Natural Resources, Climate, and Clean Energy

Energy Resources & Infrastructure Research
Electronic and Magnetic Properties at High Pressure

Dr. Andrew Cornelius
Department of Physics & Astronomy
Phone (702) 895-1727

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**
- 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

![Periodic table with localized to delocalized electron transition](image)

**Increasing Localization**

- **f-electron delocalization**
- **X-ray absorption**
- **Heavy fermions**
- **Heat Capacity**
- **Fluctuating valence**
- **X-ray fluorescence**

![Graphs and data points](image)
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

Photoemission
X-ray Emission

In-situ cell

From beamline
To XES/XAS spectrometer
From solar simulator

UHV chamber
External reservoir

Photoelectron Spectroscopy (PES, XPS, UPS)
Inverse Photoemission (IPES)
Auger Electron Spectroscopy (AES)
UV-Visible Absorption Spectroscopy (UV-Vis)
X-Ray Emission Spectroscopy (XES)
X-ray Absorption Spectroscopy (XAS)

Conduction band
Valence band
Core level
Materials for Energy Conversion

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
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<tbody>
<tr>
<td>ZnO</td>
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<tr>
<td>CdS (20 nm)</td>
<td></td>
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<tr>
<td>Cu(In,Ga)(S,Se)$_2$ (2μm)</td>
<td></td>
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<tr>
<td>Mo (2μm)</td>
<td></td>
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<tr>
<td>Na-lime glass (2 mm)</td>
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</tbody>
</table>

η = 23.35%
Areas of Research

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

http://islandlab.faculty.unlv.edu/
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.


http://islandlab.faculty.unlv.edu/
Island – Quantum computing, quantum sensing

Journal publications

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

Enhanced superconductivity in atomically thin TaS2

Proximity-induced Shiba states in a molecular junction

TiS3 transistors with tailored morphology and electrical properties

Environmental instability of few-layer black phosphorus

Ultrahigh photoresponse of few-layer TiS3 nanoribbon transistors

Gate controlled photocurrent generation mechanisms in high-gain In2Se3 phototransistors

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

http://islandlab.faculty.unlv.edu/
Economic Geology

Dr. Simon Jowitt
Department of Geoscience
simon.jowitt@unlv.edu

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 companionality; understanding how critical metal production is reliant on other metals

Be-bearing rare metal pegmatite, southern Nevada

Production and recycling of Nd

<table>
<thead>
<tr>
<th>Metal</th>
<th>75-100% By-product</th>
<th>50-75% By-product</th>
<th>25-50% By-product</th>
<th>0-25% By-product</th>
<th>Unquantified</th>
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Environmental impact of mining

- Assessing environmental impacts
- Potential of wealth from waste; assessing mining waste metal production and CO$_2$ sequestration potential

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

Understanding arsenic mobility in mining and mineral processing environments
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

Dong-Chan Lee, Ph.D.
Associate Professor
Department of Chemistry & Biochemistry
Phone: 702-895-1486
Email: dong-chan.lee@unlv.edu

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

$E_{\text{LUMO}}$  
-3.16 eV  
-3.26 eV  
-3.22 eV

$E_{\text{HOMO}}$  
-5.43 eV  
-5.45 eV  
-5.49 eV  
-5.32 eV  
-5.51 eV  
-5.40 eV
Solvent-Dependent Morphology Control through Organogelation

Solid-State Emission with High Quantum Yield

Gel-Induced Room Temperature Phosphorescence
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

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

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

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

Water (blue) pooled above a fracture intersection

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

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

Sampling Chloride as a proxy for root-driven horizontal flow

Millimeter-scale transport experiment

Seepage through gravel-sized capillary barrier materials

Hydraulic conductivity of a rock slab

2D simulation of root-driven transport
**Synthetic and coordination chemistry**
Technetium binary and ternary halide compounds
Compounds with multiple metal-metal bonds

**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$_3$O$_8$, UF$_4$) prepared at UNLV
- $^{235}$U/$^{238}$U isotopic ratio measurements using TIMS at LANL

Uranium samples prepared at UNLV
$^{235}$U/$^{238}$U Isotopic ratio: 80%
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
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/

Interview on KPNR and writeup describing the idea:

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.
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


Google Scholar: https://scholar.google.com/citations?user=uZyA2VUAAAAJ&hl=en&authuser=1
Advanced Numerical Methods for Moving Domain/Interface Multi-Physics Problems

Dr. Pengtao Sun
Professor
Department of Mathematical Sciences
Email: pengtao.sun@unlv.edu; URL: https://faculty.unlv.edu/sun/

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.