

New Materials and Applications

Advanced Materials:
Development & Analysis Research

Theoretical and Computational Condensed Matter and Materials Physics

Dr. Changfeng Chen

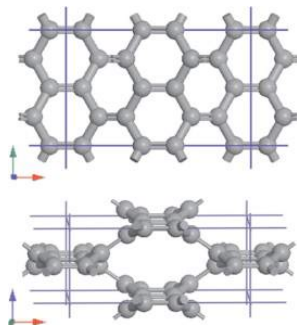
Department of Physics and Astronomy

Phone: 702-895-4230

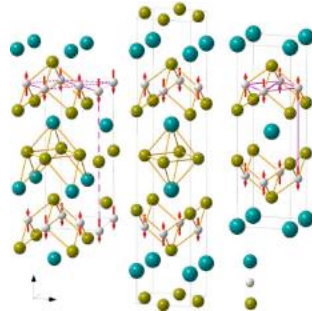
Email: chen@physics.unlv.edu

Expertise

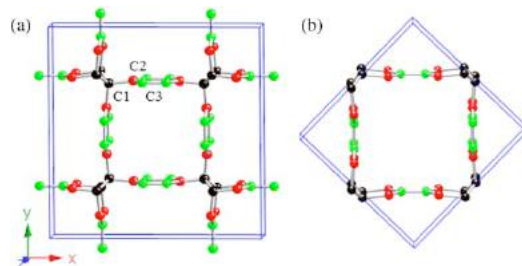
- Novel states of matter: topological insulators and semimetals
- Superior bonding structures: superhard and supertough materials
- Intriguing quantum phenomena: superconductivity and magnetism
- Extreme mechanics: stress responses to complex large strains
- Ultimate thermodynamics: materials inside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



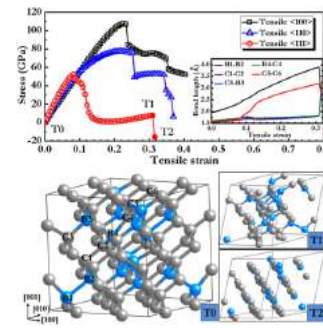
Nodal-ring Dirac semimetal states identified in bco-C₁₆ crystal [Wang, Weng, Nie, Fang, Kawazoe, Chen, **Phys. Rev. Lett.** 116, 195501 (2016)].



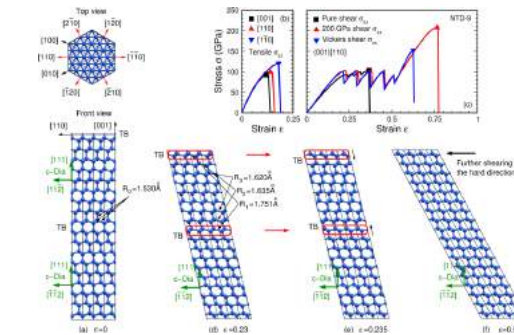
Magnetic Dirac materials CaMnBi₂ and SrMnBi₂ [Zhang, et al., **Nature Commun.** 7, 13833 (2016)].



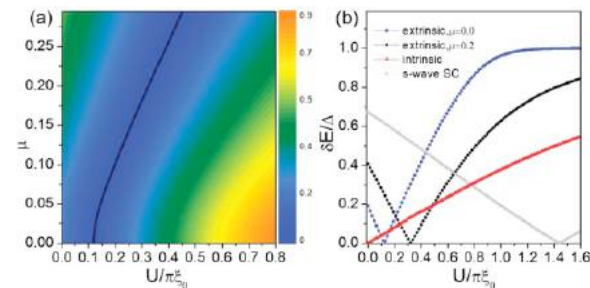
Nodal-net Dirac semimetal states in a graphene network structure [Wang, Nie, Weng, Kawazoe, Chen, **Phys. Rev. Lett.** 120, 026402 (2018)].



Superhard B₃C in diamond structure [Zhang, et al., **Phys. Rev. Lett.** 114, 015502 (2015)].



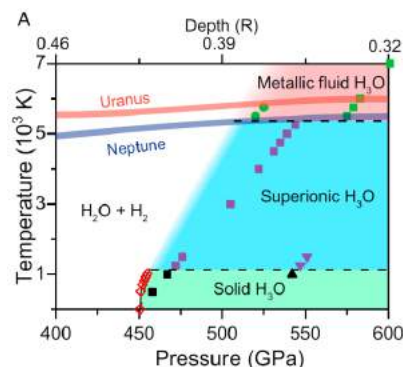
Extreme mechanics of nanotwinned diamond [Li, Sun, Chen, **Phys. Rev. Lett.** 117, 116103 (2016)].



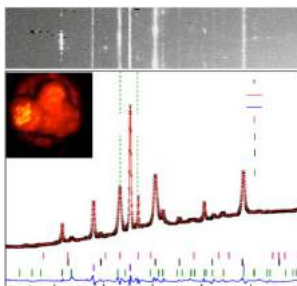
Kondo physics in 2D topological superconductors [Wang, et al., **Phys. Rev. Lett.** 122, 087001 (2019)].



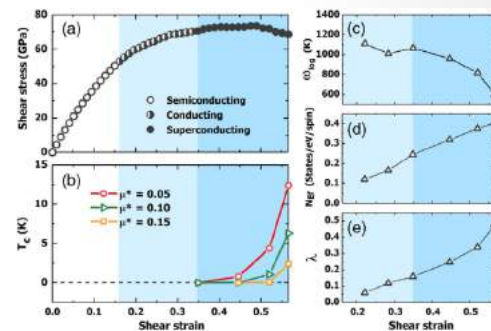
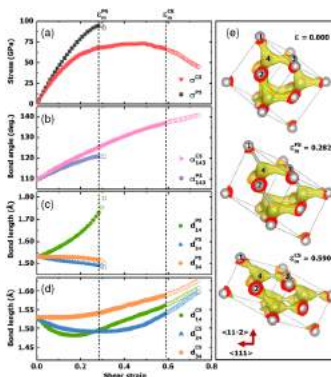
Helium-bearing compound FeO_2He predicted to stabilize at deep-Earth conditions [Zhang, et al., *Phys. Rev. Lett.* **121**, 255703 (2018)].



