

# Advanced Materials: Development & Analysis Research

# *Theoretical and Computational* Condensed Matter and Materials Physics

## **Dr. Changfeng Chen**

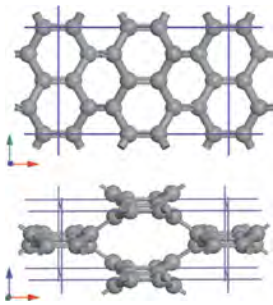
Department of Physics and Astronomy

Phone: 702-895-4230

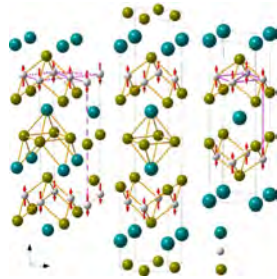
Email: [chen@physics.unlv.edu](mailto:chen@physics.unlv.edu)

## **Expertise**

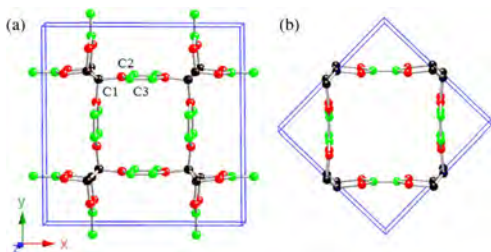
- Novel states of matter: topological insulators and semimetals
- Superior bonding structures: superhard and supertough materials
- Intriguing quantum phenomena: superconductivity and magnetism
- Extreme mechanics: stress responses to complex large strains
- Ultimate thermodynamics: materials inside Earth and other planets



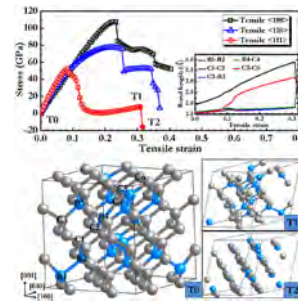
Nodal-ring Dirac semimetal states identified in bco-C<sub>16</sub> crystal [Wang, Weng, Nie, Fang, Kawazoe, Chen, *Phys. Rev. Lett.* 116, 195501 (2016)].



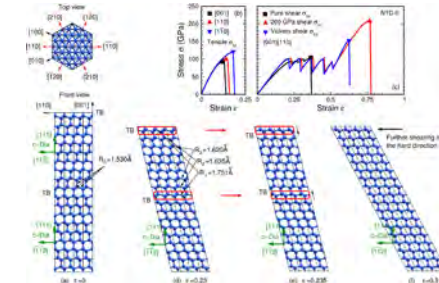
Magnetic Dirac materials CaMnBi<sub>2</sub> and SrMnBi<sub>2</sub> [Zhang, et al., *Nature Commun.* 7, 13833 (2016)].



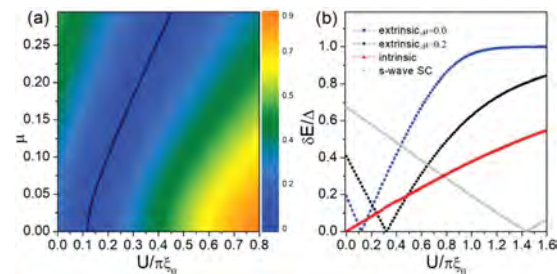
Nodal-net Dirac semimetal states in a graphene network structure [Wang, Nie, Weng, Kawazoe, Chen, *Phys. Rev. Lett.* 120, 026402 (2018)].



Superhard B<sub>3</sub>C in diamond structure [Zhang, et al., *Phys. Rev. Lett.* 114, 015502 (2015)].



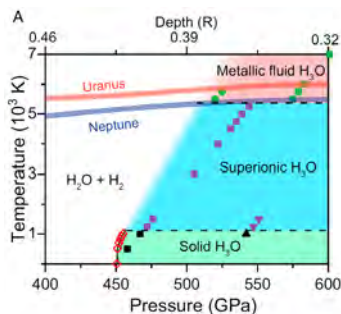
Extreme mechanics of nanotwinned diamond [Li, Sun, Chen, *Phys. Rev. Lett.* 117, 116103 (2016)].



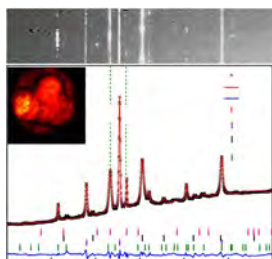
Kondo physics in 2D topological superconductors [Wang, et al., *Phys. Rev. Lett.* 122, 087001 (2019)].



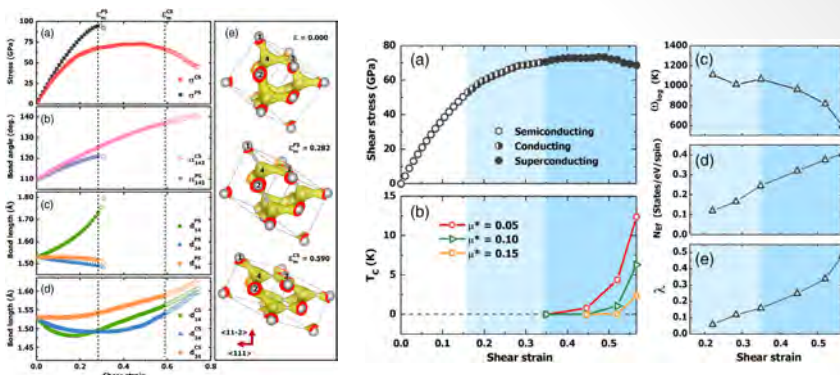
Helium-bearing compound  $\text{FeO}_2\text{He}$  predicted to stabilize at deep-Earth conditions [Zhang, et al., *Phys. Rev. Lett.* **121**, 255703 (2018)].



Prediction of novel  $\text{H}_3\text{O}$  and implications for the magnetic fields of Uranus and Neptune [Huang, et al., *Proc. Natl. Acad. Sci.* **117**, 5638 (2020)].



Pressure-stabilized divalent ozonide  $\text{CaO}_3$  and its impact on Earth's oxygen cycles [Wang, et al., *Nature Commun.* **11**, 4702 (2020)].



Metallization and superconductivity in diamond [Liu, et al., *Phys. Rev. Lett.* **123**, 195504 (2019); *Phys. Rev. Lett.* **124**, 147001 (2020)].

### Further Reading (selected papers by Chen Group, 2015-2020)

Anomalous Stress Response of Ultrahard  $\text{WB}_n$  Compounds, Li, Zhou, Zheng, Ma, Chen, *Phys. Rev. Lett.* **115**, 185502 (2015).

Ultralow-Frequency Collective Compression Mode and Strong Interlayer Coupling in Multilayer Black Phosphorus, Dong, et al., *Phys. Rev. Lett.* **116**, 087401 (2016).

Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides, Lu, Li, Ma, Chen, *Phys. Rev. Lett.* **119**, 115503 (2017).

Xenon iron oxides predicted as potential Xe hosts in Earth's lower mantle, Peng, Song, Liu, Li, Miao, Chen, Ma, *Nature Commun.* **11**, 5227 (2020).

