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



Theoretical and Computational Condensed Matter and Materials Physics

Dr. Changfeng Chen

Department of Physics and Astronomy

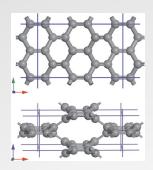
Phone: 702-895-4230

Email: chen@physics.unlv.edu

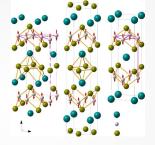
Expertise

- 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

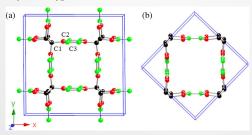




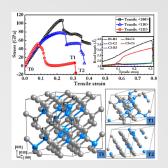
Nodal-ring Dirac semimetal states identified in bco-C₁₆ crystal [Wang, Weng, Nie, Fang, Kawazoe, Chen, *Phys. Rev. Lett.* 116, 195501 (2016)].



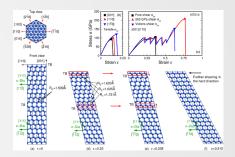
Magnetic Dirac materials CaMnBi₂ and SrMnBi₂ [Zhang, et al., *Nature Commun.* 7, 13833 (2016)].



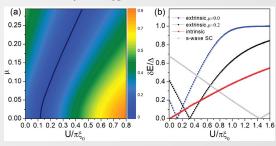
Nodal-net Dirac semimetal states in a graphene network structure [Wang, Nie, Weng, Kawazoe, Chen, *Phys. Rev. Lett.* 120, 026402 (2018)].



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



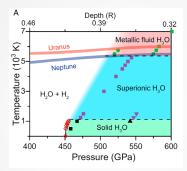
Extreme mechanics of nanotwinned diamond [Li, Sun, Chen, *Phys. Rev. Lett.* 117, 116103 (2016)].



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

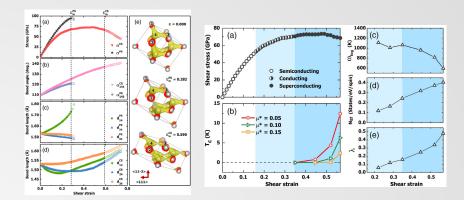


Helium-bearing compound FeO_2He predicted to stabilize at deep-Earth conditions [Zhang, et al., *Phys. Rev. Lett.* 121, 255703 (2018)].



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 CaO₃ 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)].

<u>Further Reading (selected papers by Chen Group, 2015-2020)</u>

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.* <u>116</u>, 087401 (2016).

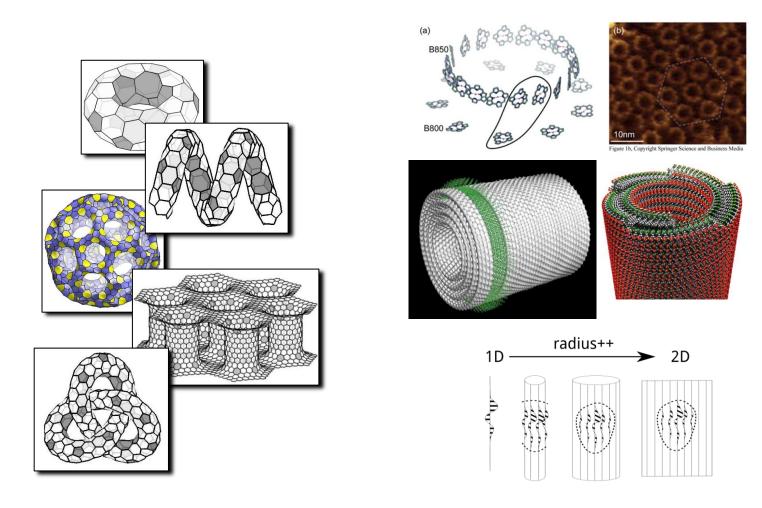
Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides, Lu, Li, Ma, Chen, *Phys. Rev. Lett.* 119, 115503 (2017).

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).