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 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).

Electronic and Magnetic Properties at High Pressure

Dr. Andrew Cornelius

Department of Physics & Astronomy

Phone (702) 895-1727

Expertise:

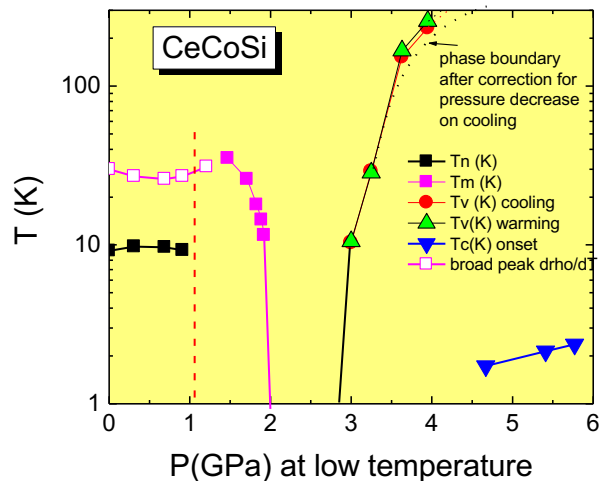
- Experimental high pressure measurements
- Magnetism
- Superconductivity

Superconductivity

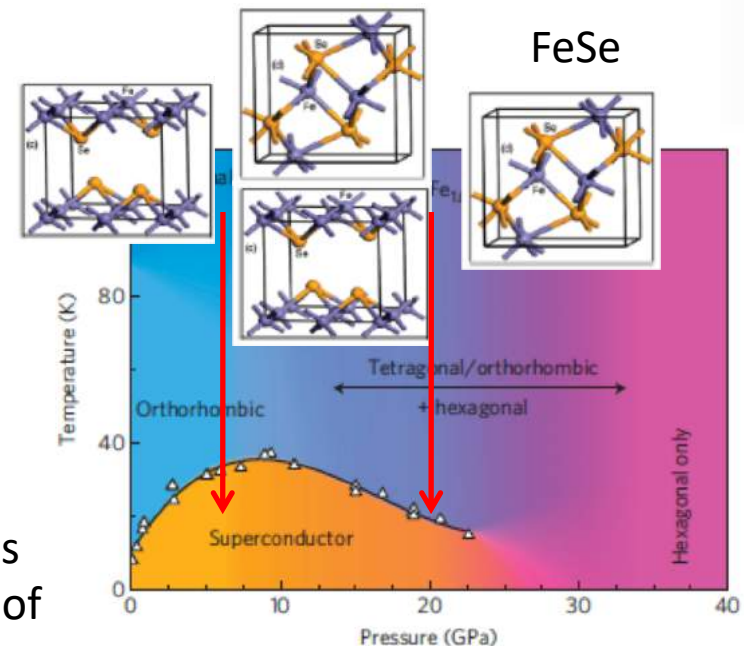


Quantum Design PPMS at UNLV

- 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

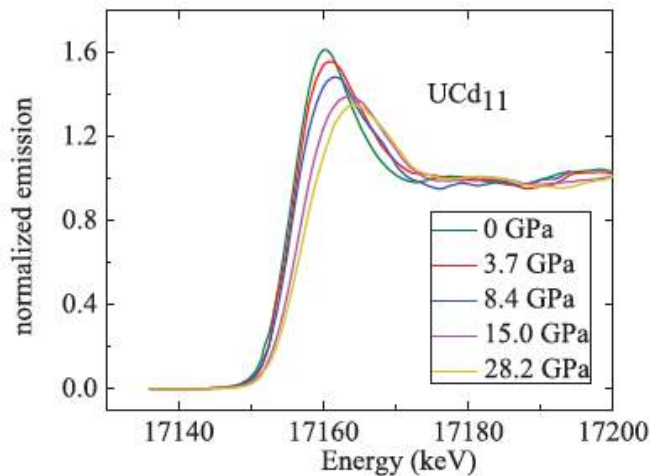
Modified periodic table

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						

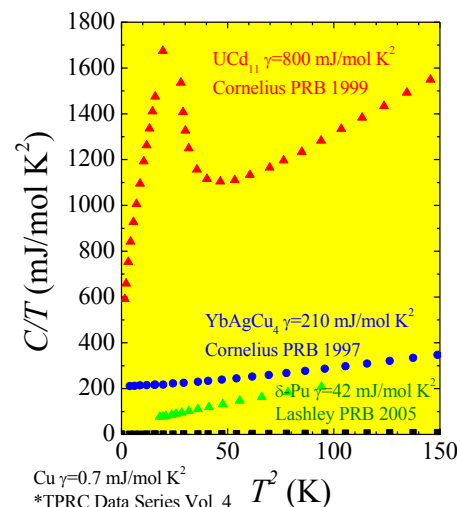
Yb³⁺

Increasing Localization

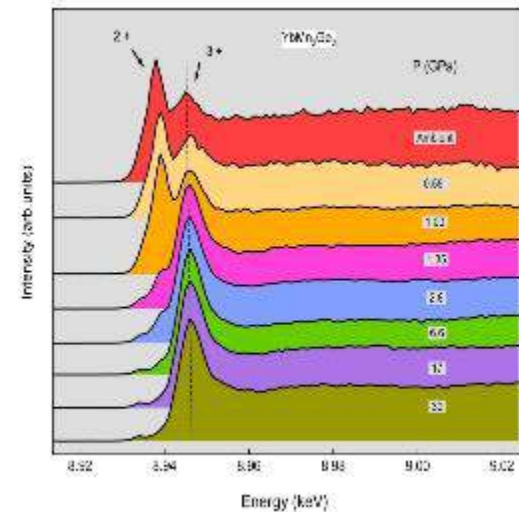
- Going from localized to delocalized electrons one often finds strong electron-electron correlations
- Correlated electron systems can yield interesting behavior: fluctuating valence, superconductivity, non-Fermi liquid, heavy fermion and many more



