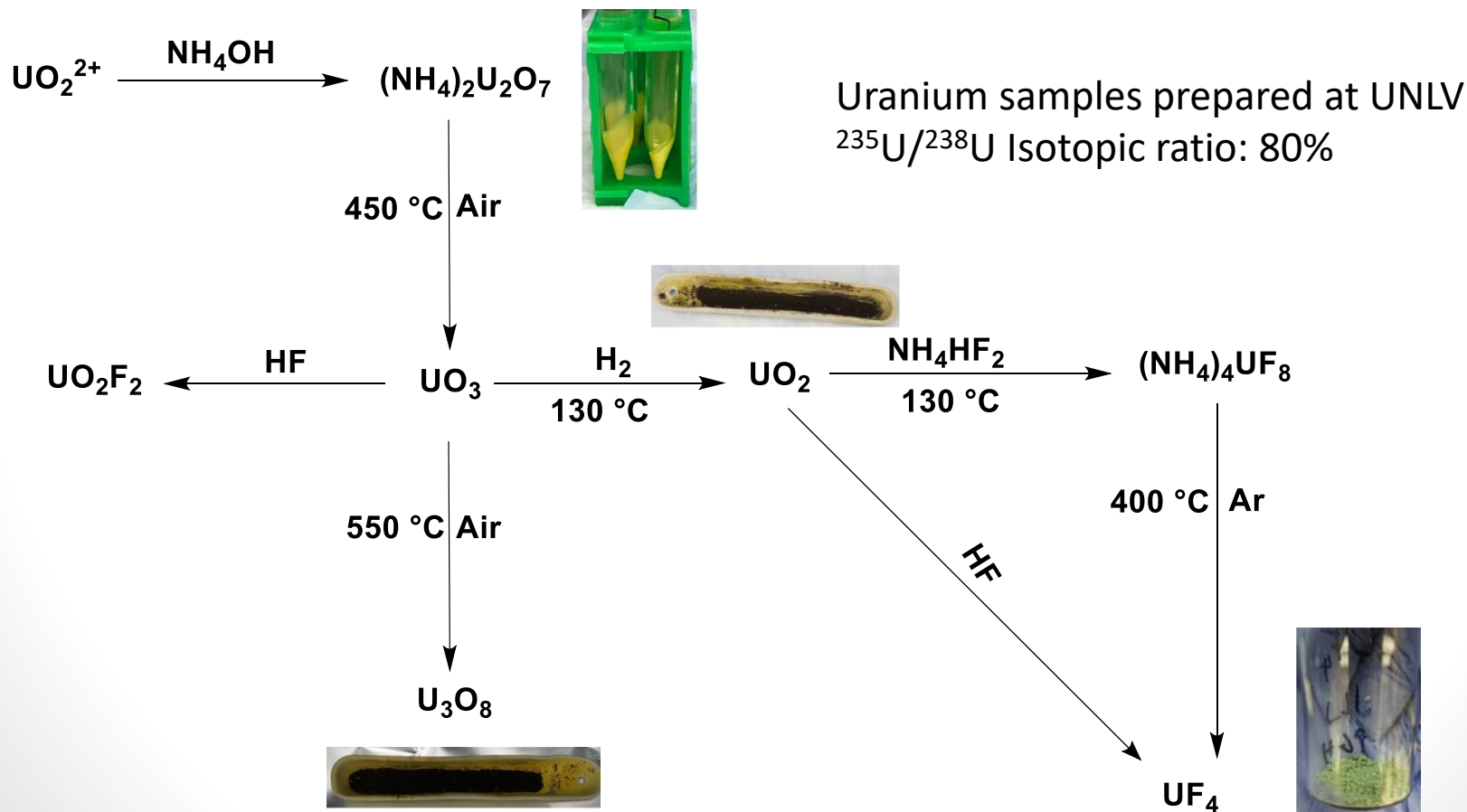


Preparation of U-Tc alloys by arc melting

→ Collaborative work relevant to nuclear forensics

Analysis of Uranium Isotopic Ratios by Thermal Ionization Mass Spectrometry (TIMS)

