# Condensed Matter & Atomic, Molecular, and Optics (AMO) Research

*Theoretical and Computational*

# Condensed Matter and Materials Physics

**Dr. Changfeng Chen**
Department of Physics and Astronomy
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Email: 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

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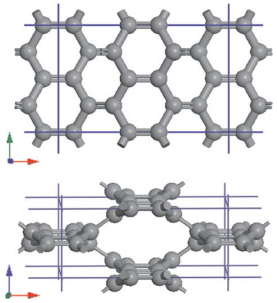
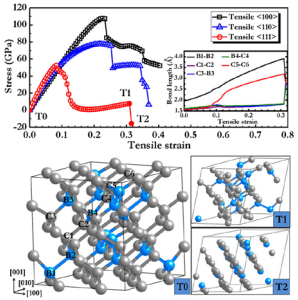
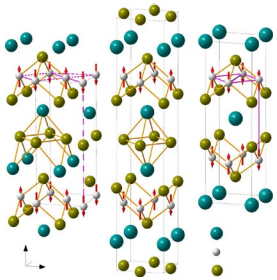


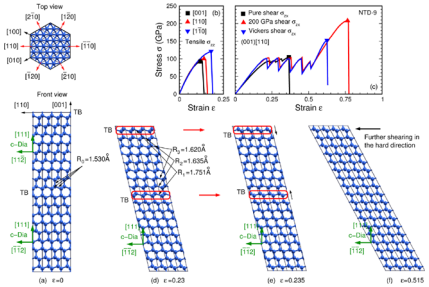
Nodal-ring Dirac semimetal states identified in bco-$C_{16}$ crystal [Wang, Weng, Nie, Fang, Kawazoe, Chen, ***Phys. Rev. Lett.*** 116, 195501 (2016)].



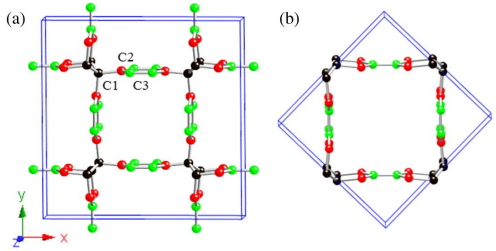

Superhard $B_3C$ in diamond structure [Zhang, et al., ***Phys. Rev. Lett.*** 114, 015502 (2015)].



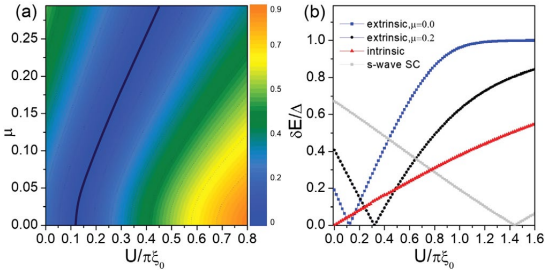
Magnetic Dirac materials $CaMnBi_2$ and $SrMnBi_2$ [Zhang, et al., ***Nature Commun.*** 7, 13833 (2016)].




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

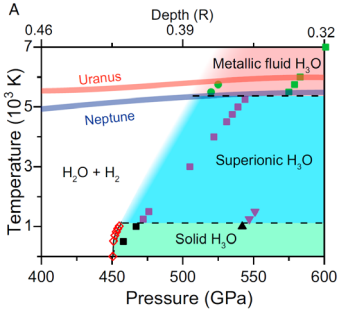



Nodal-net Dirac semimetal states in a graphene network structure [Wang, Nie, Weng, Kawazoe, Chen, ***Phys. Rev. Lett.*** 120, 026402 (2018)].

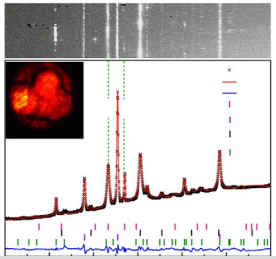



Kondo physics in 2D topological superconductors [Wang, et al., ***Phys. Rev. Lett.*** 122, 087001 (2019)].

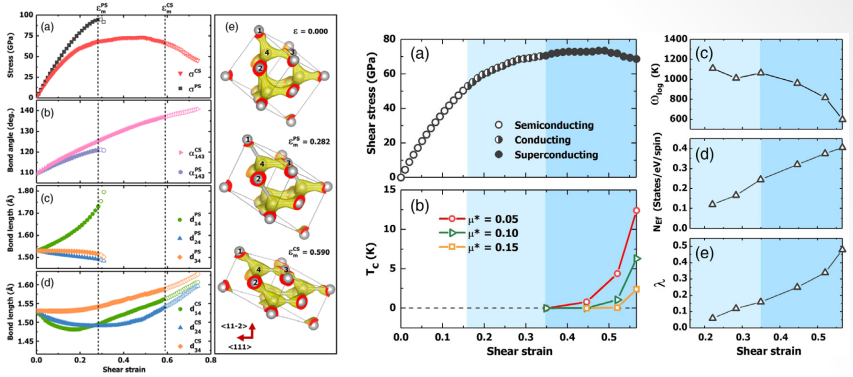
Helium-bearing compound $FeO_2He$ predicted to stabilize at deep-Earth conditions [Zhang, et al., ***Phys. Rev. Lett.*** 121, 255703 (2018)].




Prediction of novel $H_3O$ and implications for the magnetic fields of Uranus and Neptune [Huang, et al., ***Proc. Natl. Acad. Sci.*** 117, 5638 (2020)].



Pressure-stabilized divalent ozonide $CaO_3$ 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 $WB_n$ 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).

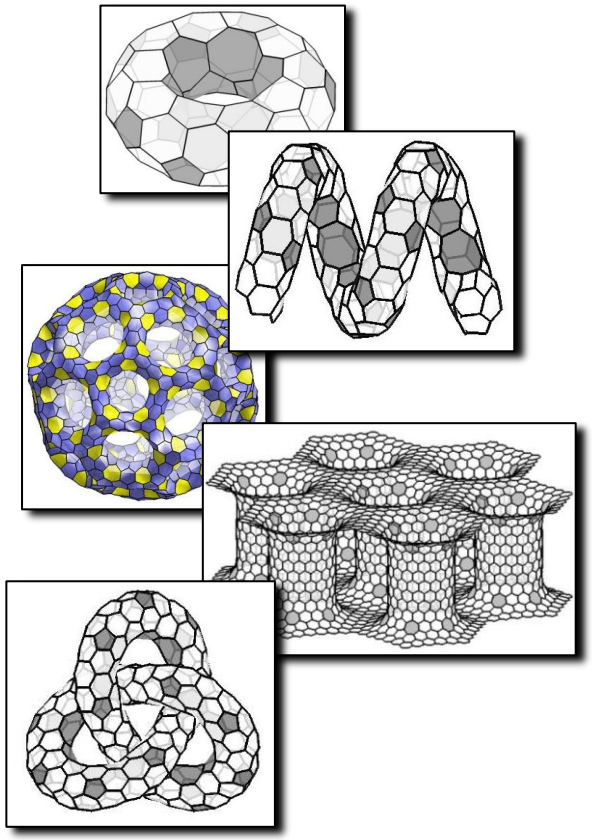
Xenon iron oxides predicted as potential Xe hosts in Earth's lower mantle, Peng, Song, Liu, Li, Miao, Chen, Ma, ***Nature Commun.*** 11, 5227 (2020).