f-electron delocalization
X-ray absorption



Heavy fermions
Heat Capacity



Fluctuating valence
X-ray fluorescence

Surface and Interface Characterization of Materials for Energy Conversion

Dr. Clemens Heske

Professor

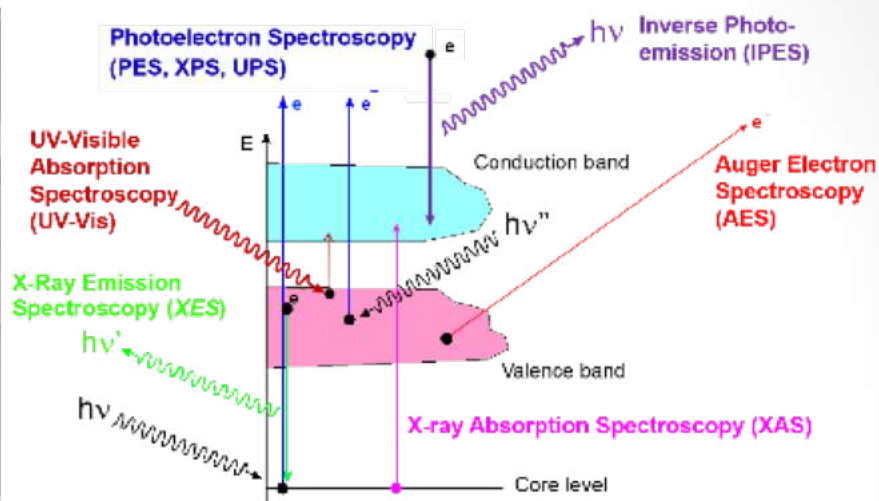
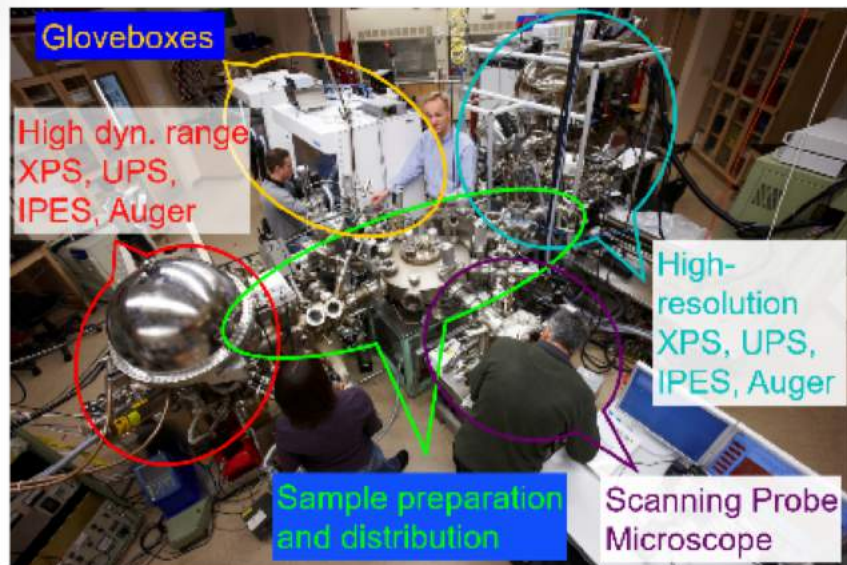
Department of Chemistry and Biochemistry

heske@unlv.nevada.edu

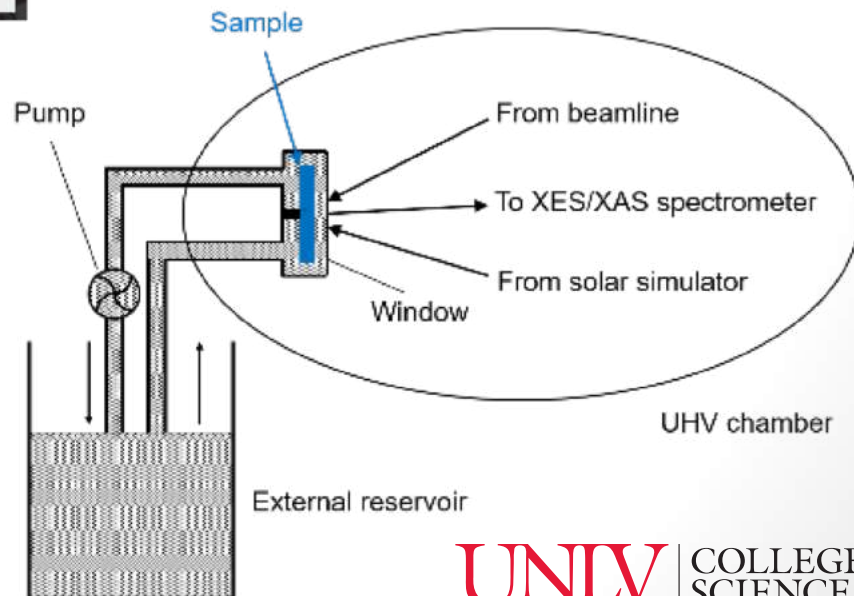
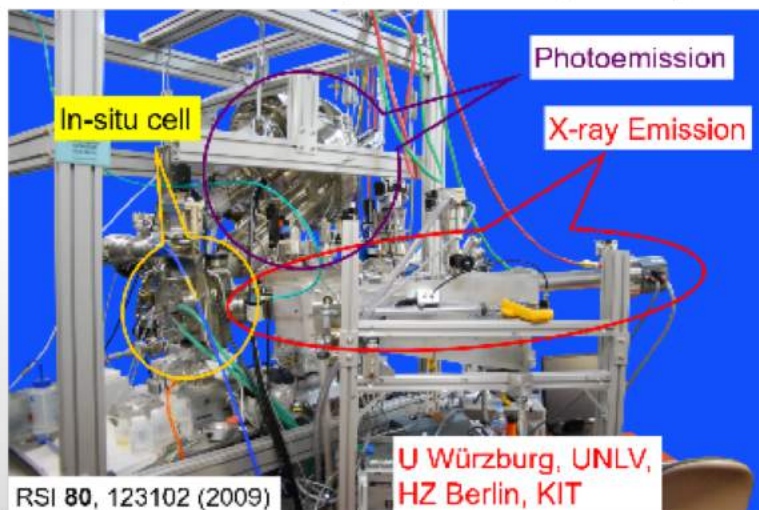
Expertise

