Physical Chemistry Research



Interfacial Photochemistry

• Dr. Jared P. Bruce

- Assistant Professor
- Department of Chemistry and Biochemistry
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Expertise

- Heterogeneous Photochemistry
- Electrocatalysis
- Photocatalysis
- Atmospheric Chemistry
- Surface Chemistry and Interfacial Characterization
- Near Ambient Pressure Photoelectron Spectroscopy



Hybrid Co-Catalyst/Photoabsorber Photochemical Interfaces

Mixing Liquid Jet Photoelectron Spectroscopy



- 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



- 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



Theoretical chemical physics

- Dr. Chern Chuang,
- Assistant Professor, Department of Chemistry and Biochemistry
- Email: <u>chern.chuang@unlv.edu</u>
- Website: <u>http://cchuang.faculty.unlv.edu/Home.html</u>
- Expertise
 - Open quantum system dynamics and spectroscopy
 - Photophysics and photochemistry of materials
 - Quantum transport
 - Quantum effects in biology
 - Exotic geometries and topologies of low dimensional materials

Theoretical chemical physics







Exotic low-dimensional materials

Photophysics of organic materials

Photochemistry under environmental control

Electrochemistry for Energy Storage, Environmental Remediation, and Biomedical Applications

Dr. Zhange Feng

- Assistant Professor
- Department of Chemistry & Biochemistry
- Email: zhange.feng@unlv.edu
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Expertise

- Water and soil remediation
- Rechargeable batteries
- Electrocatalysis
- Electrosynthesis
- Electrochemical Manufacturing
- Electrical neural stimulation

A combination of electrochemistry, *in situ* spectroscopy, and theoretical calculations to study electrified interfaces







Stephen Lepp

- Professor of Astrophysics, Department of Physics and Astronomy
- Ph.D., Physics, University of Colorado, Boulder
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Areas of Expertise

- Astrochemistry
- Interstellar Medium
- SN1987A
- Formation of first objects in the Early Universe
- Thermal Phases in Astrophysics
- X-ray chemistry

Research Summary:

I work primarily at the intersection of Atomic and Molecular Physics with Astrophysics. Making models of astronomical environments to further our understanding of them. I have modeled: interstellar clouds, star forming regions, active galactic nuclei, SN1987A, and the Early Universe.



Quantum Information and Quantum Control of Chemical Reactions

Balakrishnan Naduvalath Department of Chemistry & Biochemistry, UNLV

Areas of Expertise

- Ultracold Molecules
- Ultracold Quantum Engineered Chemistry
- Quantum control of chemical reactions
- Geometric phase effect in chemistry
- Stereodynamic control of chemical reactions

\$\$\$: NSF, DOD, NASA

Chemical reaction pathway in ultracold K+KRb collisions. Quantum engineered KRb molecules have been prepared at 300 nK. Ultracold polar molecules such as KRb are potential candidates for quantum computing and quantum information processing.

10

 $R_{KK}(a_0)$

14



KRb + K

R_{KPh} (a₀)

Controlling reaction outcome through quantum interference



Right panel: The nature of the interference can be controlled by including "geometric phase". In the image on the right, inclusion of the geometric phase enhances the reactivity. The geometric phase (that correctly describes the sign of the wave function near a conical intersection with an excited electronic state) acts as a "quantum switch" (Hazra, Balakrishnan, and Kendrick, J. Phys. A **119**, 12291 (2015) Left panel: Two paths for a chemical reaction. These two paths can interfere constructively or destructively, maximizing or minimizing the reaction rate. This quantum effect becomes magnified in the ultracold regime (Kendrick, Hazra, and Balakrishnan, Nature Comm. **6**, 7918 (2015).



References

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- N. Balakrishnan, Perspective: Ultracold molecules and the dawn of cold controlled chemistry, J. Chem. Phys. **145**, 150901 (2016).
- B. K. Kendrick, J. Hazra, and N. Balakrishnan, The Geometric Phase Appears in the Ultracold Hydrogen Exchange Reaction, Phys. Rev. Lett. **115**, 153201 (2015).
- B. K. Kendrick, J. Hazra, and N. Balakrishnan, The Geometric Phase Controls Ultracold Chemistry, Nature Communications **6**, 7918 (2015).

Technetium and Uranium Chemistry

→ Synthetic and coordination chemistry Technetium binary and ternary halide compounds Compounds with multiple metal-metal bonds



TcCl₂: a unique structure-type

Frederic Poineau, PhD Radiochemistry



→ 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

Technetium and Uranium Chemistry

Frederic Poineau, PhD Radiochemistry

\rightarrow Collaborative work relevant to nuclear forensics

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

- Uranium compounds found throughout the fuel cycle (UO₂, U₃O₈, UF₄) prepared at UNLV
- ²³⁵U/²³⁸U isotopic ratio measurements using TIMS at LANL