# Theoretical chemical physics

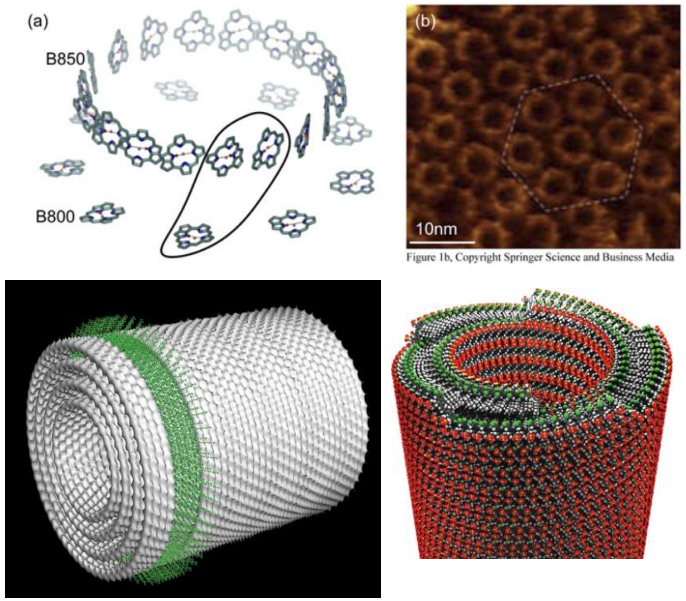

- Dr. Chern Chuang,
- Assistant Professor, Department of Chemistry and Biochemistry
- Email: chern.chuang@unlv.edu
- Website: http://cchuang.faculty.unlv.edu/Home.html


- 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

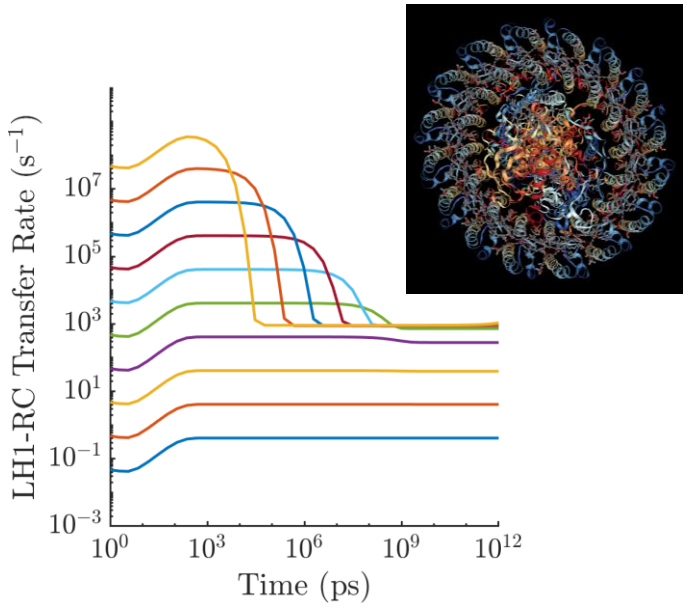
# Theoretical chemical physics

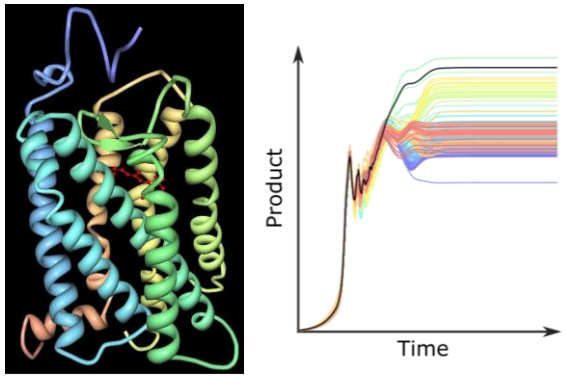


Exotic low-dimensional materials




Photophysics of organic materials




Photochemistry under environmental control

# Electronic and Magnetic Properties at High Pressure

**Dr. Andrew Cornelius**
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Phone (702) 895-1727

**Expertise**:

- Experimental high pressure measurements
- Magnetism
- Superconductivity

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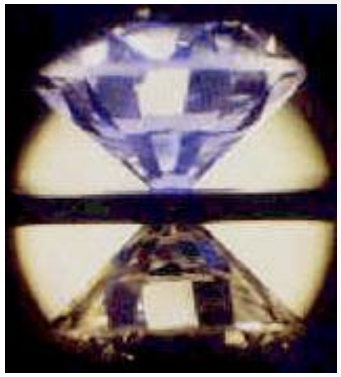
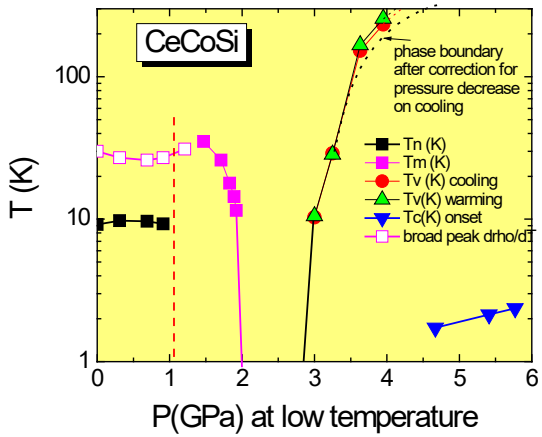
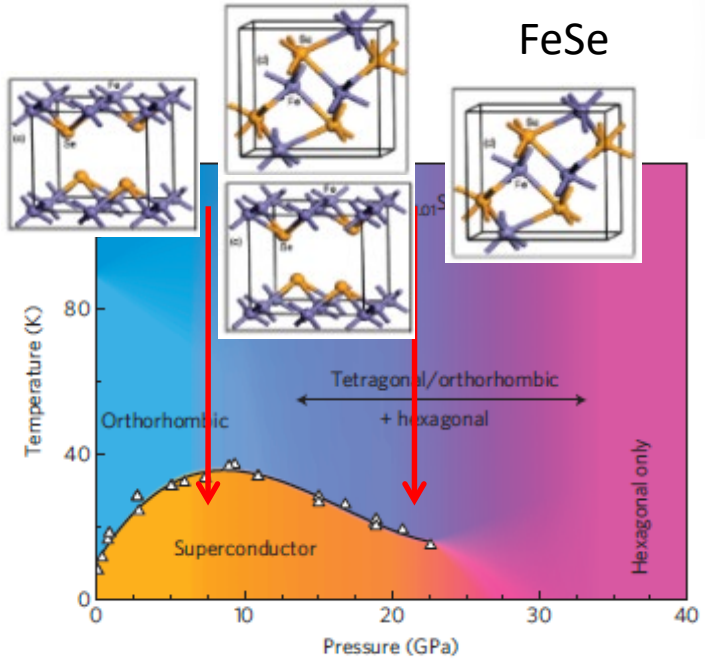
# Superconductivity