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

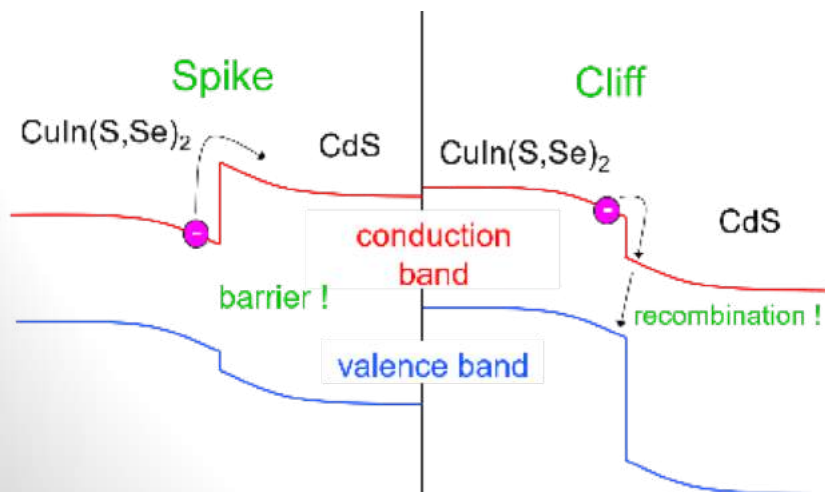
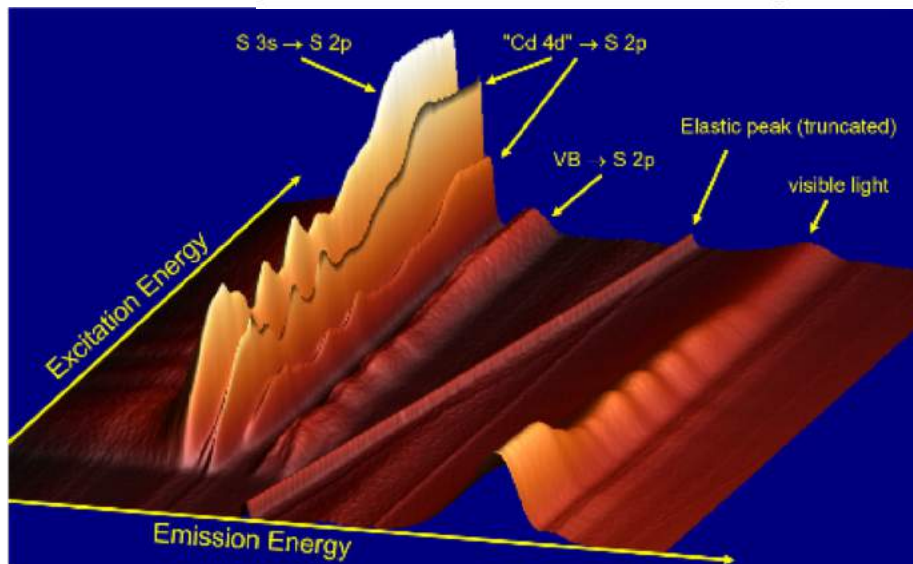
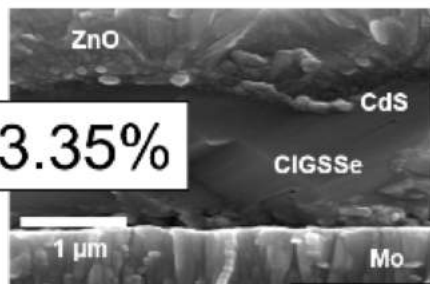
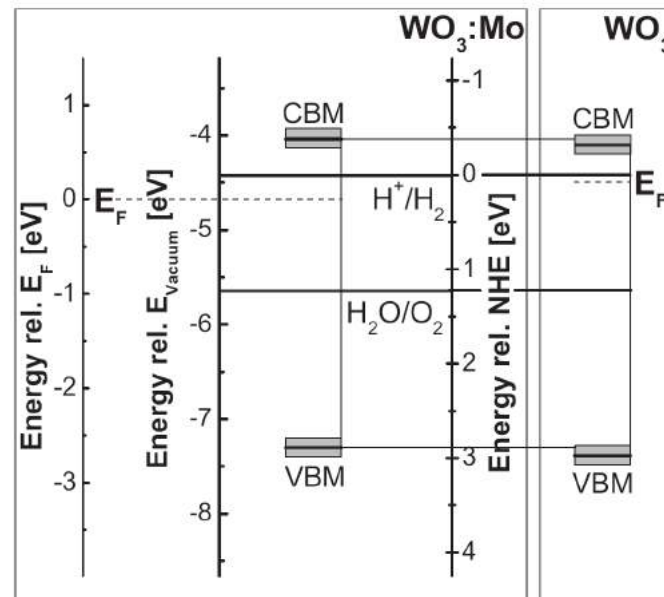
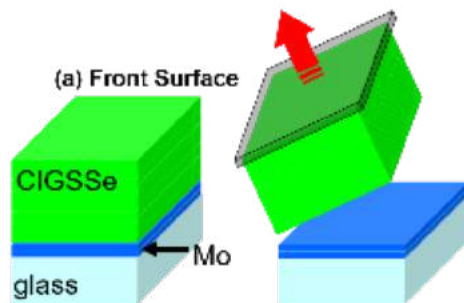
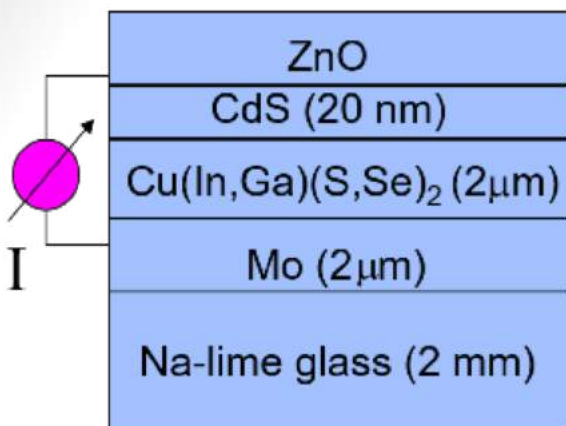
Surface and Interface Characterization