- Uranium compounds found throughout the fuel cycle (UO_2 , U_3O_8 , UF_4) prepared at UNLV
- $^{235}\text{U}/^{238}\text{U}$ isotopic ratio measurements using TIMS at LANL



Climate Change; Renewable Energy; Astronomy

Dr. George Rhee

Department of Physics and Astronomy

Phone: (702) 895-4453

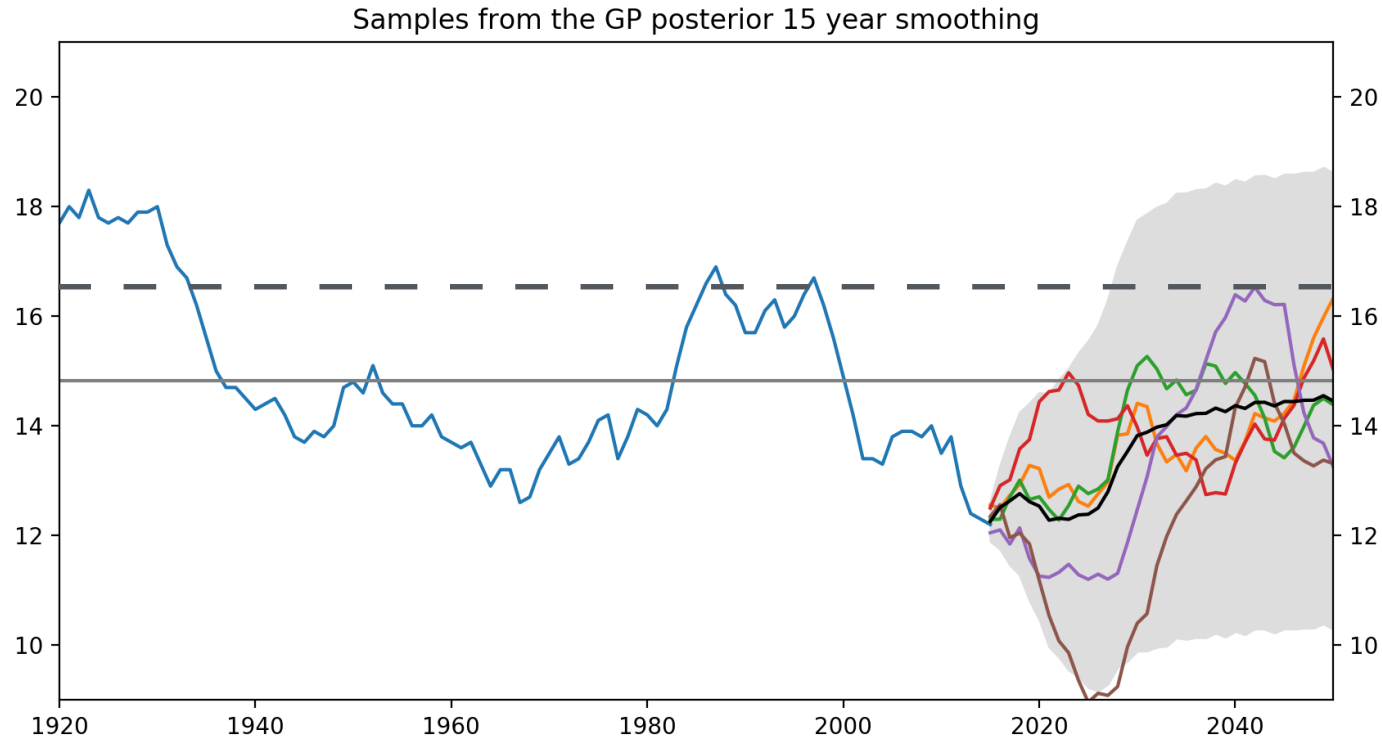
email: grhee@physics.unlv.edu

Expertise

- Observational Astronomy/Cosmology
- Renewable Energy
- Colorado River Flow Projections

Climate Change

River flow projections using statistics from tree ring data from the upper Colorado River Basin. Gaussian processes with known covariance can be used to predict properties of river flows. Figure shows predictions for Colorado river flow 2015-2050.