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)

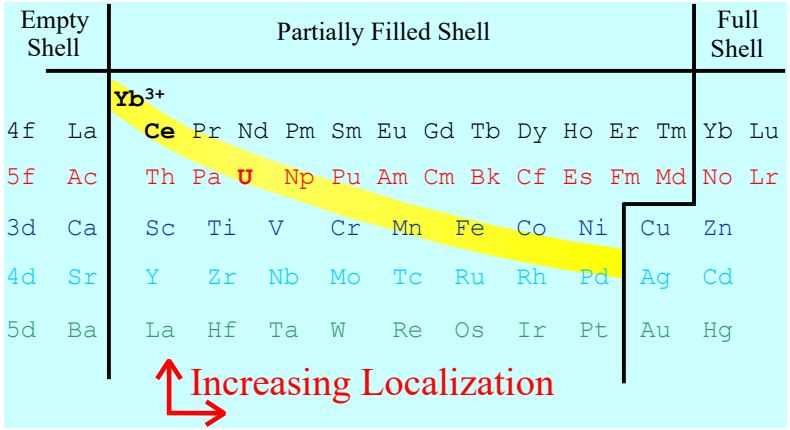




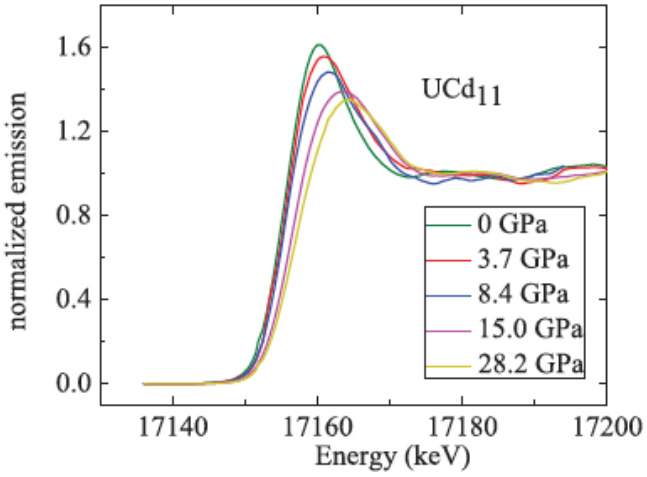

Addition of high pressure synchrotron experiments (diffraction and X-ray absorption) allows mapping of complex superconducting phase diagrams

# Correlated-Electron Systems

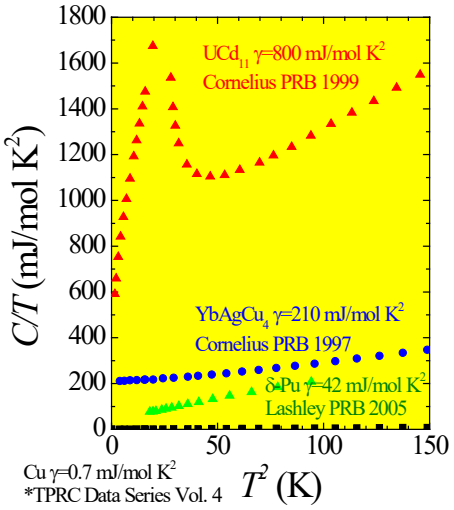



Modified periodic table

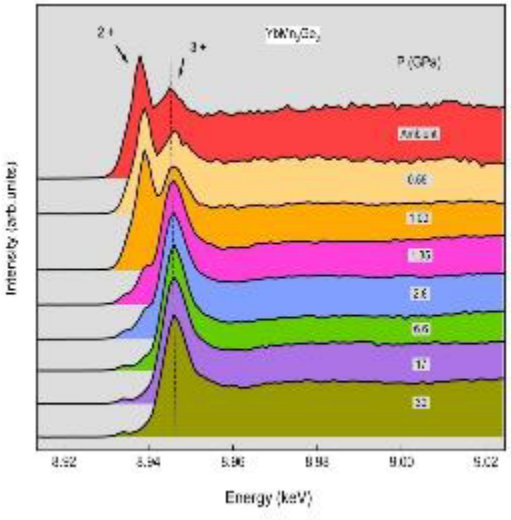
- Going from localized to delocalized electrons one often finds strong electron-electron correlations
- Correlated electron systems can yield interesting behavior: fluctuating valence, superconductivity, non-Fermi liquid, heavy fermion and many more




f-electron delocalization
X-ray absorption




Heavy fermions
Heat Capacity



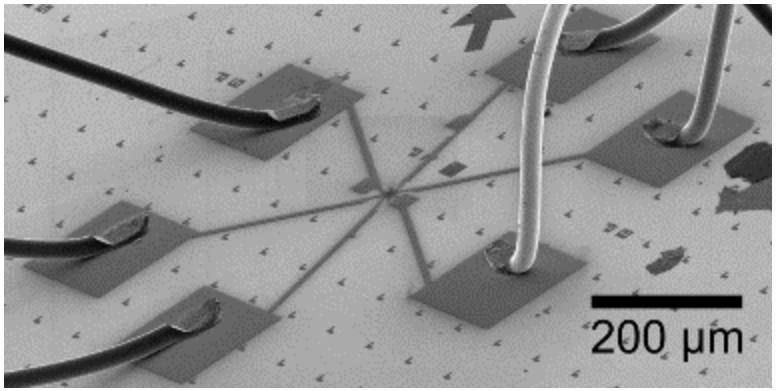

Fluctuating valence
X-ray fluorescence

# Island – Quantum computing, quantum sensing

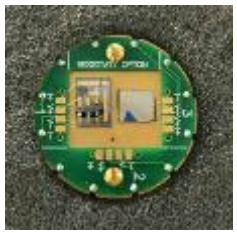
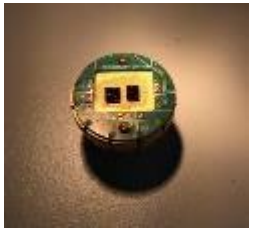
The Nanoscale Physics Group @ UNLV