SALSA: Solid And Liquid Spectroscopic Analysis



Materials for Energy Conversion

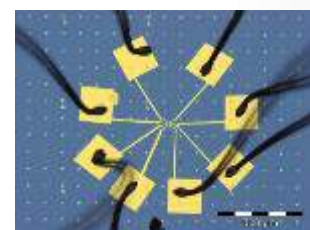
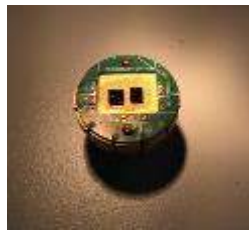
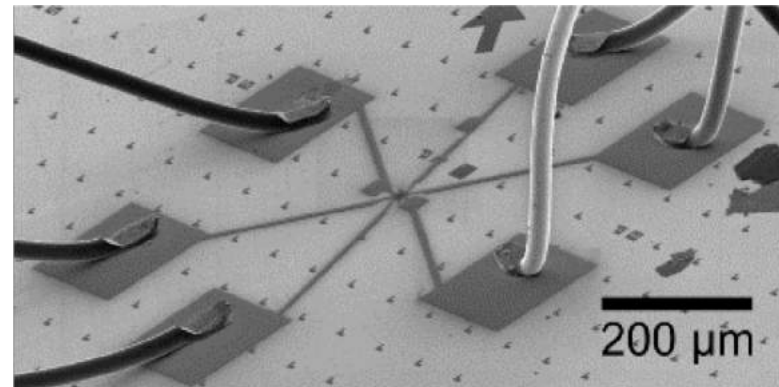


Island – Quantum computing, quantum sensing



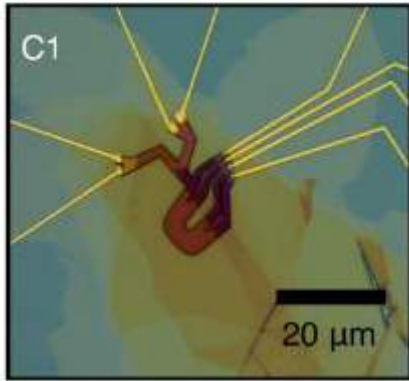
Areas of Research

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

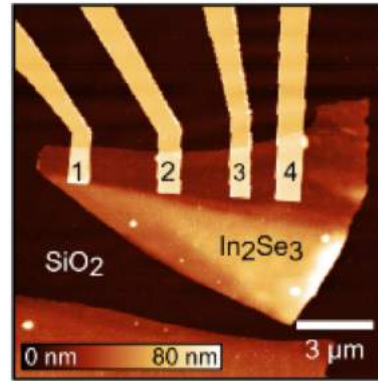


Island – Quantum computing, quantum sensing

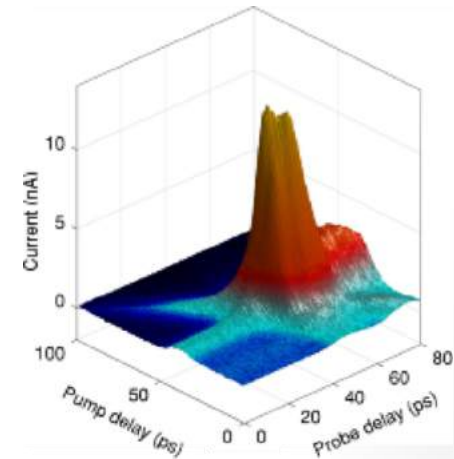
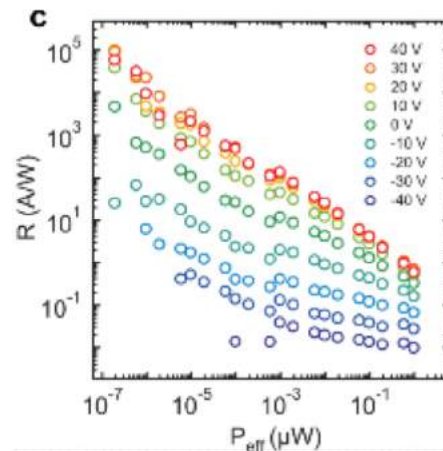
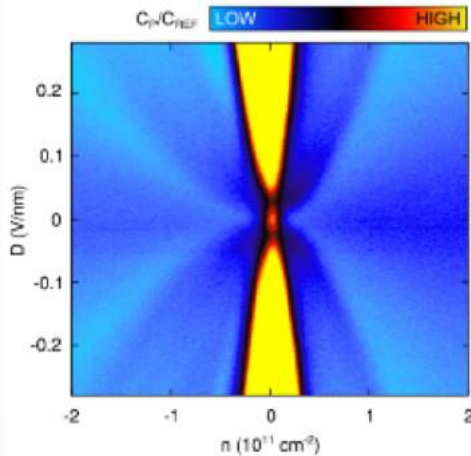
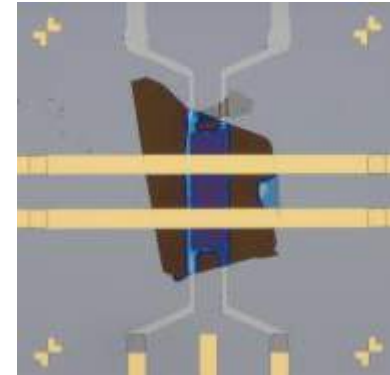
Quantum computing:
Topological phases for fault-tolerant, universal quantum computing.



