Energy Resources & Infrastructure Research
Interfacial Photochemistry

• Dr. Jared P. Bruce
  • Assistant Professor
  • Department of Chemistry and Biochemistry
  • Email: jared.bruce@unlv.edu
  • Website: jpbruce.faculty.unlv.edu

Expertise

• Heterogeneous Photochemistry
• Electrocatalysis
• Photocatalysis
• Atmospheric Chemistry
• Surface Chemistry and Interfacial Characterization
• Near Ambient Pressure Photoelectron Spectroscopy
Hybrid Co-Catalyst/Photoabsorber Photochemical Interfaces

- Metals often make good electrocatalysts
- Semiconductors make good photoabsorbers
- The combination of the two create a new, complex interface that can be leveraged to increase the efficiency of co-catalyst/photoabsorber devices

Mixing Liquid Jet Photoelectron Spectroscopy

- Dynamic processes are tricky to study at the liquid surface
- A small liquid jet (20µm dia.) is used to investigate the liquid surface
- Microfluidic chips provide mixing chamber to induce chemical reactions
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

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

Increased Localization

f-electron delocalization
X-ray absorption

Heavy fermions
Heat Capacity

Fluctuating valence
X-ray fluorescence

$\gamma = 800 \text{ mJ/mol K}^2$
Cornelius PRB 1999

$\gamma = 210 \text{ mJ/mol K}^2$
Cornelius PRB 1997

$\gamma = 82 \text{ mJ/mol K}^2$
Lashley PRB 2005

Cu$\gamma = 0.7 \text{ mJ/mol K}^2$
*TPRC Data Series Vol. 4
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

Pump
From beamline
To XES/XAS spectrometer
From solar simulator
Window
UHV chamber
External reservoir

Gloveboxes
High dyn. range
XPS, UPS, IPES, Auger
Sample preparation
and distribution
Scanning Probe Microscope

Photoelectron Spectroscopy
(PES, XPS, UPS)

UV-Visible
Absorption Spectroscopy
(UV-Vis)

X-Ray Emission
Spectroscopy (XES)

Conduction band
Valence band
Core level

Auger Electron Spectroscopy
(AES)

Inverse Photoemission (IPES)
### Materials for Energy Conversion

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

\[ \eta = 23.35\% \]
Island – Quantum computing, quantum sensing

The Nanoscale Physics Group @ UNLV

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's Lab website
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's Lab website
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**

**T1S3 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**

Island's Lab website
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

<table>
<thead>
<tr>
<th>$E_{\text{LUMO}}$</th>
<th>-3.16 eV</th>
<th>-3.26 eV</th>
<th>-3.22 eV</th>
</tr>
</thead>
</table>

| $E_{\text{HOMO}}$ | -5.43 eV | -5.45 eV | -5.49 eV | -5.32 eV | -5.51 eV | -5.40 eV |

![Chemical structures and color images](images)
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

- 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).

- 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
- Sampling Chloride as a proxy for root-driven horizontal flow
- Seepage through gravel-sized capillary barrier materials
- Hydraulic conductivity of a rock slab
- 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
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.

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
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:

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.