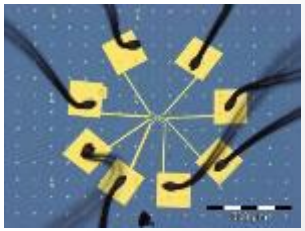
## Areas of Research

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





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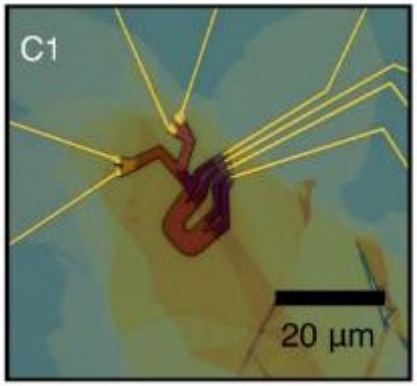
Island's Lab website

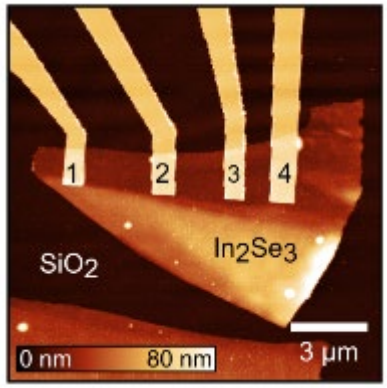
# Island – Quantum computing, quantum sensing

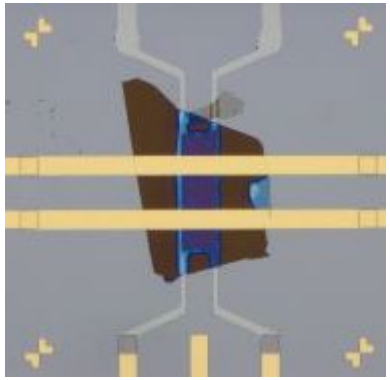
**Quantum computing:** Topological phases for fault-tolerant, universal quantum computing.

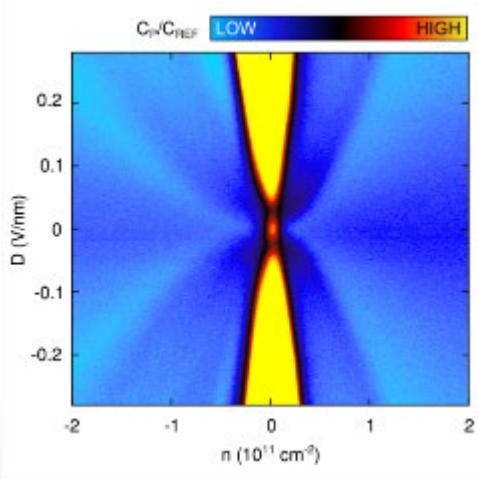
**Industry-disruptive photodetectors:** Ultra-sensitive phototransistors designed with 2D materials and heterostructures.

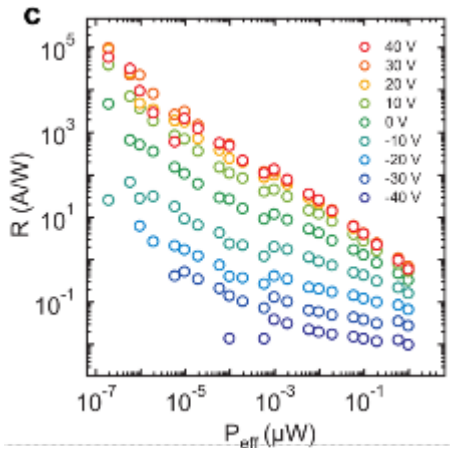
**Transient phases of driven systems:** Non-equilibrium response of pumped nanomaterials below the diffraction limit.

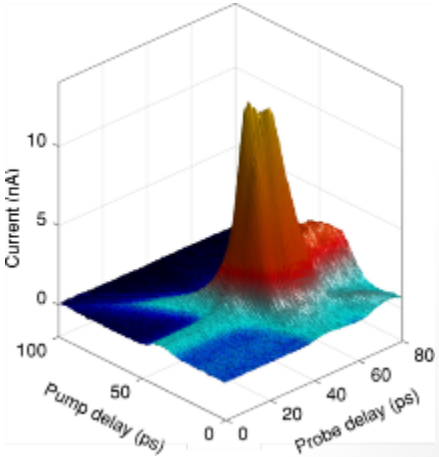





Island, J. O., et al. *Nature* **571** (2019): 85–89.

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

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

**T1S3 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 ln2Se3 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.U. Diependaal, H.S.J. van der Zant, T. Heine, and A. Castellanos- Gomez, Nanoscale, **8,** 2589 (2016). (arXiv)

Island's Lab website

# Condensed Matter Theory

Tao Pang

Department of Physics and Astronomy

University of Nevada, Las Vegas

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# Research Methods and Systems Studied

- Analytical Approach

  Quantum Hall effect; quantum transport phenomena, superconductor-insulator transitions; vibrational modes in glasses; and slow light in cold atoms.

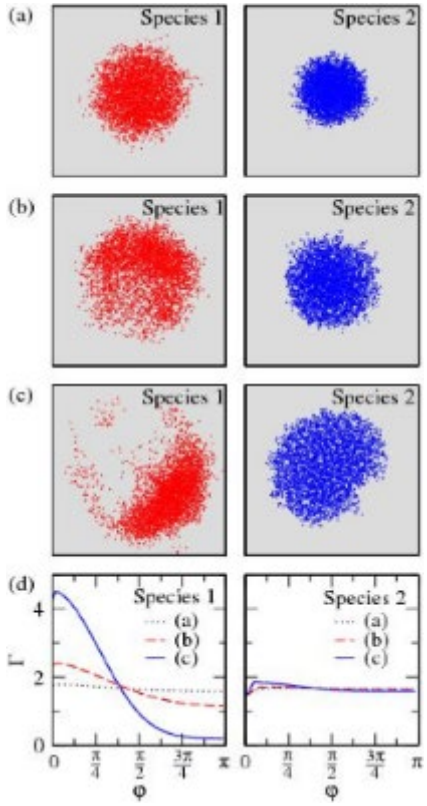
- Diffusion Quantum Monte Carlo Simulation