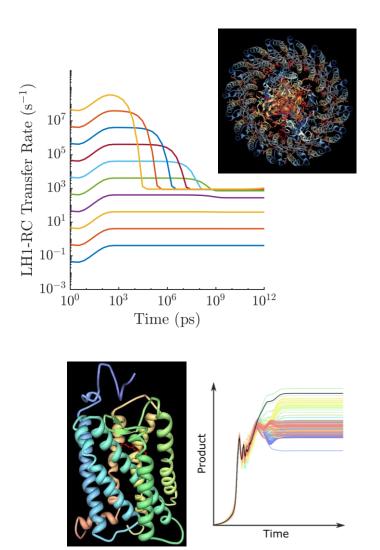
Theoretical chemical physics

- 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



Photophysics of organic materials



Photochemistry under environmental control

Exotic low-dimensional materials

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

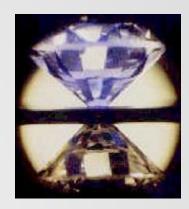


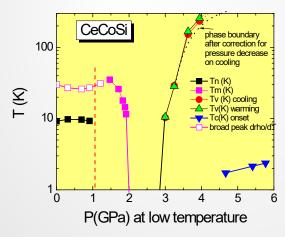
Superconductivity



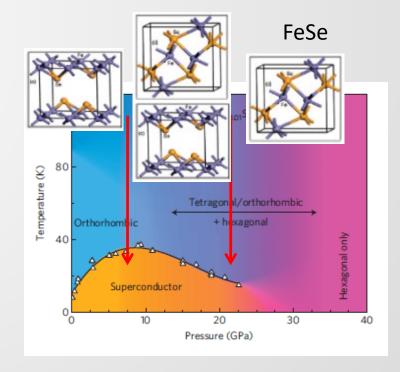
Quantum Design PPMS at UNLV

- 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)

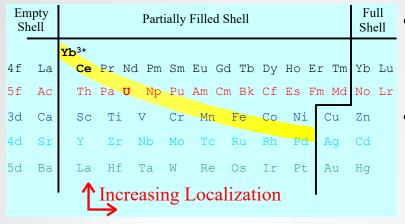




Addition of high pressure synchrotron experiments (diffraction and X-ray absorption) allows mapping of complex superconducting phase diagrams

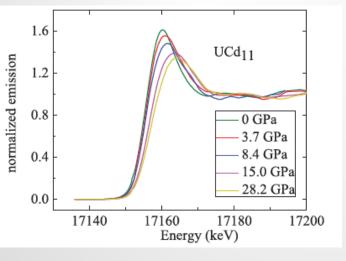


Correlated-Electron Systems

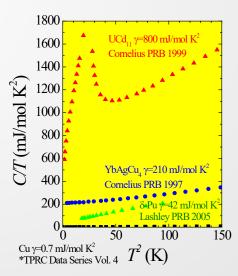


Modified periodic table

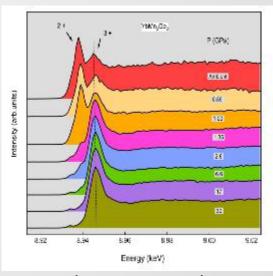
- Going from localized to delocalized electrons one often finds strong electron-electron correlations
- Correlated electron systems can yield interesting behavior: fluctuating valence, superconductivity, non-Fermi liquid, heavy fermion and many more



f-electron delocalization X-ray absorption



Heavy fermions
Heat Capacity



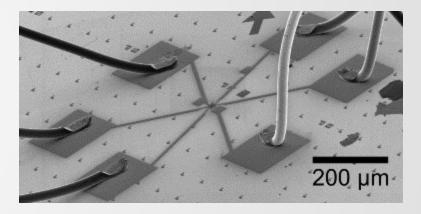
Fluctuating valence X-ray fluorescence



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



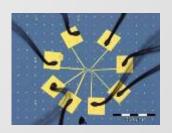










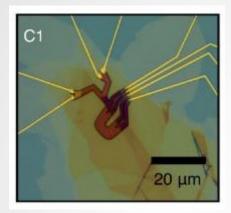


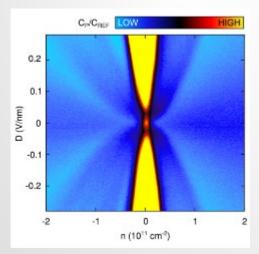


Island - Quantum computing, quantum sensing

Quantum computing:

Topological phases for faulttolerant, universal quantum computing.

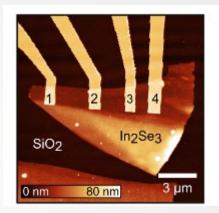


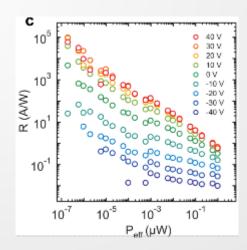


Island, J. O., et al. Nature 571 (2019): 85–89.

Industry-disruptive
photodetectors: Ultra-sensitive
phototransistors designed with

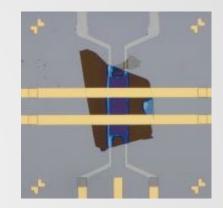
2D materials and heterostructures.

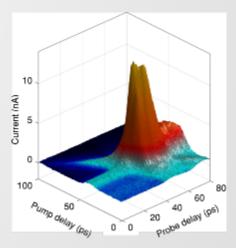




Island, J. O., et al. Nano Letters 15 (2015): 7853-7858.