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 – 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. Navarro-Moratalla*, J. O. Island*, S. Manas-Valero, E. Pinilla-Cienfuegos, A. Castellanos- Gomez, J. Quereda, G. Rubio-Bollinger, L. Chirulli, J. A. Silva-Guillin, 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)



TiS₃ 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 In₂Se₃ 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.H. Diependaal, H.S.J. van der Zant, T. Heine, and A. Castellanos- Gomez, *Nanoscale* **8**, 2589 (2016). (arXiv)



Scientific Computing and Mathematical Modeling

Dr. Jichun Li

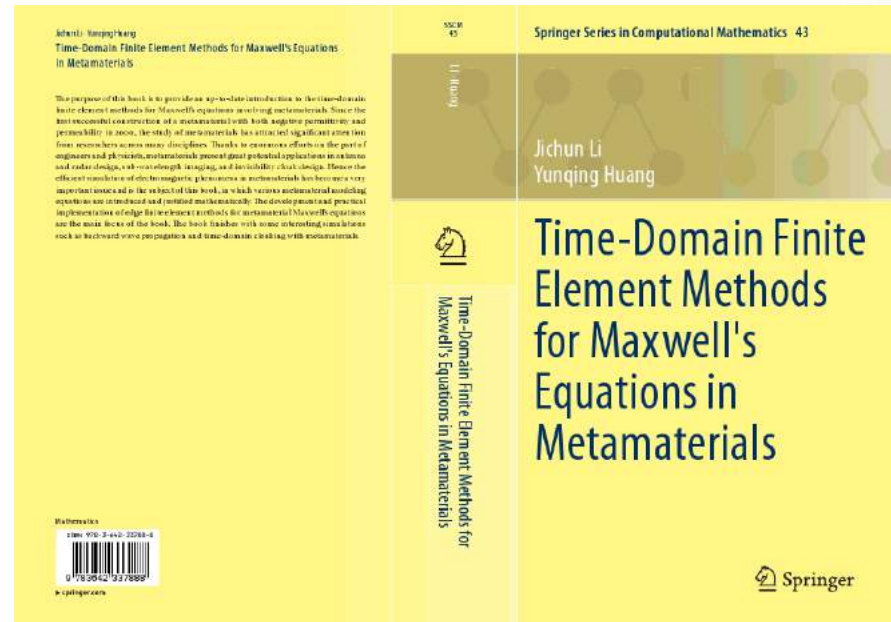
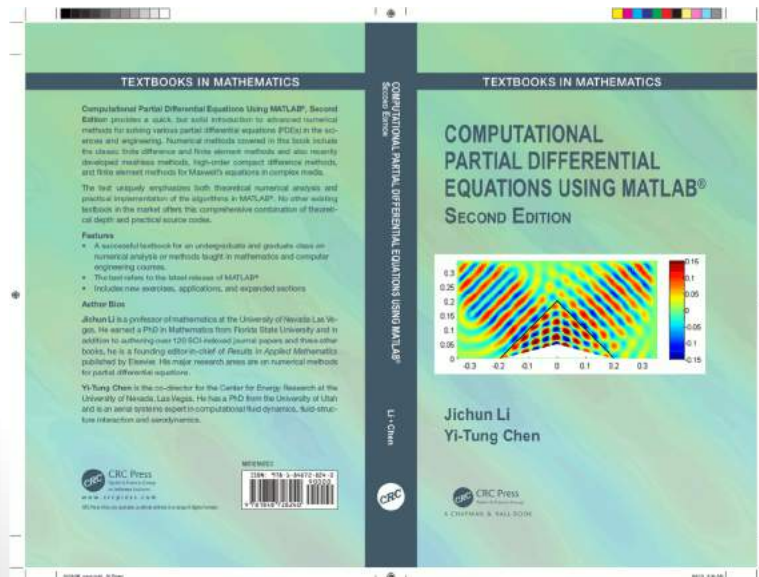
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Expertise:

Computational Electromagnetics
Numerical Methods for PDEs
Mathematical Modeling



Jichun Li et al (Mathematical modeling and analysis of optical black hole with metamaterials): Computer Methods in Applied Mechanics and Engineering 204 (2016) 501-520.