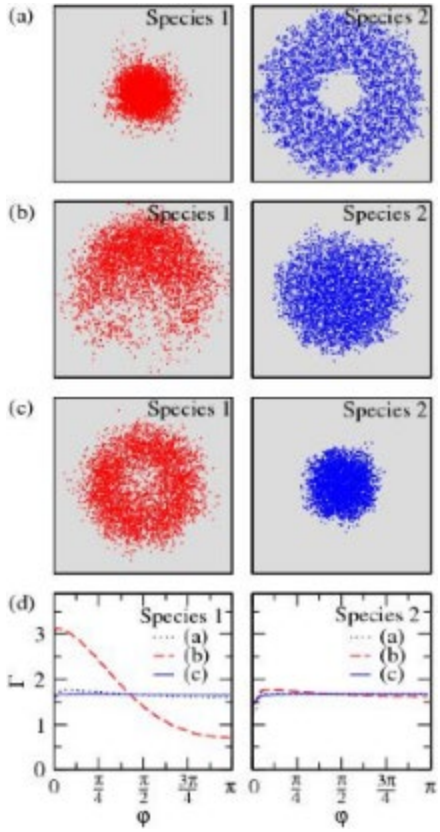
  Negative donor centers in semiconductors; hydrogen molecules in confinement; ionic hydrogen clusters; and helium clusters with modified interactions.

- Path Integral Quantum Monte Carlo Simulation

  Bosons trapped in potential wells in one dimension or two dimensions; Bose-Einstein condensation of cold atoms; and asymmetric distributions of Bose-Einstein condensates of boson mixtures.

# An Example: Asymmetry of the Mixed Bose Condensates:




Asymmetric distributions of two Bose-Einstein condensates in the same trap with different cluster parameters.

H. Ma and T. Pang, Phys. Rev. A **70**, 063606 (2004).

# 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

**Expertise:**
*Useful Hard X-ray photochemistry*
High pressure
Spectroscopy
*Ion Beam Nuclear Transmutation Doping*
*High quality synthesis of vaccines using tuned hard x-rays*

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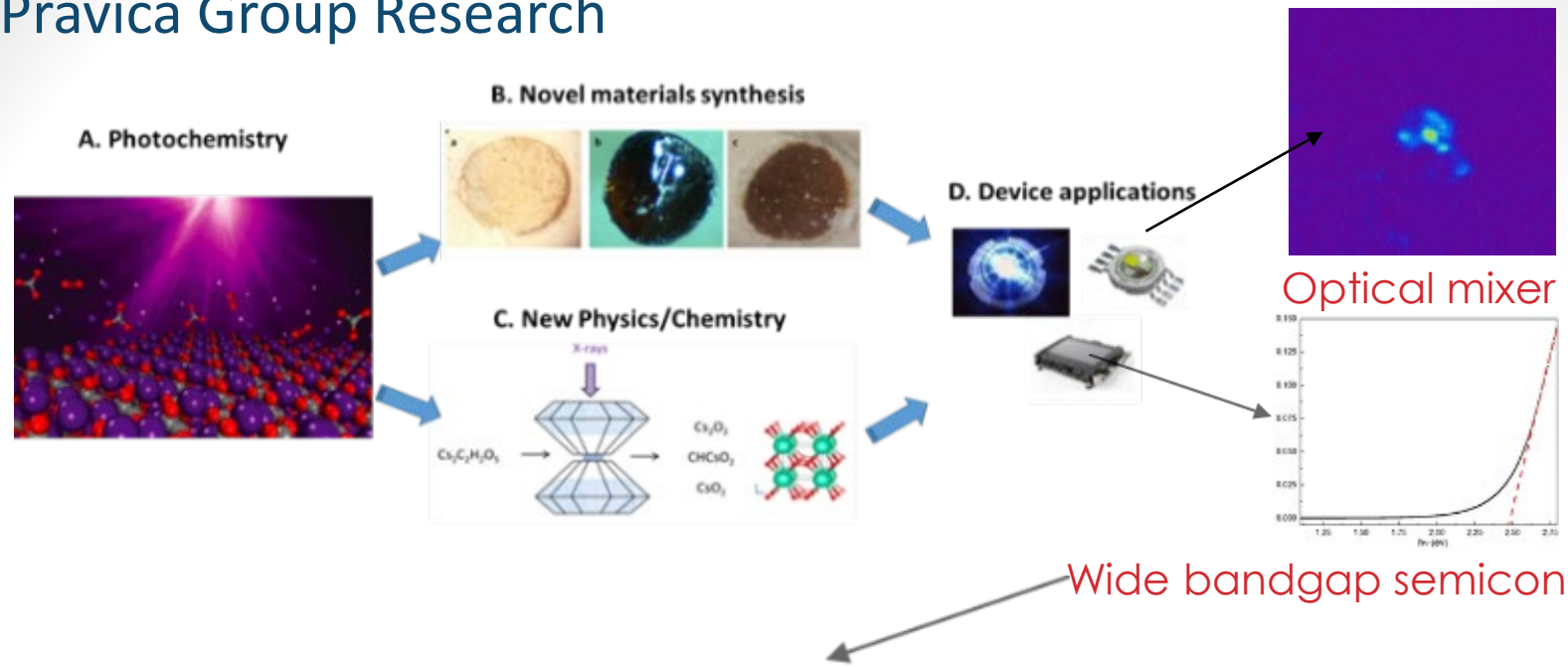
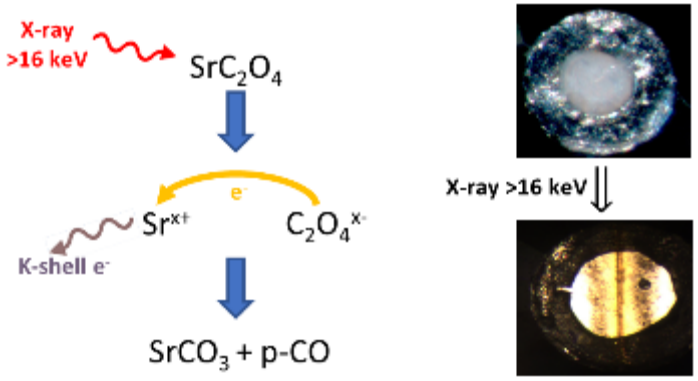
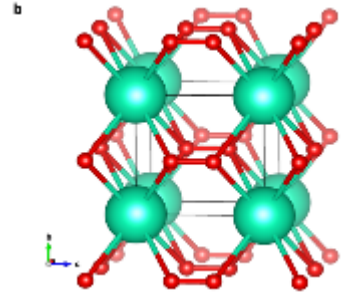
# Pravica Group Research