Renewable Energy

Created an online calculator allowing the user to choose supply and demand options to make plans to zero out emissions in Nevada by 2050.

<http://nv2050.physics.unlv.edu/>. I

Interview on KPNR and writeup describing the idea:

<https://knpr.org/desert-companion/2018-12/do-math>

Supply Choices

Nuclear Energy	<input type="text" value="no nuclear energy ever"/>	⬇
Wind energy	<input type="text" value="add two new wind farms by 2050"/>	⬇
Hydroelectric power	<input type="text" value="Lake Mead dries up by 2030 and generation stops"/>	⬇
Geothermal Energy	<input type="text" value="increase generation by 3% per year"/>	⬇
Rooftop Solar power	<input type="text" value="keep rooftop solar at its 2015 value"/>	⬇
Solar PV power plants	<input type="text" value="solar PV increases by 10 percent a year to 2050"/>	⬇
Concentrating Solar Power	<input type="text" value="build one new Tonopah plant every ten years"/>	⬇
Solar Thermal (hot water)	<input type="text" value="increase to 10% of demand by 2050"/>	⬇
Electricity imports	<input type="text" value="keep electricity imports at 0.15 GW"/>	⬇
Carbon Capture and Storage	<input type="text" value="no CCS, business as usual"/>	⬇

Demand Choices

International aviation	<input type="text" value="factor of three increase in international visitors by 2050"/>	⬇
Nevada transport	<input type="text" value="electrify transport completely by 2050"/>	⬇
Nevada freight	<input type="text" value="business as usual freight travels by road"/>	⬇
Industry growth	<input type="text" value="energy demand increases by 1.5% per year"/>	⬇
Commercial heating and cooling	<input type="text" value="5% increase in efficiency"/>	⬇
Commercial light and appliances	<input type="text" value="energy demand increases by 25% by 2050"/>	⬇
Home heating and cooling	<input type="text" value="energy demand increases by 1.5% per year"/>	⬇
Home lighting and appliances	<input type="text" value="electricity demand increases by 70% from 2015 to 2050"/>	⬇
Home insulation	<input type="text" value="no extra effort on home insulation"/>	⬇
Average home temperature	<input type="text" value="no thermostat adjustment"/>	⬇

Astrophysics

Interested in:

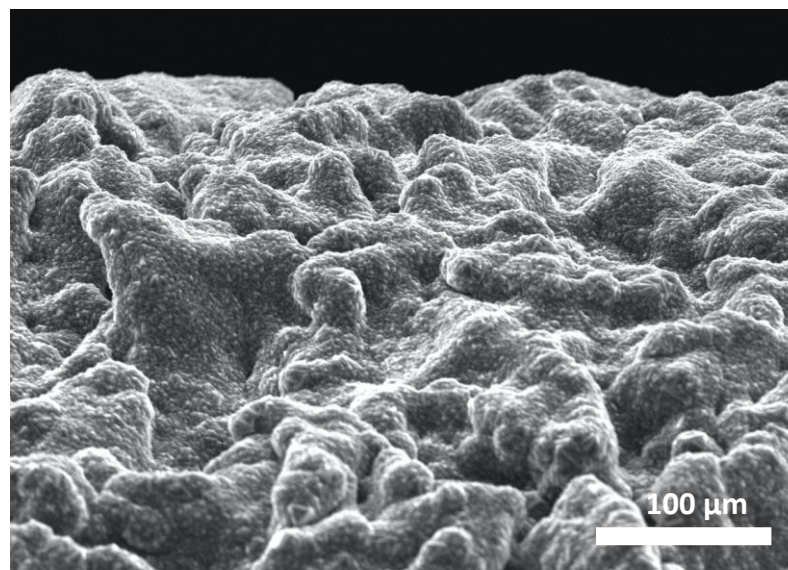
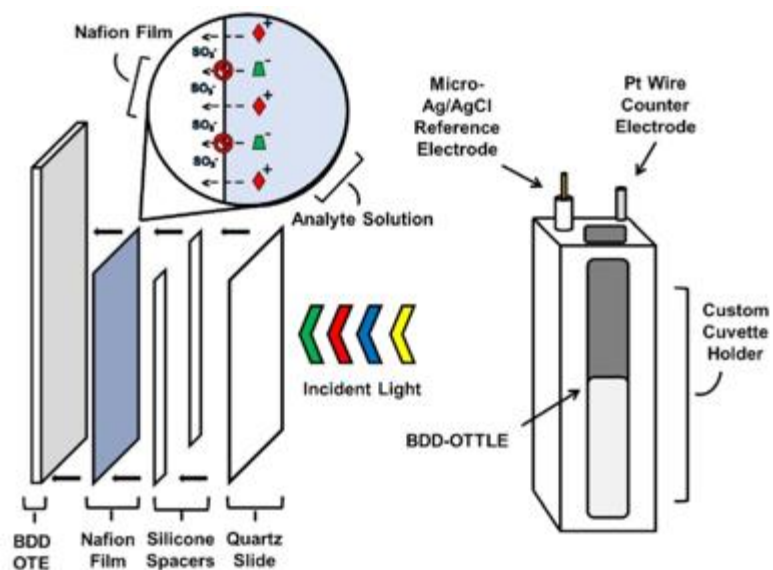
Dark matter distribution in galaxies inferred from the rotation of neutral hydrogen gas in disks

Properties of galaxies in extreme low density environments (voids)

Measuring the masses of black holes using the variability of the central region in Seyfert galaxies and quasars.
spectral and brightness measurements

Electrochemistry and Spectroelectrochemistry in molten salts for the development of the molten salt nuclear reactor

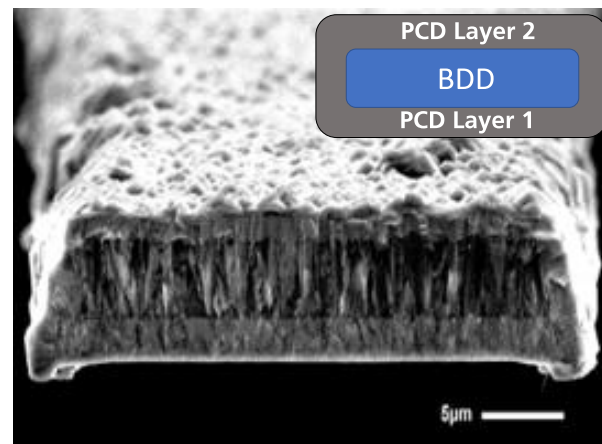
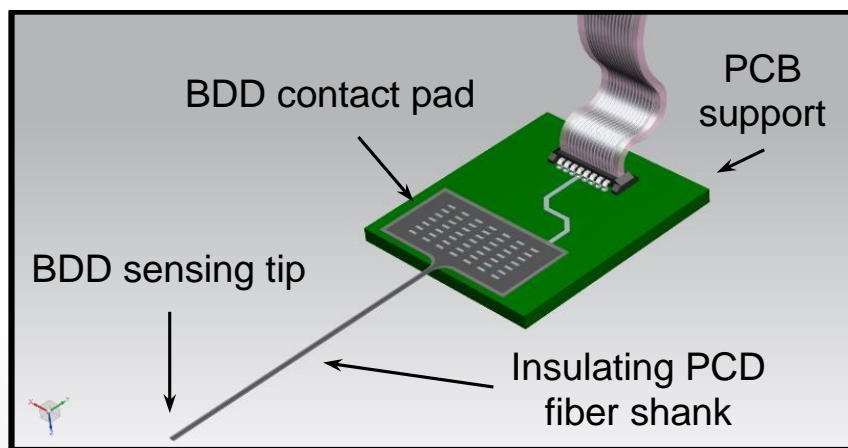
- Fundamental redox and thermodynamic properties of nuclear fuel can be gained using electrochemistry and spectroelectrochemistry.
- Diamond electrodes are specifically amenable to use as the sensing material due to its robustness and tunable properties