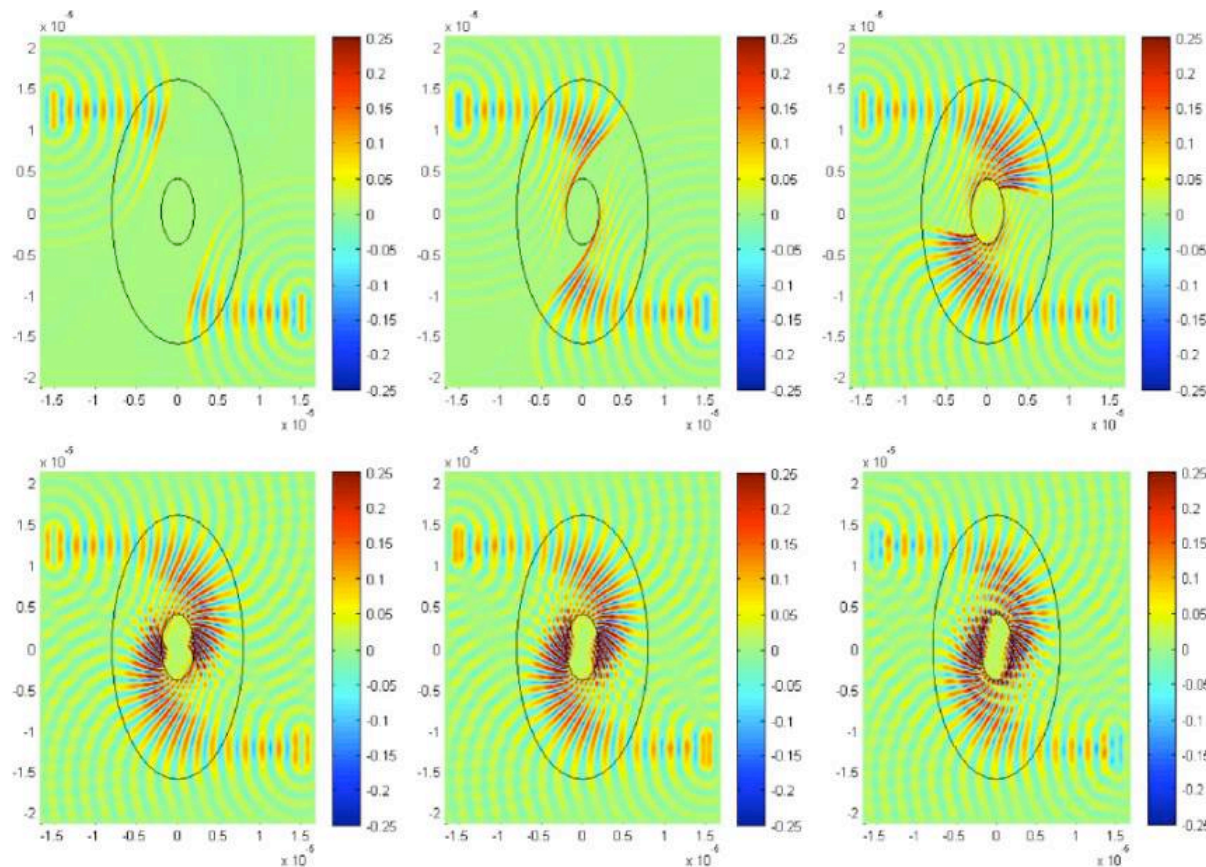
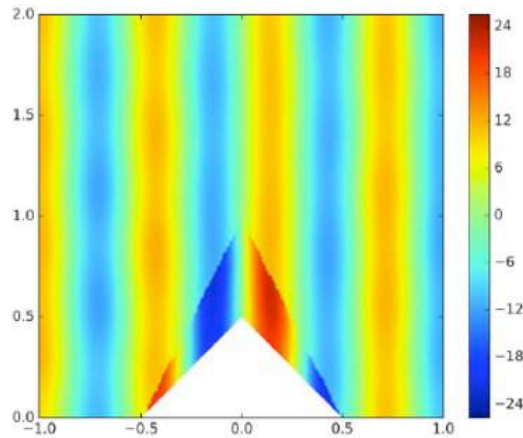
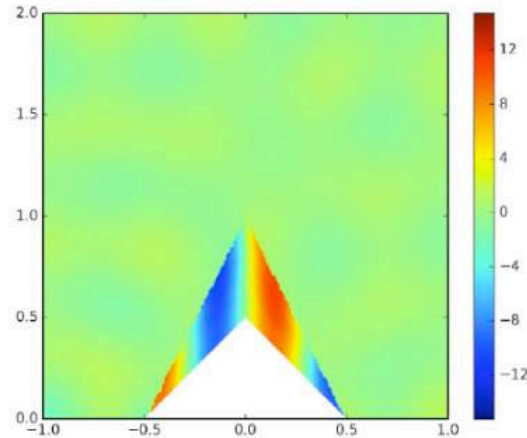


Fig. 4.5. Example 2. Magnetic fields H_z at various time steps for the elliptical OBHs simulation. Top left: 1600 steps. Top middle: 2400 steps. Top right: 3600 steps. Bottom left: 4800 steps. Bottom middle: 5200 steps. Bottom right: 8000 steps.

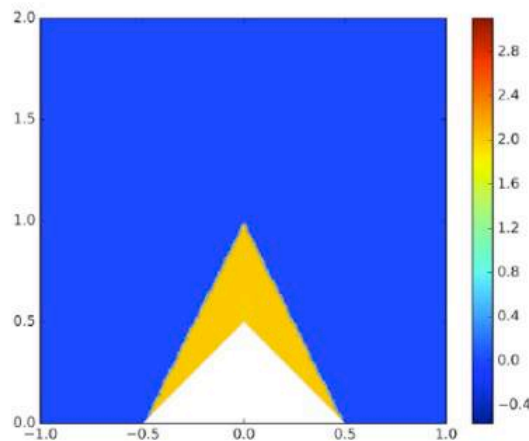
Jichun Li et al (Optimal control for electromagnetic cloaking metamaterial design): Computer and Mathematics with Applications 79 (2020) 1165-1176.