# Electronic and Magnetic Properties at High Pressure

**Dr. Andrew Cornelius**

Department of Physics & Astronomy

Phone (702) 895-1727

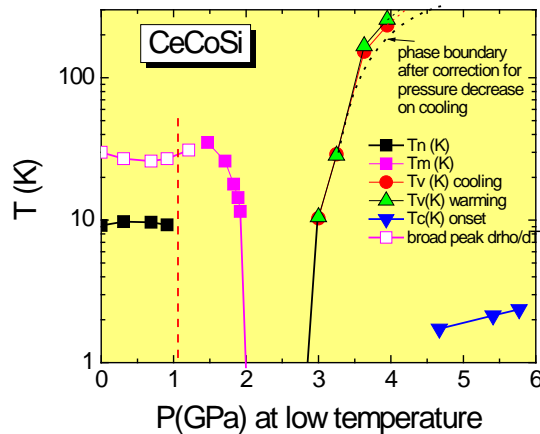
## **Expertise:**

- Experimental high pressure measurements
- Magnetism
- Superconductivity

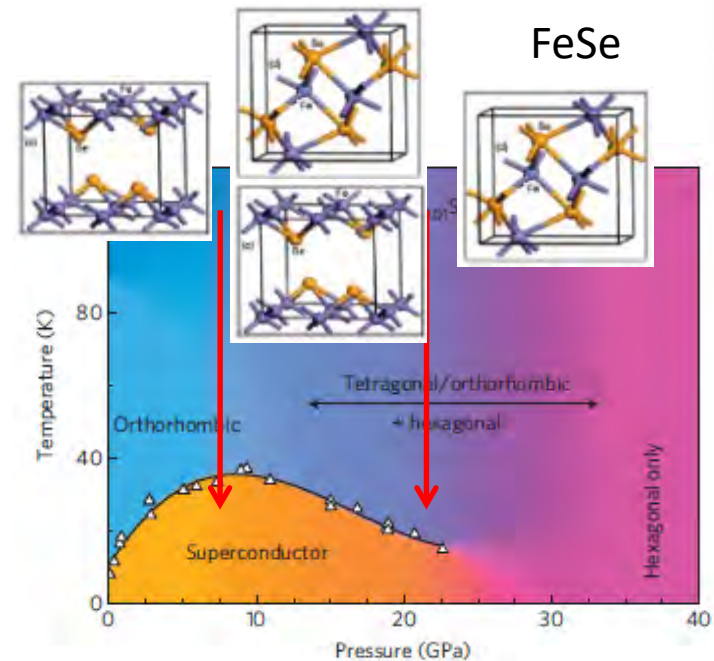
# Superconductivity

## 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





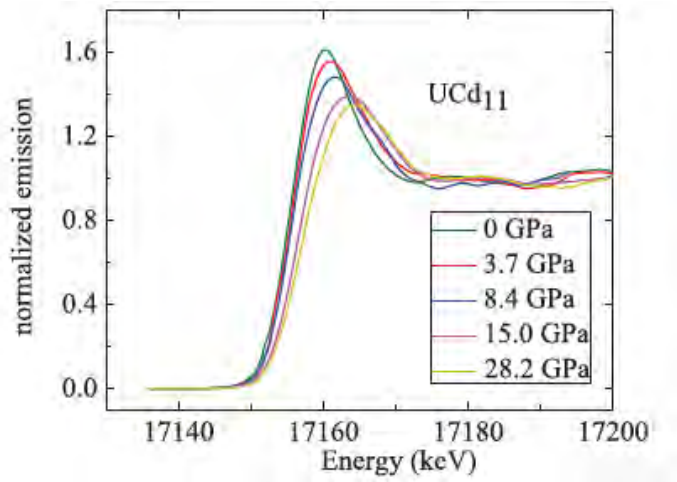
# Correlated-Electron Systems

Modified periodic table

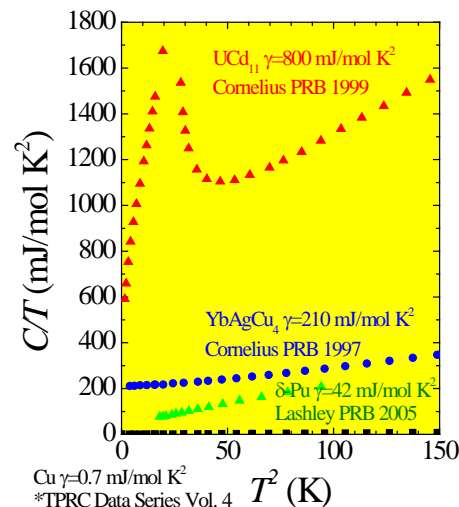
Empty Shell	Partially Filled Shell														Full Shell		
4f	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
5f	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		
3d	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn						
4d	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd						
5d	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg						

↑ Increasing Localization

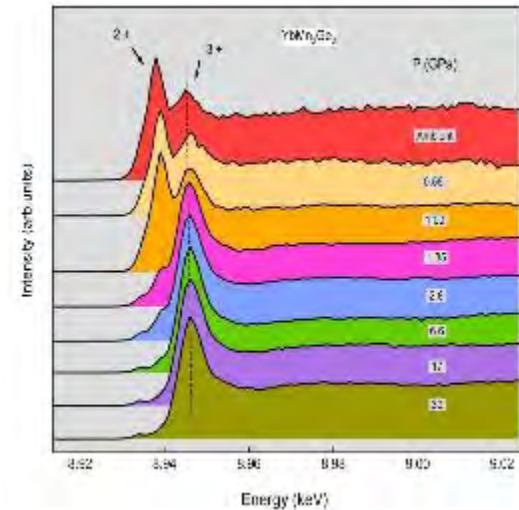
- Going from localized to delocalized electrons one often finds strong electron-electron correlations
- Correlated electron systems can yield interesting behavior: fluctuating valence, superconductivity, non-Fermi liquid, heavy fermion and many more



f-electron delocalization  
X-ray absorption



Heavy fermions  
Heat Capacity



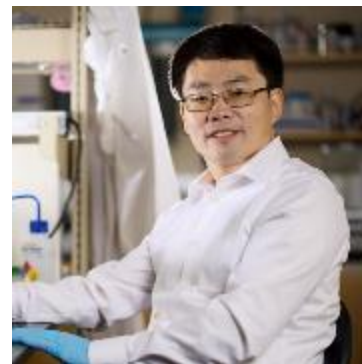
Fluctuating valence  
X-ray fluorescence

# Electrochemistry for Energy Storage, Environmental Remediation, and Biomedical Applications

- **Dr. Zhange Feng**
- Assistant Professor
- Department of Chemistry & Biochemistry
- Email: [zhange.feng@unlv.edu](mailto:zhange.feng@unlv.edu)
- Website: <https://zfeng.faculty.unlv.edu/>

## 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**

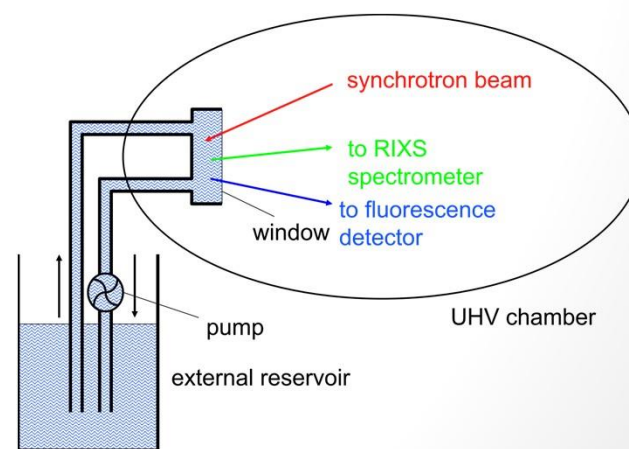
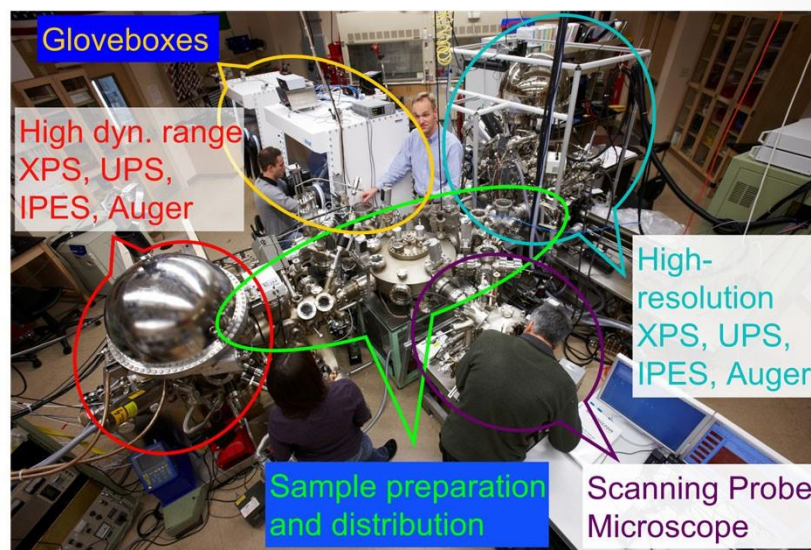


# Surface and Interface Characterization of Materials for Energy Conversion

- **Dr. Clemens Heske**
- Professor
- Department of Chemistry and Biochemistry
- Email: [heske@unlv.nevada.edu](mailto:heske@unlv.nevada.edu)
- Website: <https://heske.faculty.unlv.edu//>