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

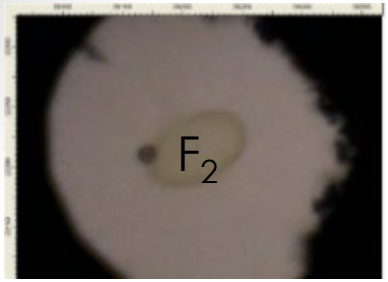
*Useful hard x-ray photochemistry*

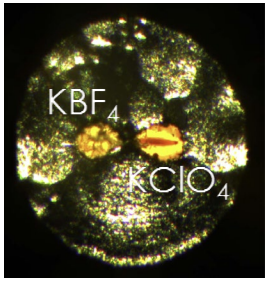


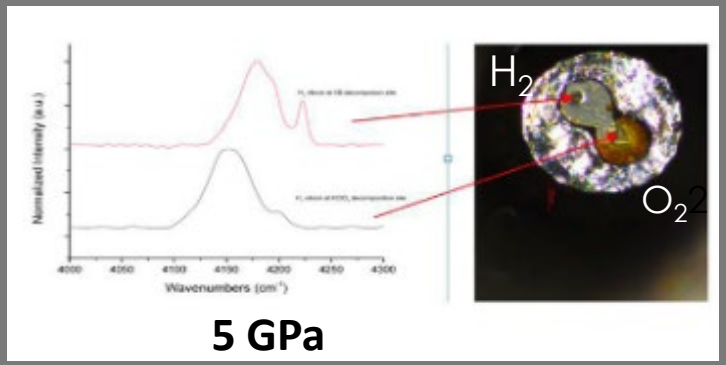
Novel structures of known materials produced With hard x-rays and high pressure (e.g. $CsO_2$)

# High Pressure Fluorine Chemistry



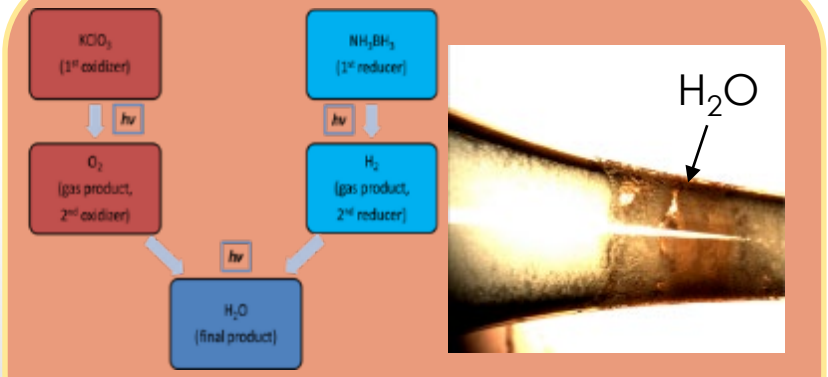




$$2F_2 + O_2 \xrightarrow{h\nu} 2OF_2 \text{ @ 3 GPa}$$




**5 GPa**

Molecular mixtures at high pressure

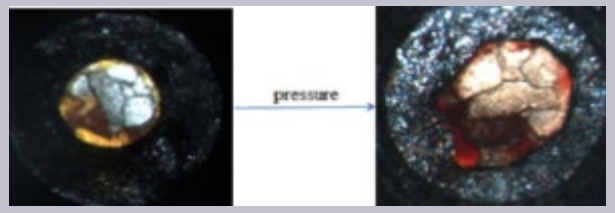






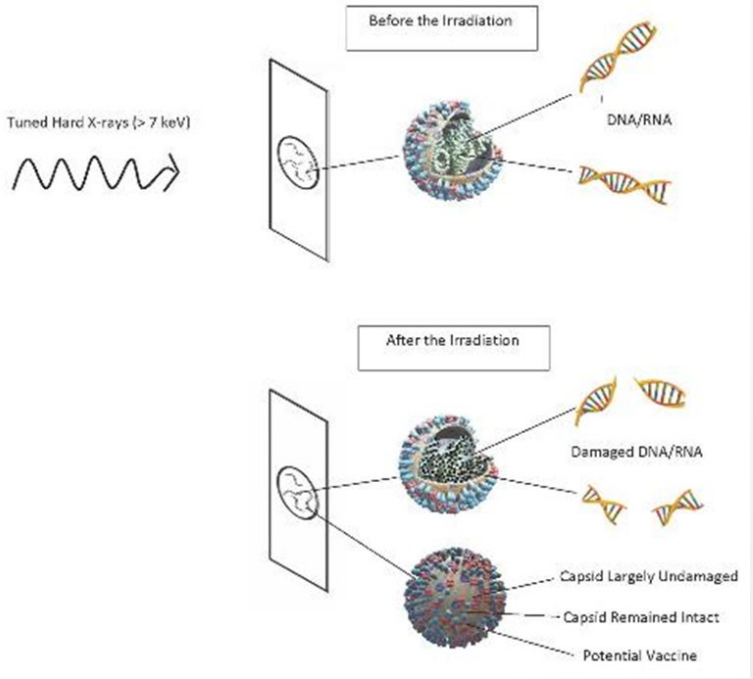
X-ray induced combustion

## Inner shell chemistry at high pressure



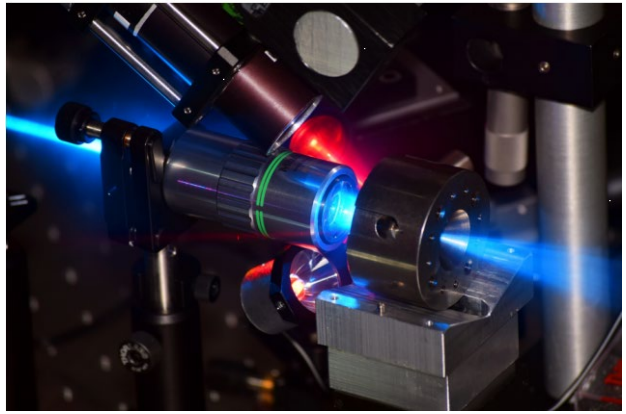

$$XeF_2 \xrightarrow{h\nu} Xe + F_2 \text{ (\textit{in situ} x-ray fluorination)}$$

$$HgF_2 + F_2 \xrightarrow{h\nu} HgF_4$$

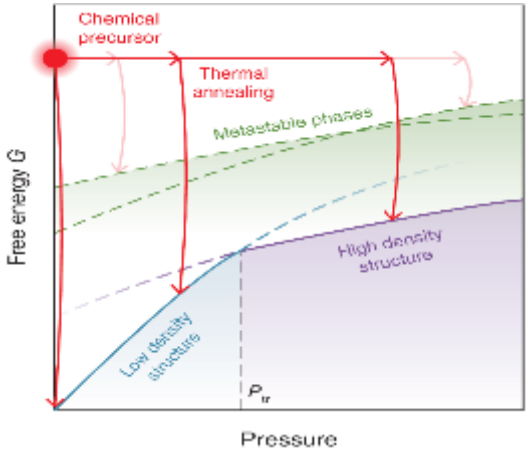


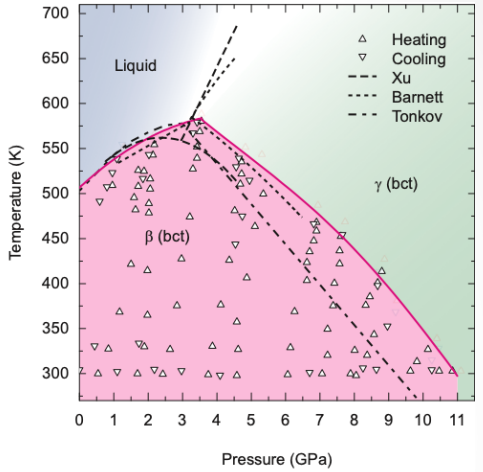

Using tuned hard x-rays to damage viruses to create high quality vaccines by targeting specific molecular groups/bonds that resonantly absorb x-ray energy leading to decomposition chemistry.