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 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

- Dr. Tao Pang
- Professor of Physics
- Department of Physics and Astronomy
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- Website: physics.unlv.edu/~pang/



Expertise

- Theoretical and computational studies of novel materials, such as cold atoms and molecules, superconductors and superfluids, and other highly correlated systems.
- Path-integral and diffusion quantum Monte Carlo simulations and other first-principles calculations.
- Functional variation, correlated-basis, mean-field, and other analytical approaches.



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.

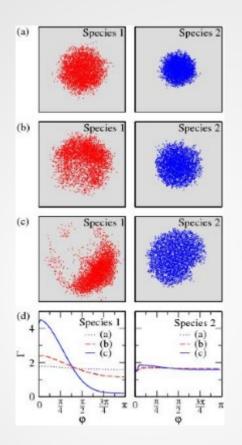
Diffusion Quantum Monte Carlo Simulation

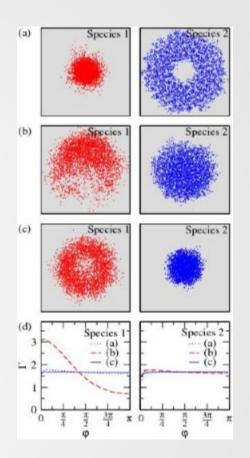
Negative donor centers in semiconductors; hydrogen molecules in confinement; ionic hydrogen clusters; and helium clusters with modified interactions.

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

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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

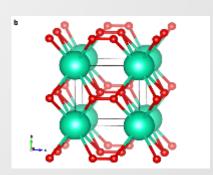


B. Novel materials synthesis C. New Physics/Chemistry C. New Physics/Chemistry Control of the control of the

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

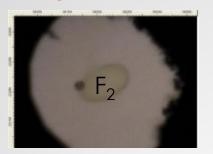
Useful hard x-ray photochemistry

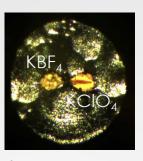




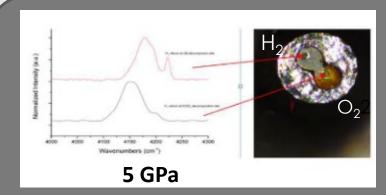
Novel structures of known materials produced With hard x-rays and high pressure (e.g. CsO₂)

High Pressure Fluorine Chemistry

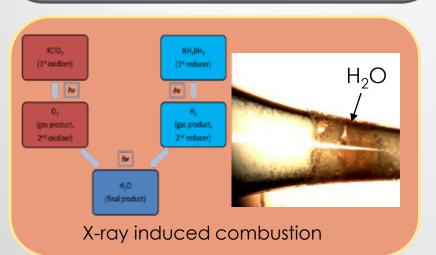


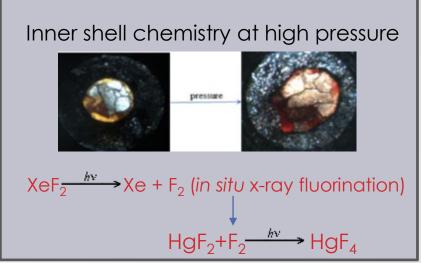


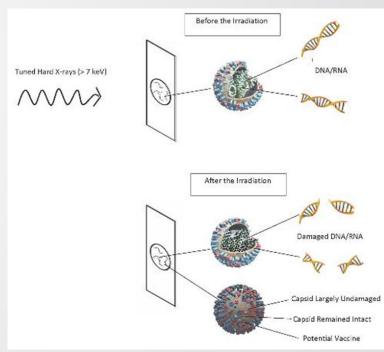
 $2F_2 + O_2 \rightarrow 2OF_2 @ 3 GPa$



Molecular mixtures at high pressure



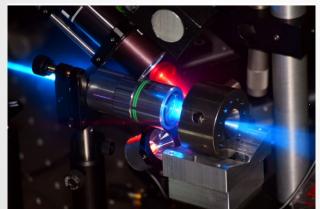




Using tuned hard x-rays to damage viruses to create high quality vaccines by targeting specific molecular groups/bonds that resonantly absorb x-ray energy leading to decomposition chemistry.