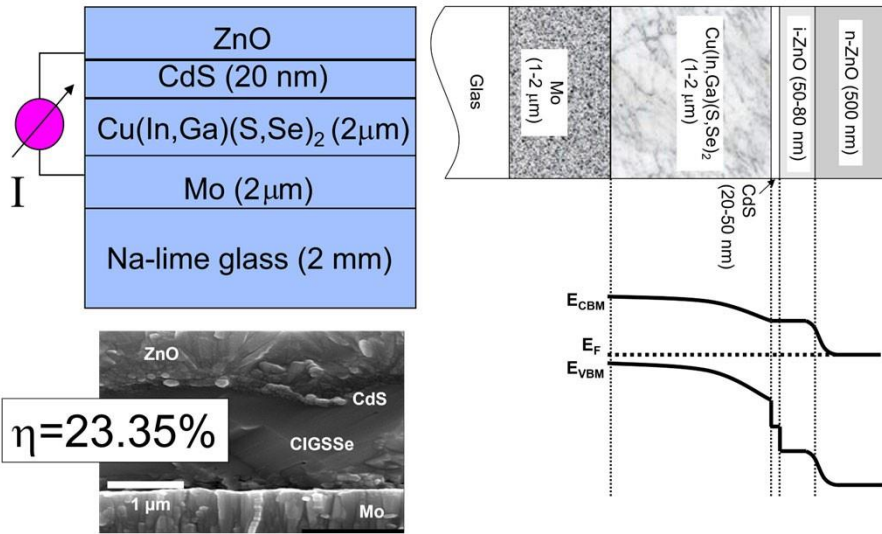
## Expertise

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

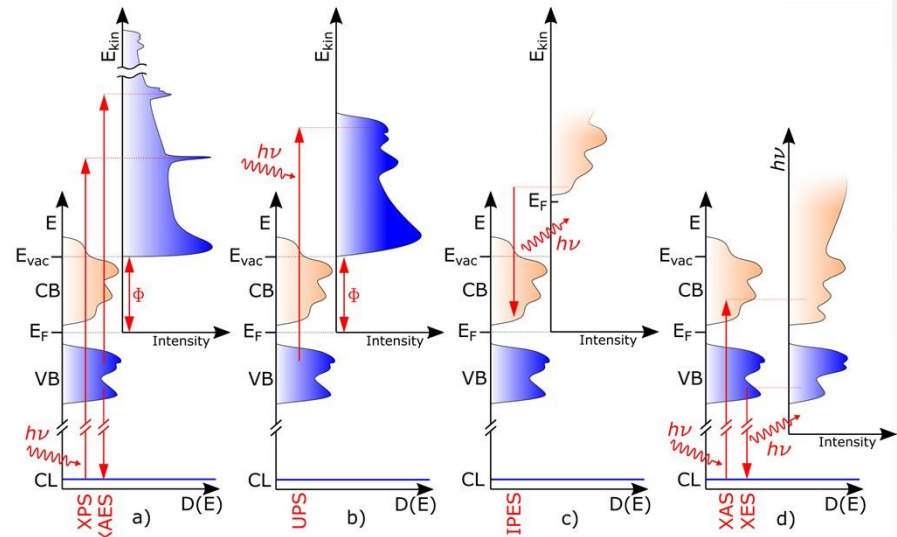


# Surface and Interface Characterization of Materials for Energy Conversion

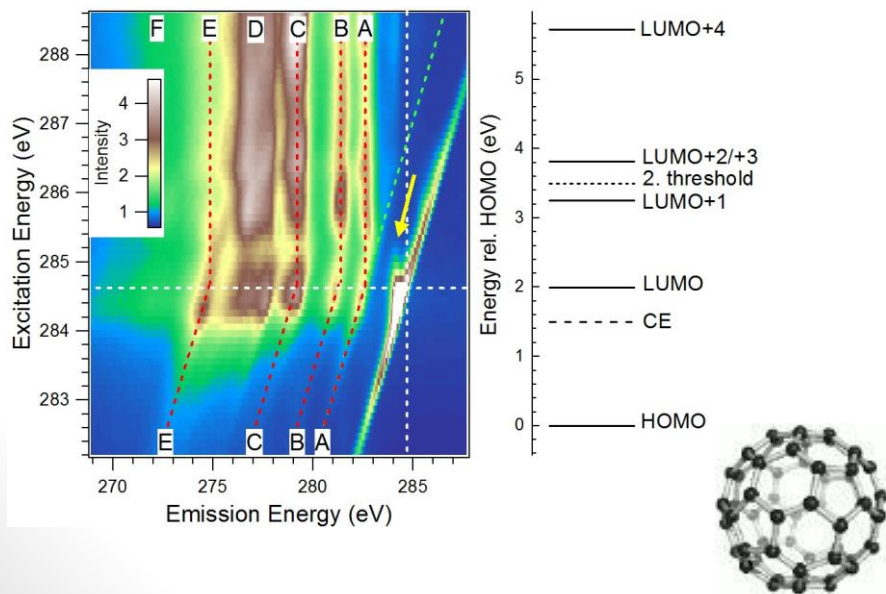
## Cu(In,Ga)(S,Se)<sub>2</sub> Thin-Film PV Device



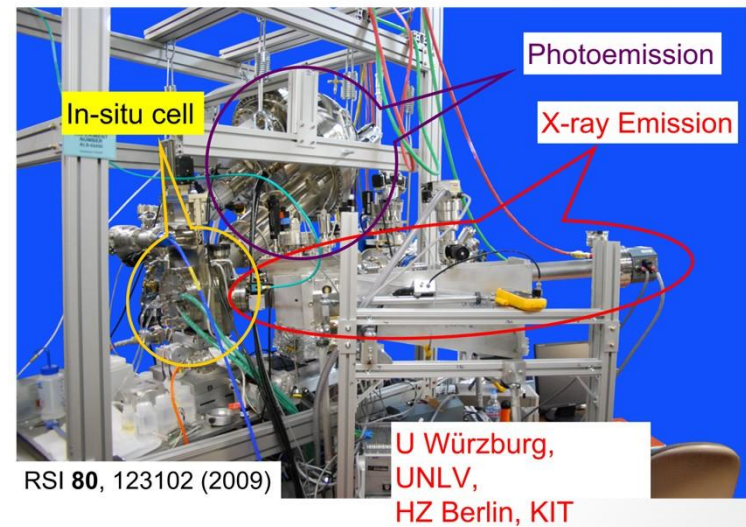
## Method development



## Electronic structure of C<sub>60</sub>



## SALSA: Solid And Liquid Spectroscopic Analysis





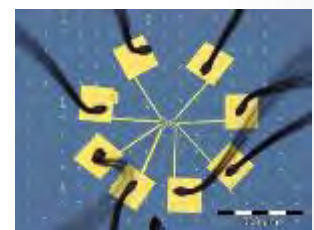
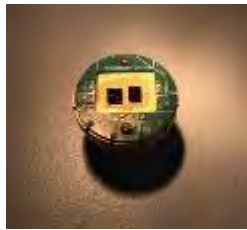
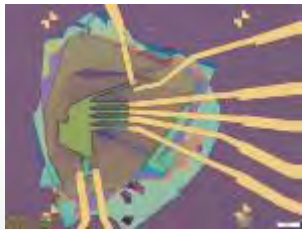
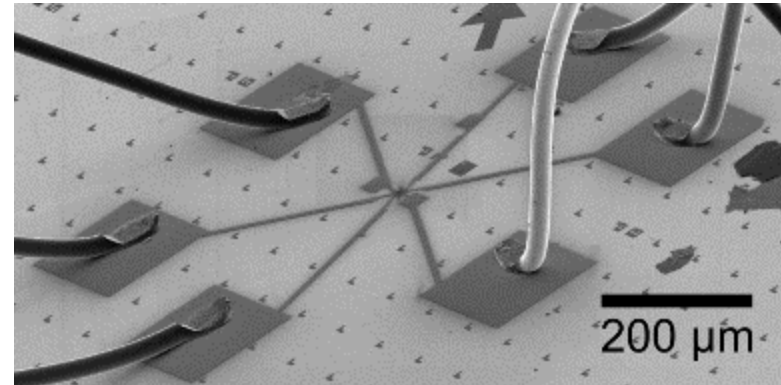
# Island – Quantum computing, quantum sensing



The Nanoscale Physics Group @ **UNLV**

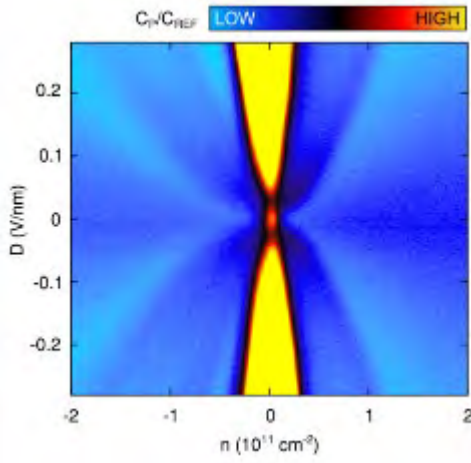
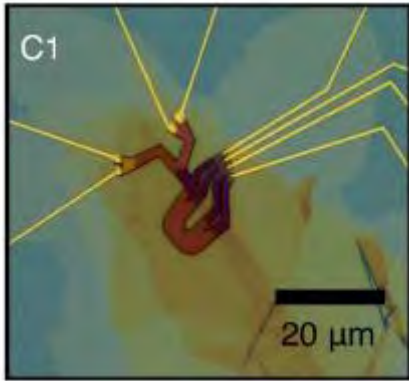
## Areas of Research