# Salamat Group – Collaboration with MSTS

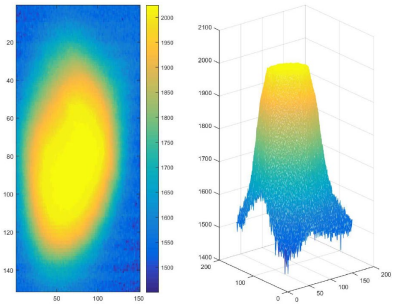


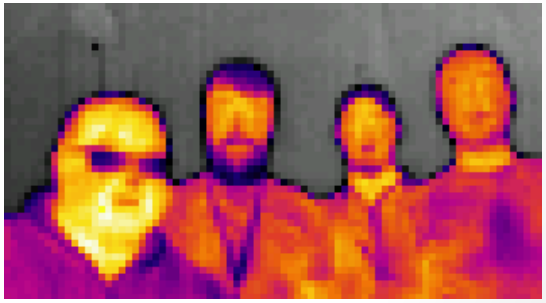
Metrology – accurate mapping of P, V, T




High temperature modelling – understanding emissivity under extreme conditions





Los Alamos NATIONAL LABORATORY

MSTS MISSION SUPPORT AND TEST SERVICES LLC

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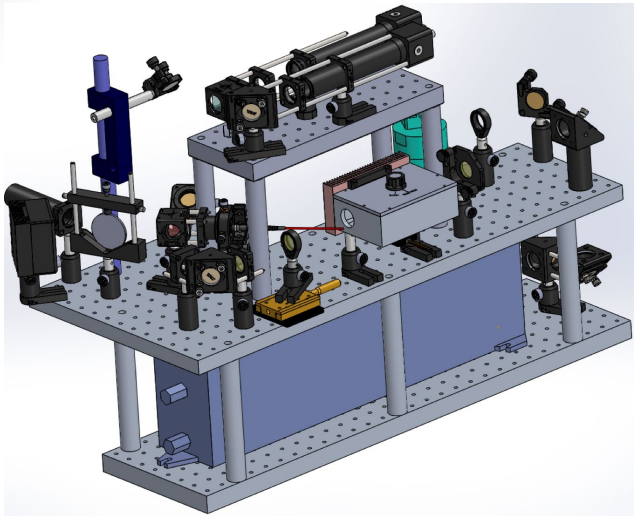
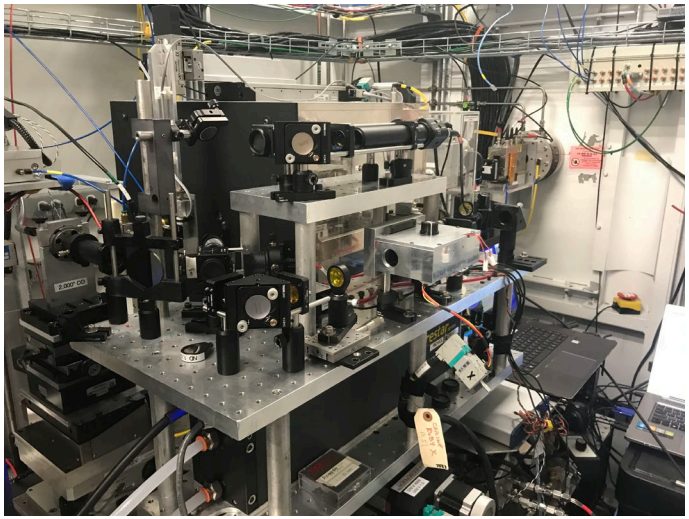
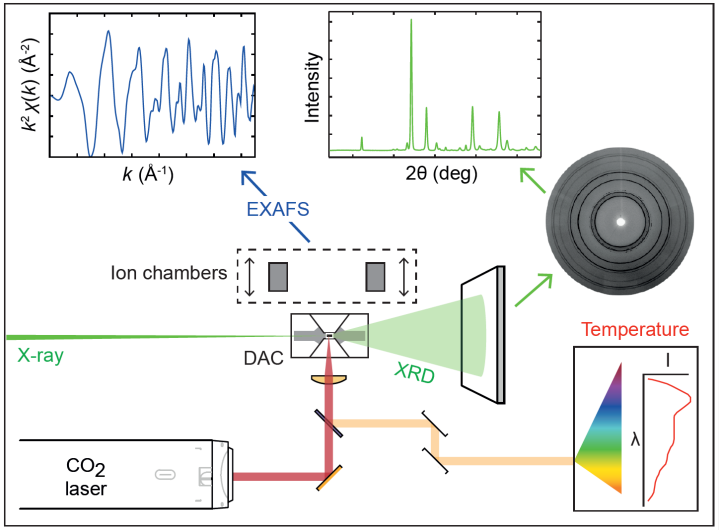
# Warm dense matter – probed using EXAFS



- Development of a $CO_2$ 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: $La_2Sn_2O_7$ 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 $CaCO_3$ at lower mantle pressures Physical Review M 2, 013605 (2018)

(5) D. Smith, J. S. Smith, C. Childs, E. Rod, R. Hrubiak, G. Shen, A. Salamat*, A $CO_2$ 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)

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# Zhou Lab – Experimental AMO physics


- **Dr. Yan Zhou**
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- 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