Salamat Group – Collaboration with MSTS





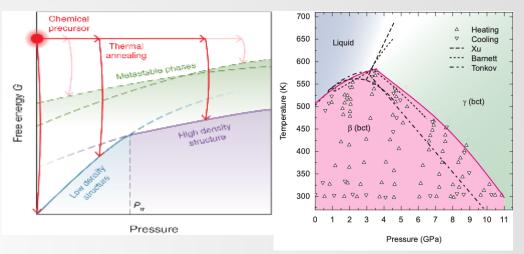




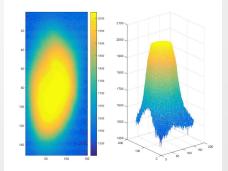




Metrology – accurate mapping of P, V, T



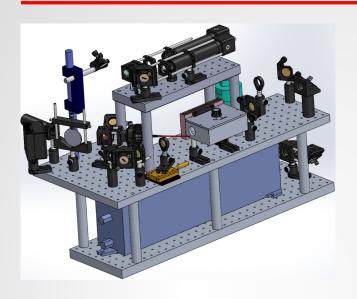
High temperature modelling – understanding emissivity under extreme conditions



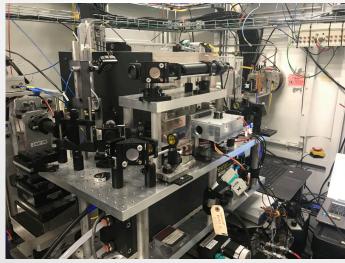


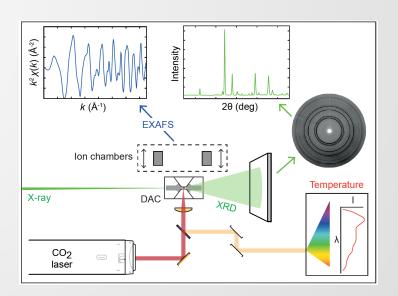


Warm dense matter – probed using EXAFS



- Development of a CO₂ 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: La₂Sn₂O₇ 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 CaCO₃ 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 CO₂ 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)



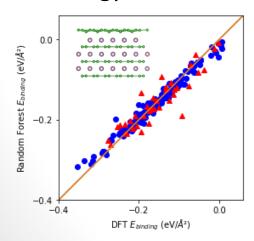
Computational Materials Science

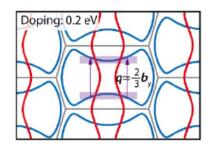
- Dr. Luqing Wang
- Assistant Professor Physics
- Department of Physics and Astronomy
- Email: luqing.wang@unlv.edu
- Office: BPB 232



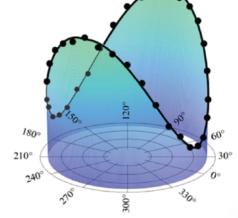
Expertise

- 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 Electronic and Quantum



2D Electro-Mechanics



Zhou Lab – Experimental AMO physics

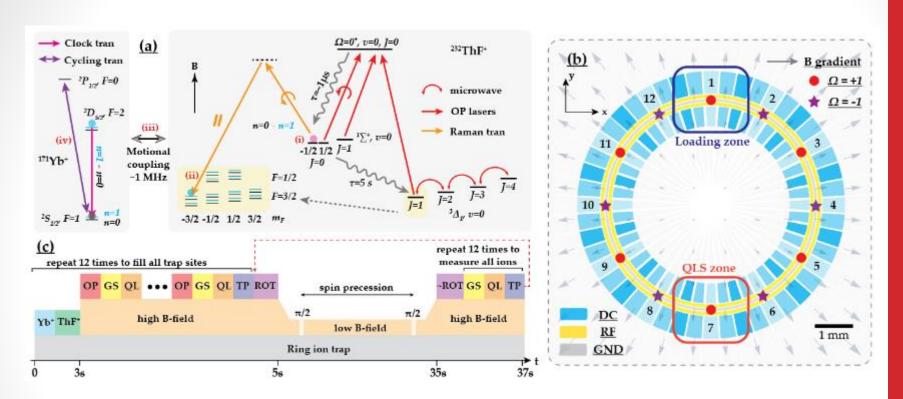
- Dr. Yan Zhou
- Assistant Professor
- Department of Physics and Astronomy
- Email: yan.zhou@unlv.edu
- Website: https://www.physics.unlv.edu/~yanzhou/index.html

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



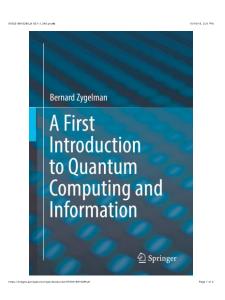
- On-chip Quantum sensors
- Entanglement between atomic ions and molecular ions
- Scalability and multiplexing measurements
- New table-top platform to investigate nuclear physics

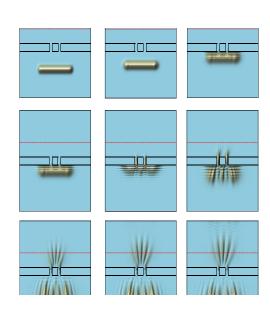


Bernard Zygelman

- 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 nonradiative 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+molecularion*, 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.