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



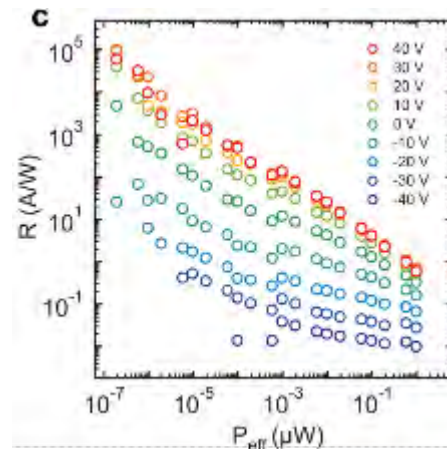
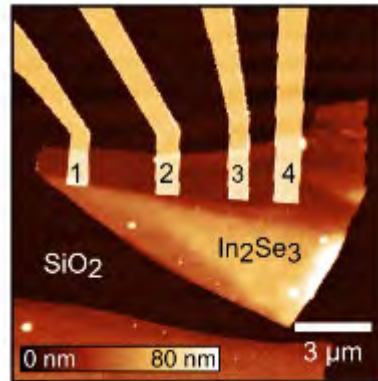
# Island – Quantum computing, quantum sensing

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



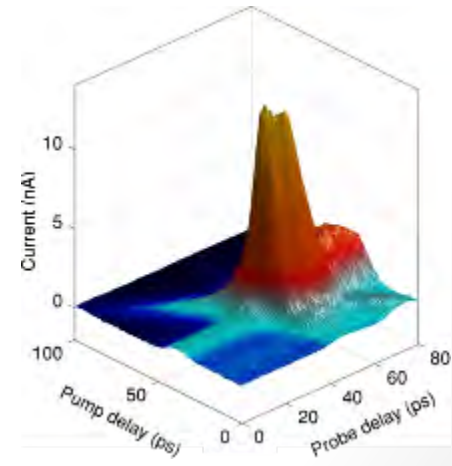
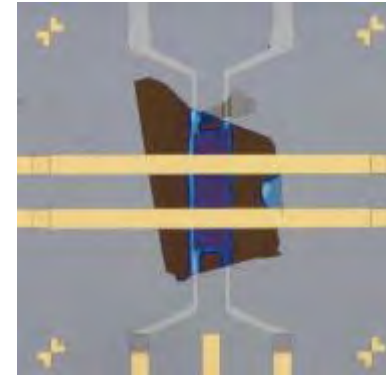
Island, J. O., et al. *Nature* **571** (2019): 85–89.

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



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

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



# 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 TaS<sub>2</sub>**

E. Navano-Moiatalla\*, J.O. Island\*, S. Manas-Valero, E. Pinilla-Cienfuegos, A. Castellanos-Gomez, J. Queieda, G. Rubio-Bollinger, L. Chirulli, J.A. Silva-Guilin, 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)

## **TiS<sub>3</sub> 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 TiS<sub>3</sub> 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)

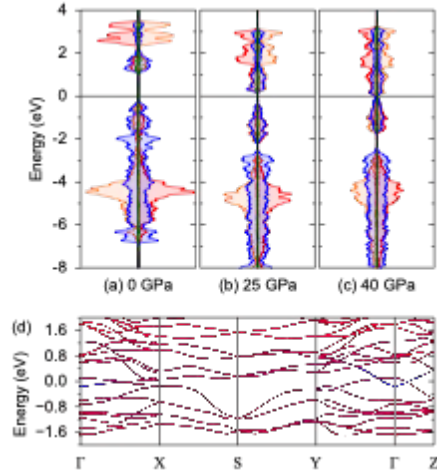
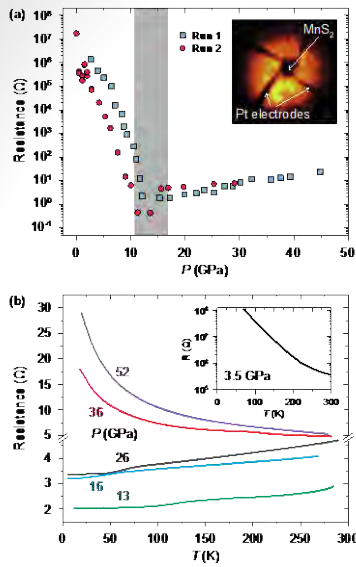
## **Gate controlled photocurrent generation mechanisms in high-gain In<sub>2</sub>Se<sub>3</sub> phototransistors**

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 MoSe<sub>2</sub> by uniaxial strain**

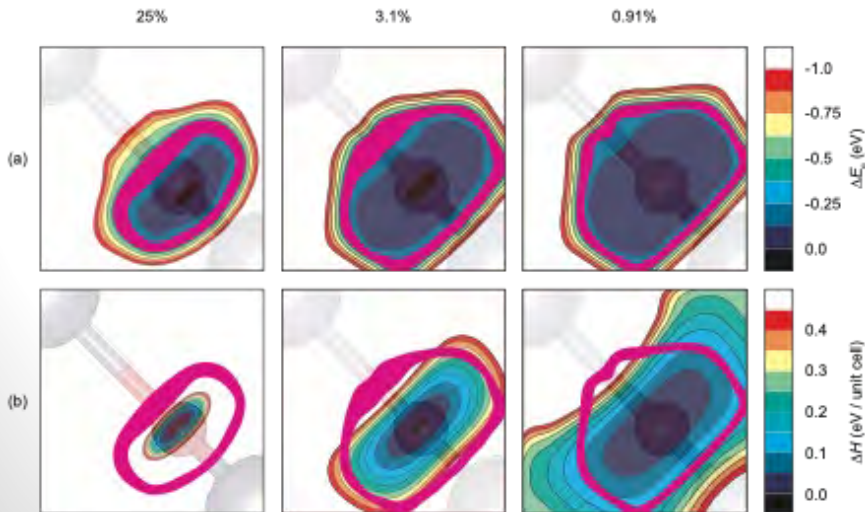
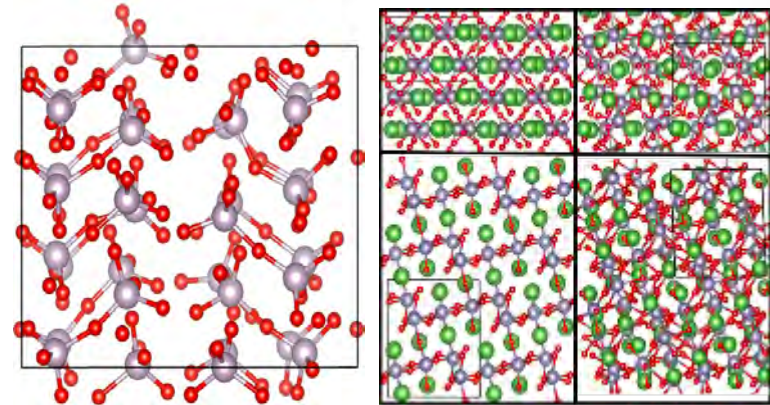
J.O. Island, A. Kuc, E.U. Diependaal, H.S.J. van der Zant, T. Heine, and A. Castellanos-Gomez, *Nanoscale*, **8**, 2589 (2016). (arXiv)





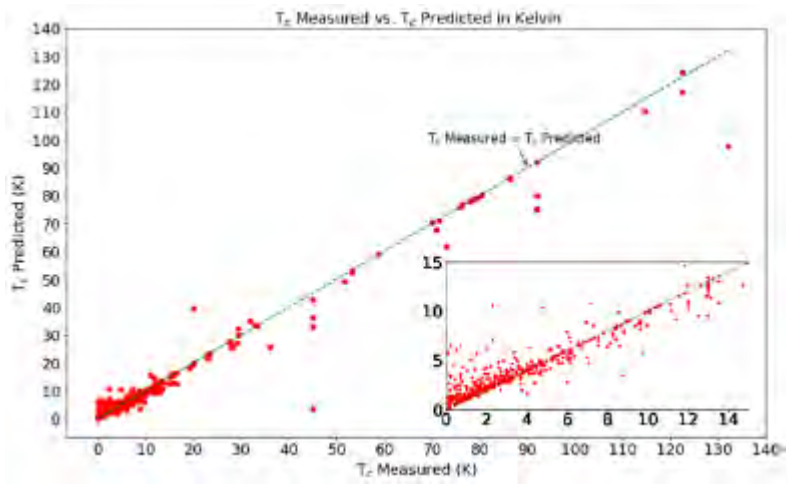
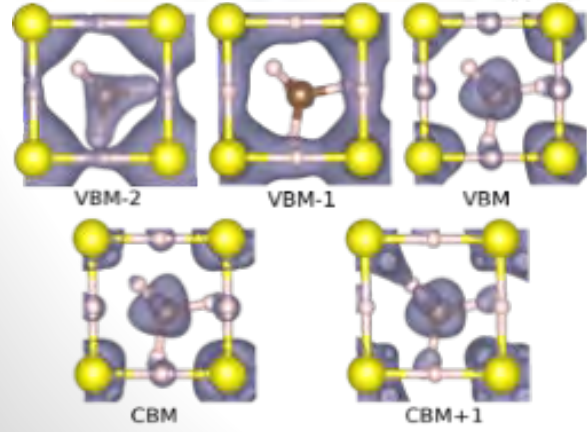
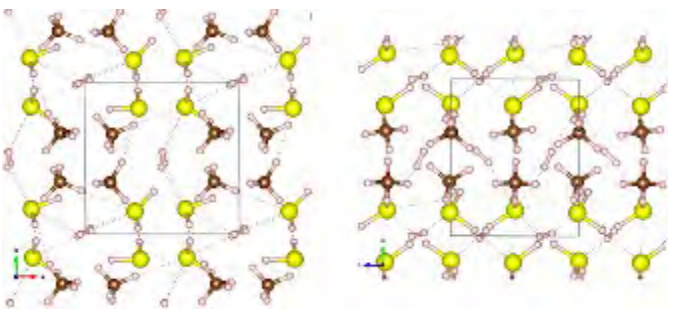
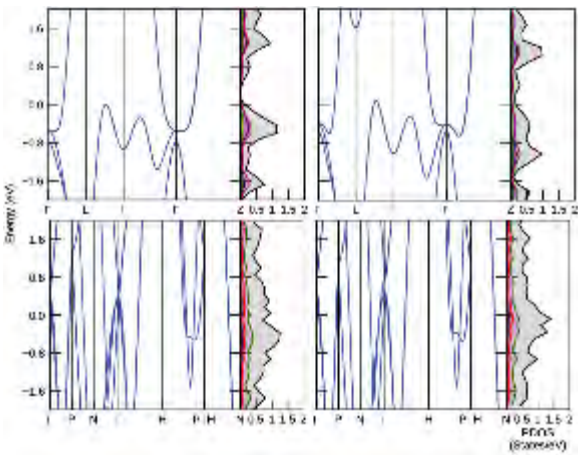
We primarily perform electronic structure simulations to understand pressure driven phenomenon particularly related to correlated electron systems and changes in bonding.