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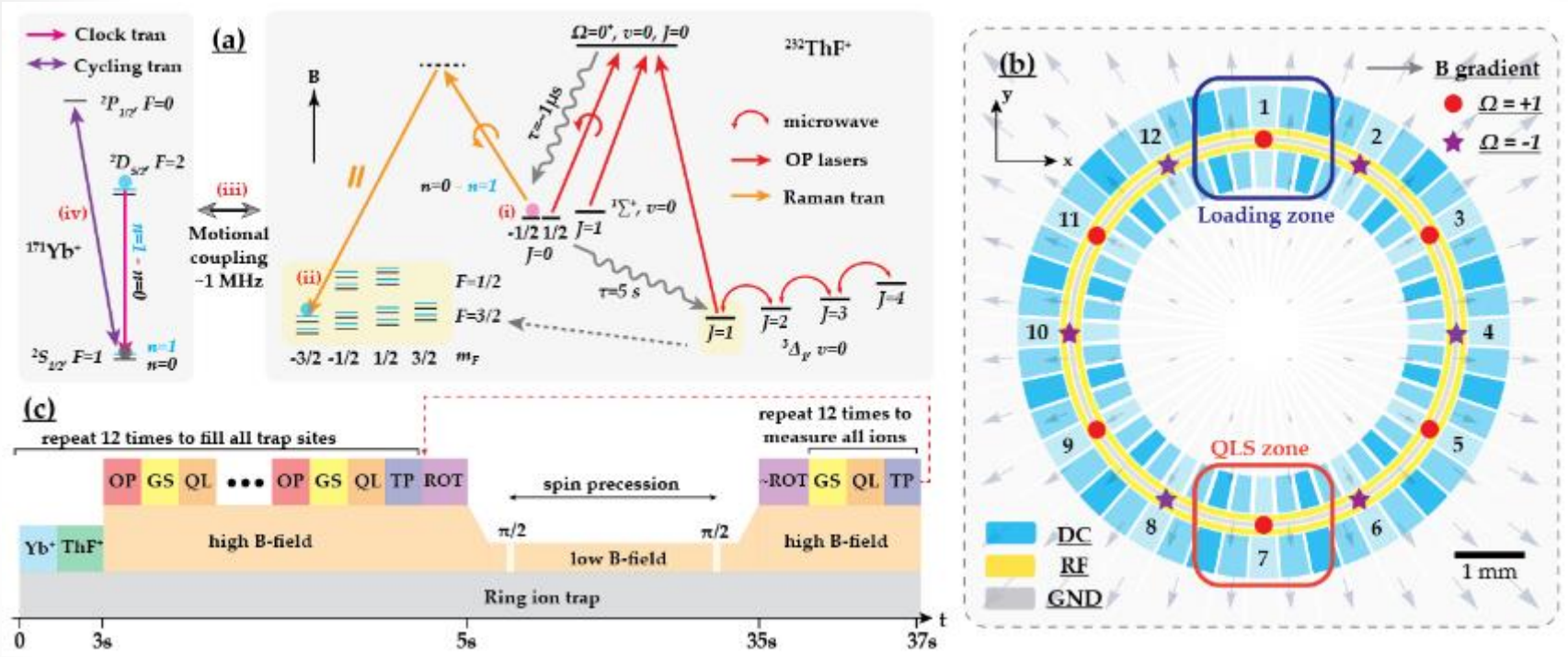
# Search for *T,P*-odd symmetry violation




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

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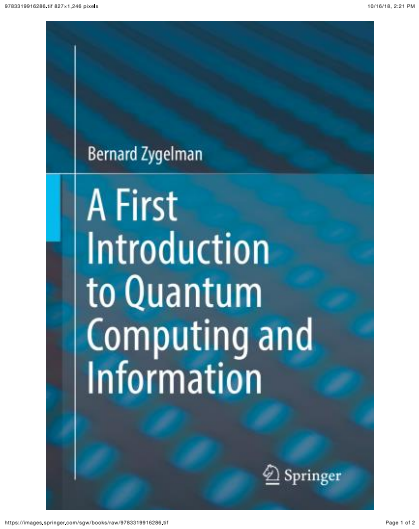
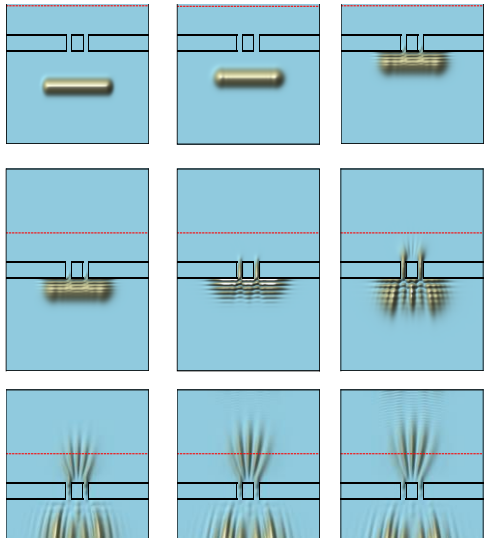
# Bernard Zygelman

- Quantum Computing and Information
- Computational Physics
- Atomic and Molecular Processes in Plasmas
- Quantum Workforce Development

# Research Expertise and Activities

- Over 70 publications, h-index 27-Google Scholar
- Work funded by AFOSR, DOE, IAEA, NSF, NASA, W. M. Keck Foundation
- Topics include remote sensing of the thermosphere, matter-anti-matter interactions, QED, radiative and non-radiative charge transfer in hot plasmas, atomic processes in the early universe, ultra-cold physics, geometric phase and magnetism, quantum computing and information

# Relevant Publications


1. B. Zygelman, *Appearance of gauge potentials in atomic collision physics*, Physics Letters A, 125, 476, 1987; (Re-printed in Geometric Phases in Physics ed. A. Shapere and F. Wilczek (Nobel laurate in Physics) ).

2. Sharma, R, Zygelman, von Esse, F., Dalgarno, A., Geophys. *On the relationship between the population of the fine structure levels of the ground electronic state of atomic oxygen and the translational temperature*, Geophysics Res. Lett., 21, 1731, 1994

3. Stancil, P. C. and Zygelman, B., *Kinematic Isotope Effects in Low Energy Electron Capture*, Phys. Rev. Lett. 75, 1495,1995

4. Zygelman, B. Saenz, A. Froelich, P. and Jonsell, S., *Cold collisions of atomic hydrogen with anti-hydrogen atoms: An optical potential approach*, Phys Rev A. 69, 042715, 2005

5. Zygelman, B. *Hyperfine Level–changing Collisions of Hydrogen Atoms and Tomography of the Dark Age Universe*, Ap. J, 622, 1356, 2005

6. Zygelman B. Lucic Z., and Hudson E., *Cold ion-atom chemistry driven by spontaneous radiative relaxation: a case study for the formation of the YbCa+molecular ion*, J. Phys. B 47, 015301, 2013

7. B. Zygelman, *Geometric-phase atom optics and interferometry*, Phys. Rev. A., 92, 043620, 2015

8. B. Zygelman, *A First Introduction to Quantum Computing and Information*, Springer-Nature, 2018.