SEM image of diamond film

Detection of clinically- and environmentally-relevant analytes with electrochemical sensors

- The all-diamond microfiber electrodes are a supremely biocompatible electrode. With the advantageous properties of diamond electrodes, the suite of potential analytes is expanded.
- The conductive BDD core is covered along the shank with undoped diamond, thereby making the device non-reactive.
- The batch-fabricated nature of these devices make them attractive compared to others.



Publication track record

“Polymer-coated Boron Doped Diamond Optically Transparent Electrodes for Spectroelectrochemistry” C.A Rusinek, M. Becker, R. Rechenberg, D. Zhao, K. Ojo, N. Kaval, and W.R. Heineman. *Electroanalysis*, 2016, 28, 2228-2236.

“Fabrication and characterization of boron doped diamond microelectrode arrays of varied geometry” C.A Rusinek, M. F. Becker, R. Rechenberg, T. Schuelke, *Electrochemistry Communications*, 2016, 73, 10-14

“Large-scale, All Polycrystalline Diamond Structures Transferred on Flexible Parylene-C Films for Neurotransmitter Sensing” B. Fan, Y. Zhu, R. Rechenberg, C.A Rusinek, M.F. Becker, W. Li, *Lab-on-a-Chip*, 2017, 17, 3159-3167.

“Isatin Detection using an All Boron-doped Diamond 3-in-1 Sensing Platform” M. Ensich, V.Y. Maldonado, G. M. Swain, R. Rechenberg, M.F. Becker, T. Schuelke, C.A Rusinek, *Analytical Chemistry*, 2018, 90, 1951-1958.

“Analysis of Ag(I) Biocide in Water Samples using Anodic Stripping Voltammetry with a Boron-doped Diamond Disk Electrode” V.Y. Maldonado, P.J. Espinoza, C.A Rusinek, G.M. Swain, *Analytical Chemistry*, 2018, 90 (11), 6477–6485.

“All Diamond Microfiber Electrodes for Neuroelectrochemistry” C.A Rusinek, Y. Guo, R. Rechenberg, E. Purcell, C. McKinney, M.F Becker, W. Li, *Journal of the Electrochemical Society*, 2018, 165 (12), G3087-G3092.

“Indium Tin Oxide Film Characteristics for Cathodic Stripping Voltammetry” M. Ensich, B. Wehring, G.D Landis, M.F Becker, T. Schuelke, C.A Rusinek, *ACS Applied Materials and Interfaces*, 2019, 11 (18), 16991-17000.

“Determination of Lead with a Copper-Based Electrochemical Sensor” W. Kang, X. Pei, C.A Rusinek, A Bange, E.N Haynes, W.R Heineman, I. Papautsky. *Analytical Chemistry*, 2017, 89, 3345-3352.

Google Scholar:

<https://scholar.google.com/citations?user=uZyA2VUAAAAJ&hl=en&authuser=1>

Advanced Numerical Methods for Moving Domain/Interface Multi-Physics Problems

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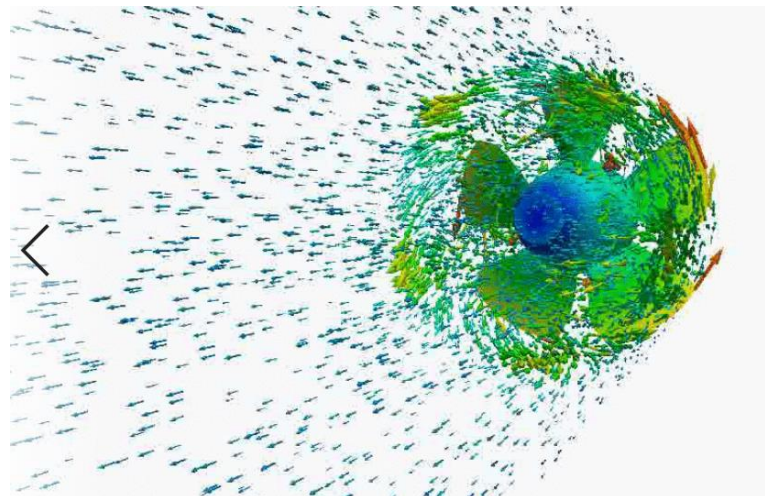
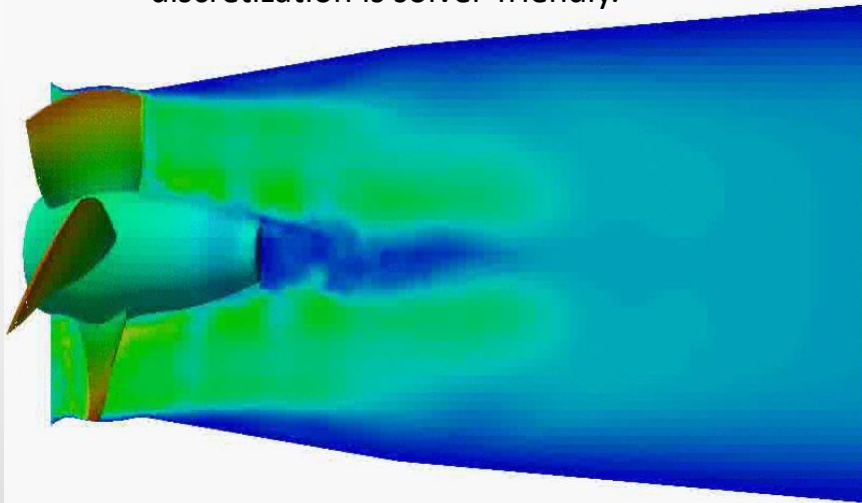
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Expertise

- Numerical Solutions of Partial Differential Equations (PDE)
- Numerical Analysis (Well-posedness, Stability, Convergence)
- Finite Element/Volume/Difference Methods
- Scientific and Engineering Computing
- Fluid-Structure Interaction (FSI) Modeling and Simulation
- Fuel Cell Dynamics, Fluid Dynamics, Electrohydrodynamics

Fluid-Hydro Turbine Interaction Problems

- Hydroelectric power generating system produces renewable energy and remains crucial for society and industry. The most significant part of this system is the hydro turbine interacting with the water flow, which involves elastic solid materials and viscous fluids and belongs to the category of fluid-structure interaction (FSI). The developments of mathematical models and numerical methodologies are critical in practice for efficient simulations of the hydro turbine, which in turn guides the design and evaluation.
- We approach the challenges in different aspects. First, based on the observation that the hydro turbine, although exhibiting large rotations, has relatively small deformation, we develop linearized elasticity equations that alleviate the burden on nonlinear solver and improves the well-posedness of spatial discretization. Second, we propose a new approach to solve the arbitrary Lagrangian-Eulerian mesh motion for rotating structure. Moreover, we analyzed the well-posedness and convergence of the finite element discretization and demonstrated the discretization is solver-friendly.



Hemodynamic Fluid-Structure Interaction (FSI) Problems

- FSI simulation has become the most promising solution method to solve the hemodynamic problem existing in the clinical cardiovascular system. However, the complexity of cardiovascular environment, the artificial heart pump model, the vascular rupture, the aneurysm progression and the aortic dissection cause the deficiency of the existing FSI simulation package towards the clinical demands.
- We devoted our research to the new modeling and numerical techniques for the bloodstream-vascular-stent graft/artificial heart pump interaction problems, aiming at overcoming numerical difficulties and challenges, and developed advanced numerical methodologies to improve the efficiency and accuracy of corresponding FSI simulations. and to deliver more instructive numerical results to medical professionals for helping out patients on an efficient and accurate diagnosis and treatment.