This includes molecular dynamics to understand the thermal behavior of materials and melts,



as well as crystal structure prediction and the electronic response to pressure driven perturbations in crystalline lattices.

Our group is also focused on understanding and predicting high temperature superconductivity in pressurized systems. As part of the team that reported room temperature superconductivity in a carbonaceous sulfur hydride system, we have been focused on understanding the molecular pathway to that system, the fundamental interactions driving its superconductivity, and building machine learning tools to predict such properties in new materials.



# Scientific Computing and Mathematical Modeling

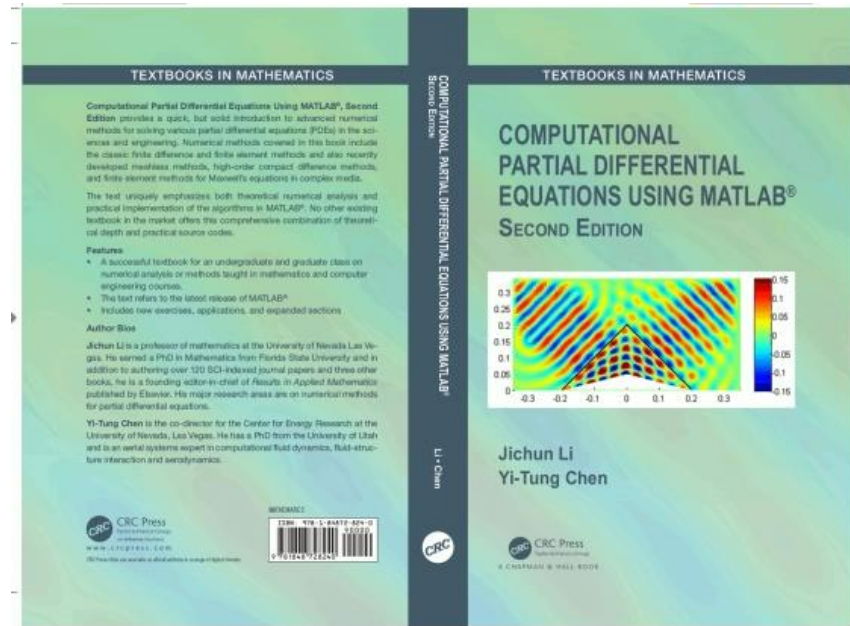
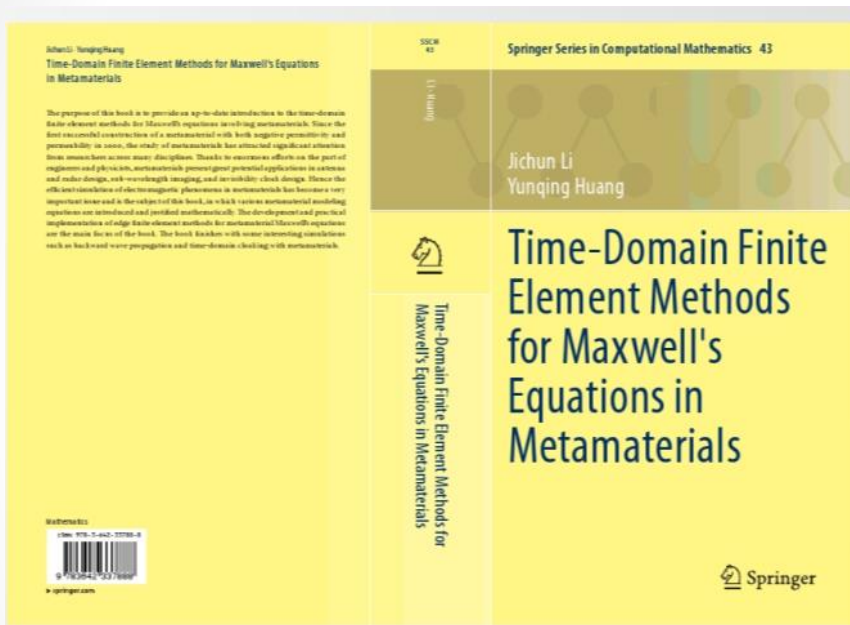
- **Dr. Jichun Li**
- Full Professor
- Department Mathematical Sciences
- Email: [jichun.li@unlv.edu](mailto:jichun.li@unlv.edu)
- Website: <http://faculty.unlv.edu/jichun/>

## Expertise

- Computational Electromagnetics: wave propagation in metamaterials, graphene, and other complex media.
- Develop, analyze, and implement various numerical methods for solving various Differential Equations (DEs) in sciences and engineering.
- Machine Learning; Math finance; Numerical Analysis.



# Published over 2 books, and over 140 SCI papers



In 2023, ranked #1097 (out of total 1138) in United States and #2638 in the world in The 2nd edition of Research.com ranking of the best scholars in the arena of Mathematics: <https://research.com/scientists-rankings/mathematics/>

# Novel chemistry and biology using highly ionizing radiation

**Michael Pravica, Ph.D.**

Professor of Physics

Department of Physics and Astronomy

Phone: (702)895-1723

Email: [michael.Pravica@unlv.edu](mailto:michael.Pravica@unlv.edu)

**Expertise:**

*Useful Hard X-ray photochemistry*

High pressure

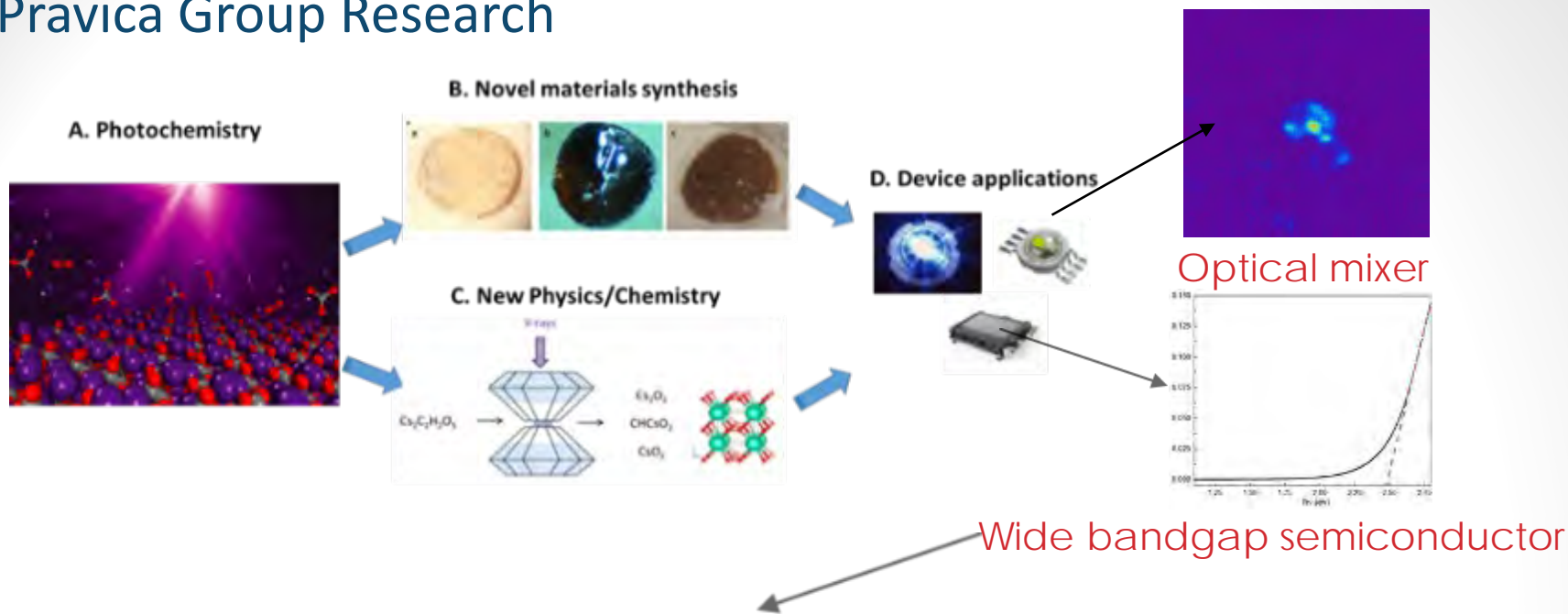
Spectroscopy

*Ion Beam Nuclear Transmutation Doping*

*High quality synthesis of vaccines using tuned hard x-rays*

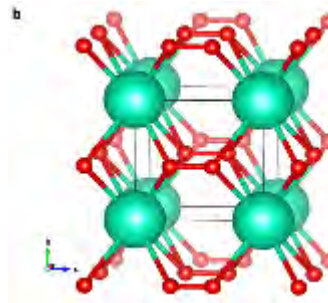


# Pravica Group Research



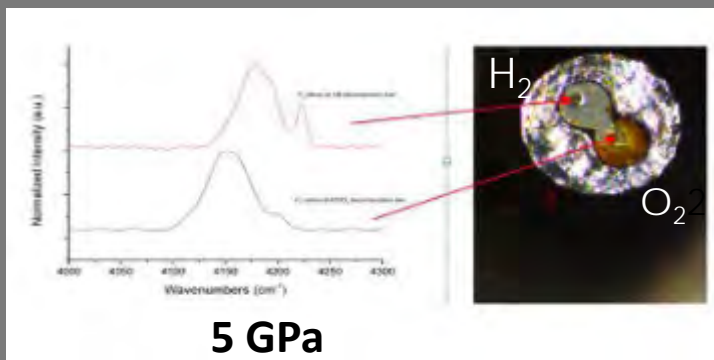
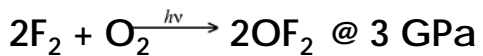
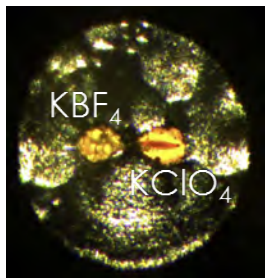
Radiation-hardened sensors/direct energy conversion devices for EXTREME CONDITIONS or tuned solar materials

## Useful hard x-ray photochemistry



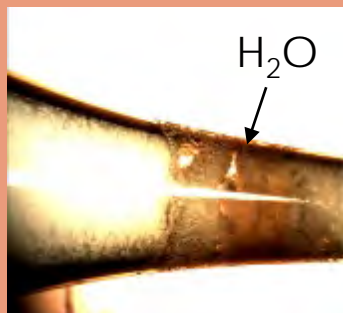
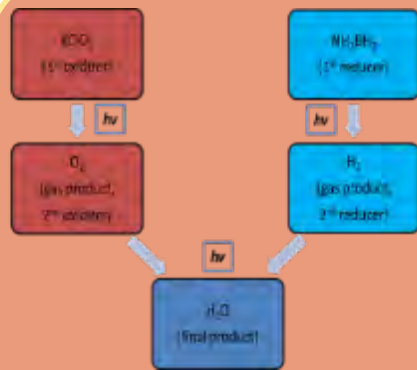
Novel structures of known materials produced With hard x-rays and high pressure (e.g. CsO<sub>2</sub>)

# High Pressure Fluorine Chemistry



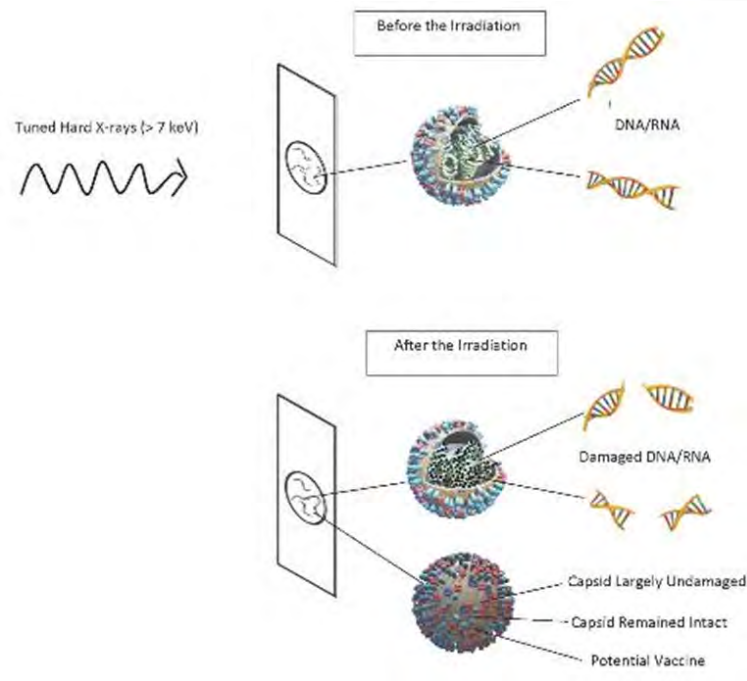
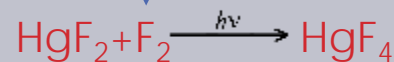
5 GPa

Molecular mixtures at high pressure



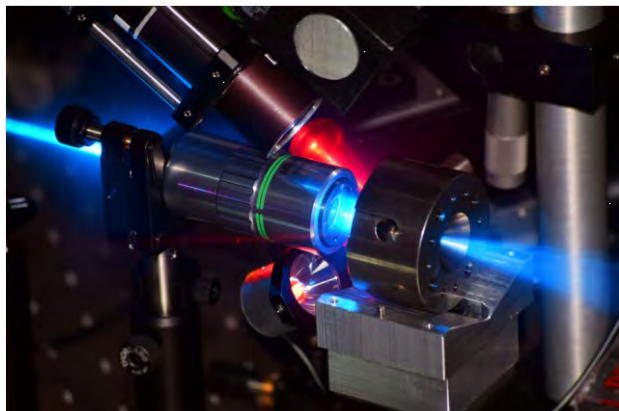
X-ray induced combustion

## Inner shell chemistry at high pressure

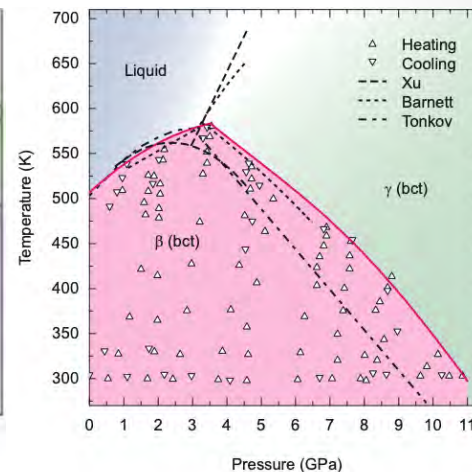
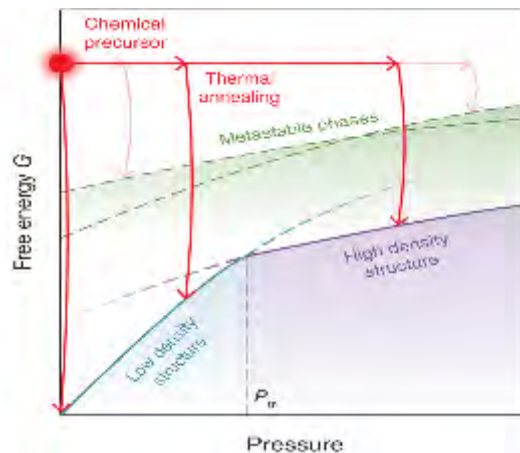


Using tuned hard x-rays to damage viruses to create high quality vaccines by targeting specific molecular groups/bonds that resonantly absorb x-ray energy leading to decomposition chemistry.

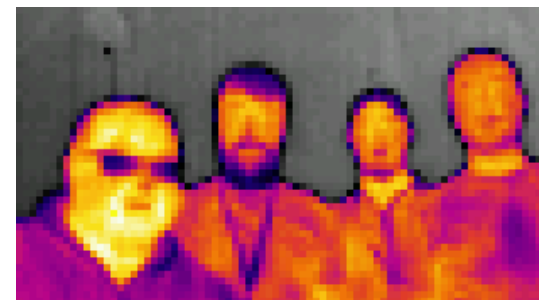
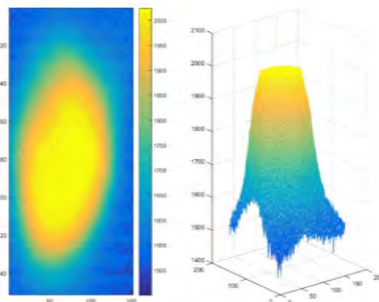
# Salamat Group – Collaboration with MSTS



Metrology – accurate mapping of P, V, T

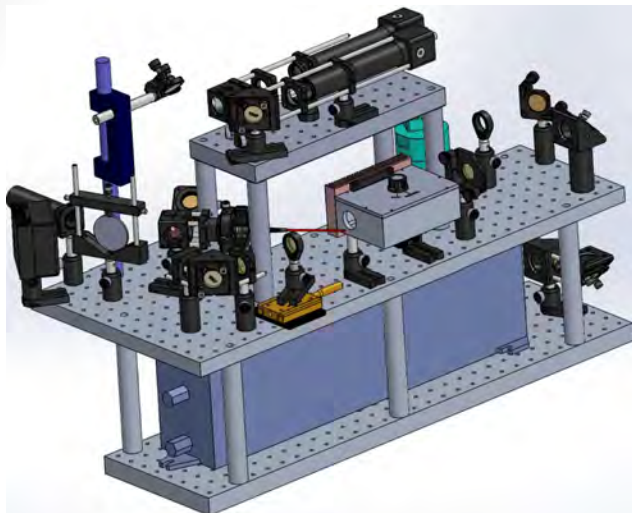


High temperature modelling – understanding emissivity under extreme conditions

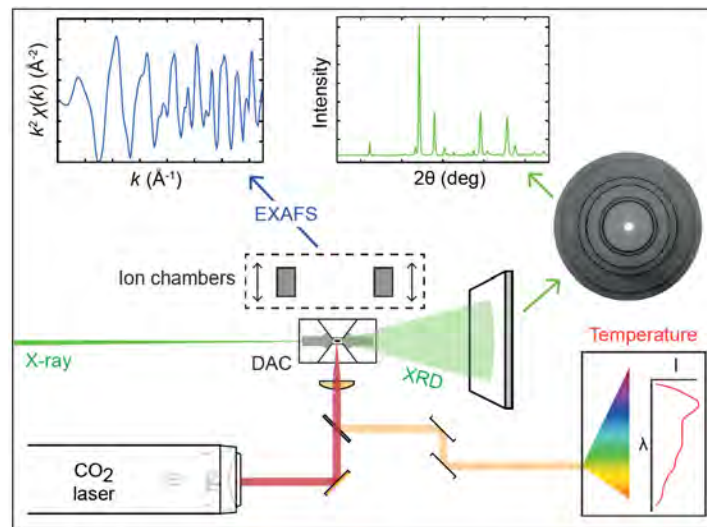
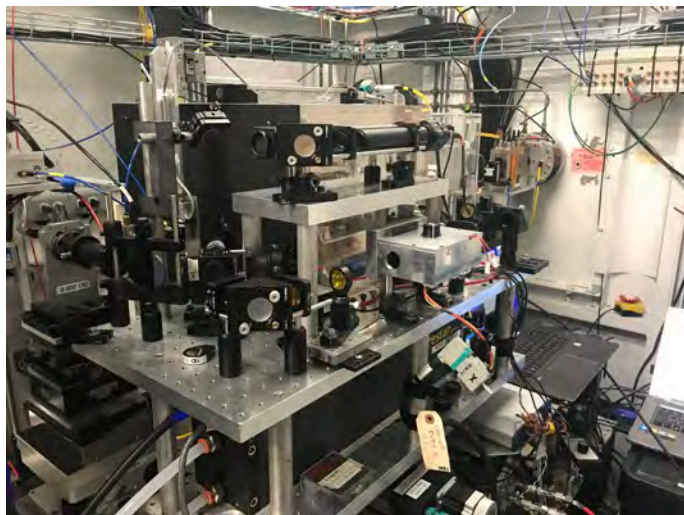




# Warm dense matter – probed using EXAFS



- Development of a CO<sub>2</sub> laser heating
- Direct heating of non-metallic systems in a DAC
- First HTHP EXAFS measurements of insulators
- In situ and post heating measurements
- Determining absolute temperature from X-ray spectroscopy



# Publications

---

- (1) D. Smith, D. Sneed, N. Dasenbrock-Gammon, E. Snider, G. A. Smith, C. Childs, J. S. Pigott, N. Velisavljevic, C. Park, K. V. Lawler, R. P Dias, A. Salamat\*, Anomalous Conductivity in the Rutile Structure Driven by Local Disorder [The Journal of Physical Chemistry Letters 10 18 5351-5356 \(2019\)](#)
- (2) J. Kearney M. Grauzinyte D. Smith A. Gulans D. Sneed C. Childs, J. Hinton C. Park J. S. Smith, E. Kim, S. D. S. Fitch, A. L. Hector, C. J. Pickard J. A. Flores-Livas, A. Salamat\*, Pressure tuneable visible range band gap in the ionic spinel tin nitride [Angewandte Chemie International Edition, 57, 11623-11628 \(2018\)](#)
- (3) C. Childs, K. V. Lawler, A. L. Hector, S. Petitgirard, O. Noked, J. S. Smith, D. Daisenberger, L. Bezacier, M. Jura, C. J Pickard, A. Salamat\*, Covalency is Frustrating:  $\text{La}_2\text{Sn}_2\text{O}_7$  and the Nature of Bonding in Pyrochlores under High Pressure Temperature Conditions [Inorganic chemistry, 57, 15051-15061, \(2018\)](#)
- (4) D. Smith, K. V. Lawler, M. Martinez-Canales, A. W. Daykin, Z. Fussell, G. A. Smith, C. Childs, J. S. Smith, C. J. Pickard, and A. Salamat\*, Postaragonite phases of  $\text{CaCO}_3$  at lower mantle pressures [Physical Review M 2, 013605 \(2018\)](#)
- (5) D. Smith, J. S. Smith, C. Childs, E. Rod, R. Hrubik, G. Shen, A. Salamat\*, A  $\text{CO}_2$  laser heating system for in situ high pressure-temperature experiments at HPCAT [Review of Scientific Instruments 89, 083901 \(2018\)](#)
- (6) R. Briggs, D. Daisenberger, O. T. Lord, A. Salamat, E. Bailey, M. J. Walter, P. F. McMillan\*, High-pressure melting behavior of tin up to 105 GPa [Physical Review B 95, 054102 \(2017\)](#)
- (7) M. Zaghoo, A. Salamat, I. F. Silvera\*, A first order phase transition to metallic hydrogen. [Physical Review B 93, 155128 \(2016\)](#)
- (8) A. Salamat\*, R. Fischer, R. Briggs, M. I. McMahon, S. Petitgirard, In situ synchrotron X-ray diffraction in the laser heated diamond anvil cell: melting phenomena and synthesis of new materials. [Coordination Chemistry Reviews 277-278, 15 \(2014\)](#)

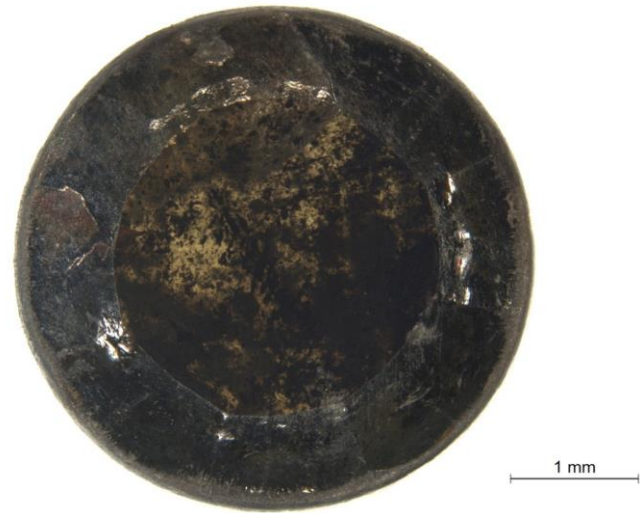


# Research Oliver Tschauner

- **Dr. Oliver Tschauner**
- Professor of Research
- Department Geoscience
- Email: [oliver.Tschauner@unlv.edu](mailto:oliver.Tschauner@unlv.edu)
- Website: <https://geoscience.unlv.edu/people/department-faculty/oliver-tschauner/>

## Expertise

- Crystallography.
- Mineralogy.
- Physics and Chemistry at high pressure.
- Dynamic compression.



Natural diamond with CO<sub>2</sub> inclusions  
at a pressure of 20000  
atmospheres

# Selected Publications

- ♦ Discovery of davemaite,  $\text{CaSiO}_3$ -perovskite as a mineral from the lower mantle. O. Tschauner, S. Huang, S. Yang, M. Humayun, W. Liu, S. N. Gilbert Corder, H. A. Bechtel, J. Tischler, G. R. Rossman, **Science** 374, 891-894 (2021).
- ♦ Ice-VII inclusions in diamonds – evidence for aqueous fluid in the Earth’s deep mantle O. Tschauner, S. Huang, E. Greenberg, V.B. Prakapenka, C. Ma , G. R. Rossman, A.H. Shen, M. Newville, A. Lanzirotti, K. Tait, **Science** 359, Issue: 6380, 1136 (2018) 10.1126/science.aao3030.
- ♦ Discovery of Bridgmanite – the most abundant mineral in Earth, in a shocked meteorite, O. Tschauner, C. Ma, J. Beckett, C. Prescher, V. Prakapenka, G. Rossman, **Science** 346, 1100 (2014), DOI: 10.1126/science.1259369
- ♦ Is merrillite shock-transformed whitlockite? Implications for the water budget of Mars, C. Adcock, O. Tschauner, E. Hausrath, A. Udry, Y. Cai, S.N. Luo, **Nature Communications** 8, Article Number: 14667 (2017).
- ♦ Tissintite ( $\text{Ca, Na, } \square$ )  $\text{AlSi}_2\text{O}_6$ , a Highly Defective, Shock-Induced, High-Pressure Pyroxene in the Tissint Martian Meteorite. Chi Ma, Oliver Tschauner, John Beckett, Yang Liu, George Rossman, Kirill Zuravlev, Vasili Prakapenka, Przemyslaw Dera and Lawrence A. Taylor, **Earth Planet. Sci. Lett.** 422,194-205 (2015).
- ♦ Ahrensite,  $\gamma\text{-Fe}_2\text{SiO}_4$ , a new shock-metamorphic mineral from the Tissint meteorite: Implications for the Tissint shock event on Mars. Ma, C. ; Tschauner, O.; Beckett, J.R.; Liu, Y.; Rossman, G.R.; Sinogeikin, S.V.; Smith, J.S.; Taylor, L.A. **Geochim. Cosmochim. Acta** 184, 240-256 (2016). DOI: 10.1016/j.gca.2016.04.042
- ♦ Tschauner, O., Ma, C. (2023). Discovering High-Pressure and High-Temperature Minerals. In: Bindi, L., Cruciani, G. (eds) **Celebrating the International Year of Mineralogy. Springer Mineralogy.** Springer, Cham. [https://doi.org/10.1007/978-3-031-28805-0\\_8](https://doi.org/10.1007/978-3-031-28805-0_8)

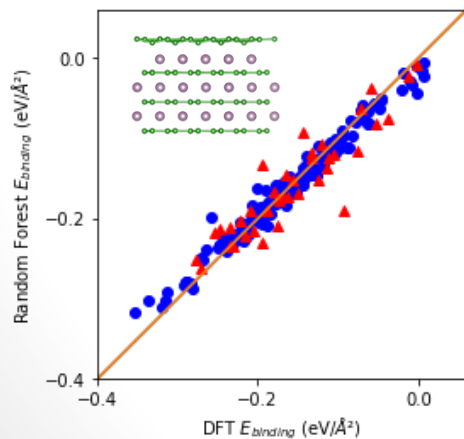
# Computational Materials Science

- **Dr. Luqing Wang**
- Assistant Professor - Physics
- Department of Physics and Astronomy
- Email: luqing.wang@unlv.edu
- Office: BPB 232

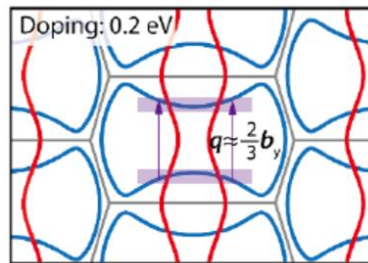


## Expertise

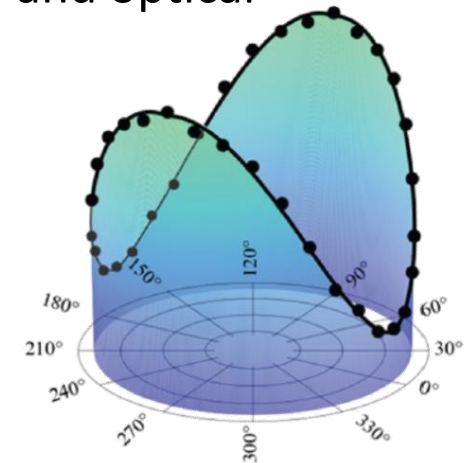
- Density functional theory calculations and machine learning.
- Two-dimensional (2D) materials functionalization and quantum effect.
- Electronic, mechanical, thermodynamic, chemical and optical properties of materials.
- Energy conversion & sustainability.



2D Materials Synthesis



2D Electronic and Quantum



2D Electro-Mechanics

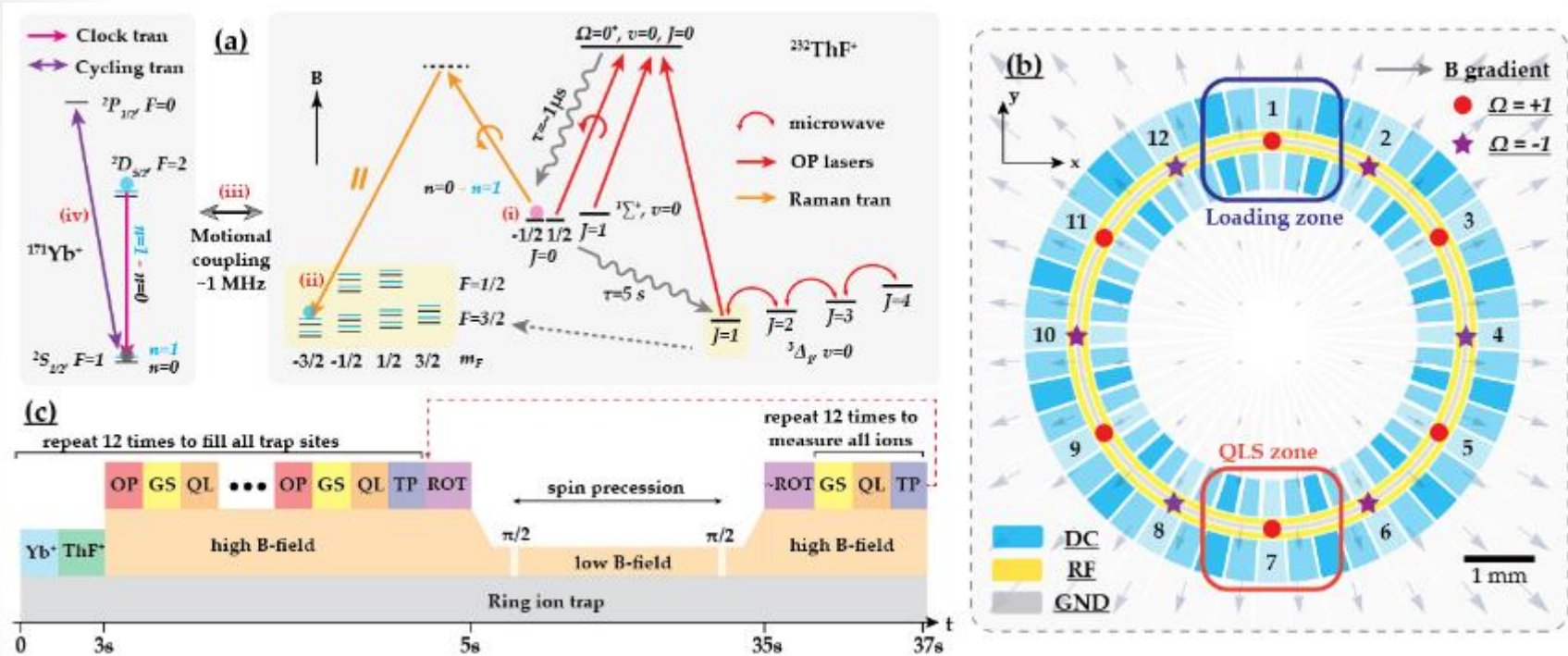
# Zhou Lab – Experimental AMO physics

- **Dr. Yan Zhou**
- Assistant Professor
- Department of Physics and Astronomy
- Email: yan.zhou@unlv.edu
- Website: <https://www.physics.unlv.edu/~yanzhou/index.html>

## Research projects

- Explore new physics beyond the Standard Model by precision measurements using quantum logically controlled molecular ions
- Precision metrology and spectroscopy using optical frequency combs
- Quantum transducer – link ion trap and superconducting quantum computers
- Experimental astrochemistry – cold ion-radical collisions

# Search for $T, P$ -odd symmetry violation



- On-chip Quantum sensors
- Entanglement between atomic ions and molecular ions
- Scalability and multiplexing measurements
- New table-top platform to investigate nuclear physics