(a) $\nabla_h \times E_h$

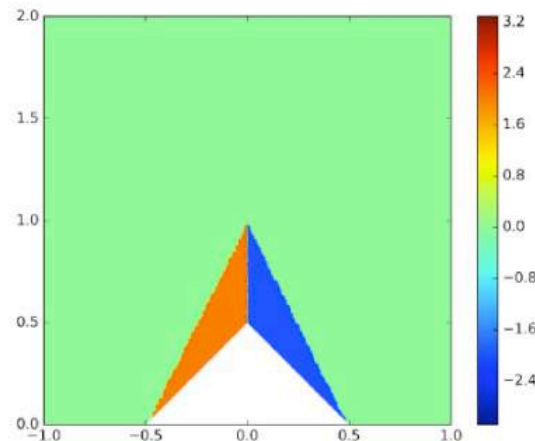


(b) $\nabla_h \times (E_h - E_w)$



(c) Optimized ϵ_1 , exact $\epsilon_1 = 2$

$\min \epsilon_1 = 2.00617032$ and $\max \epsilon_1 = 2.00996683$



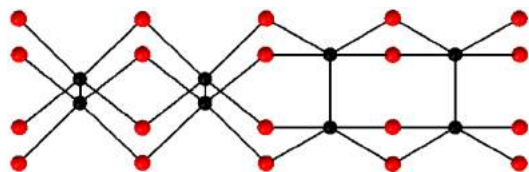
(d) Optimized ϵ_2 , exact $\epsilon_2 = -2 \cdot \text{sgn}(x)$

$\min \epsilon_2 = -2.00261751$ and $\max \epsilon_2 = 2.02687675$

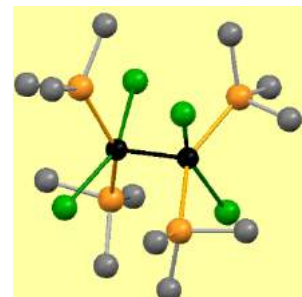
→ Synthetic and coordination chemistry

Technetium binary and ternary halide compounds

Compounds with multiple metal-metal bonds



TcCl_2 : a unique structure-type



$\text{Tc}_2\text{Cl}_4(\text{PMe}_3)_4$

→ 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

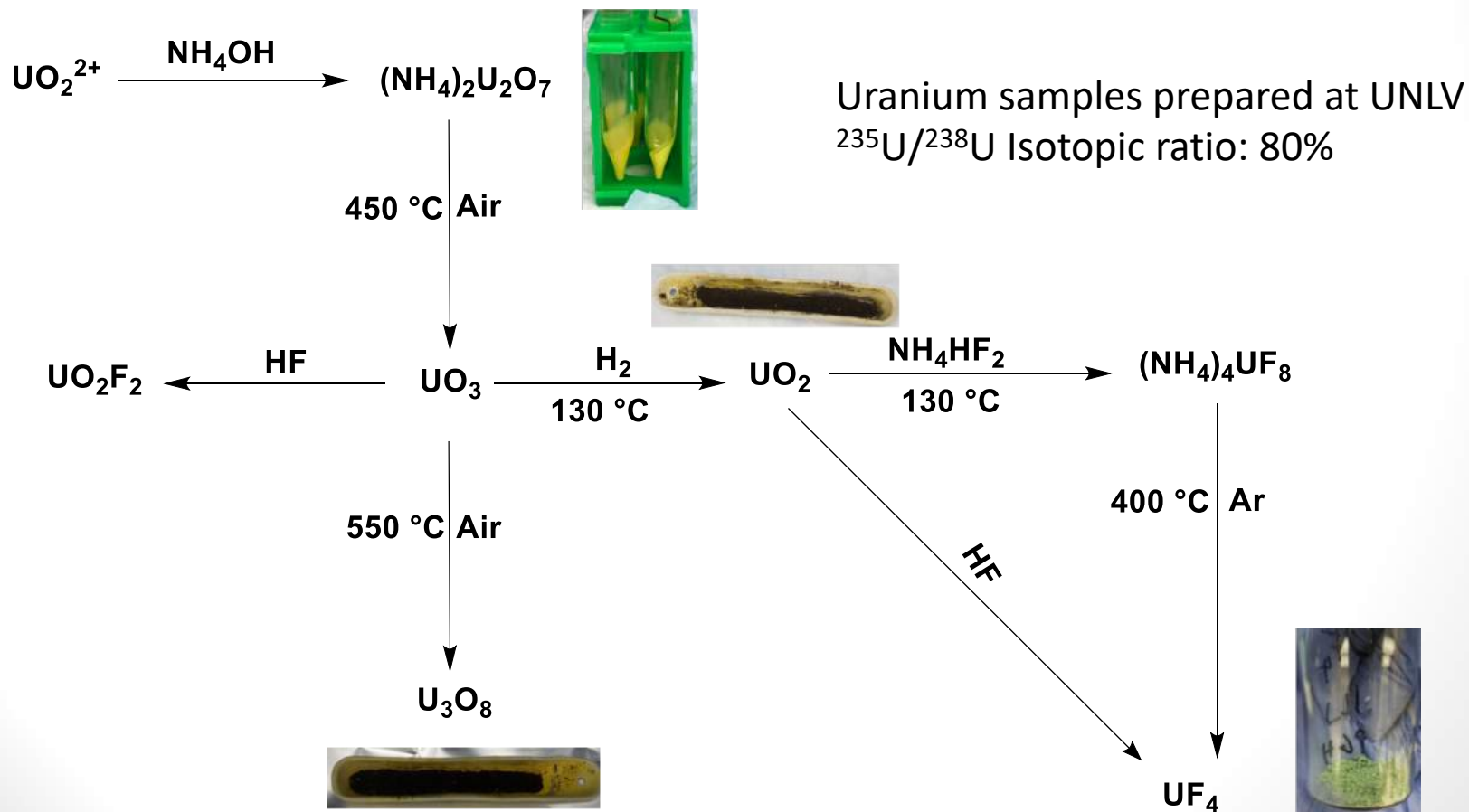


Preparation of U-Tc alloys by arc melting

→ Collaborative work relevant to nuclear forensics

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

- Uranium compounds found throughout the fuel cycle (UO_2 , U_3O_8 , UF_4) prepared at UNLV
- $^{235}\text{U}/^{238}\text{U}$ isotopic ratio measurements using TIMS at LANL



Novel Chemistry Using Highly Ionizing Radiation

Michael Pravica, Ph.D.

Professor of Physics

Department of Physics and Astronomy

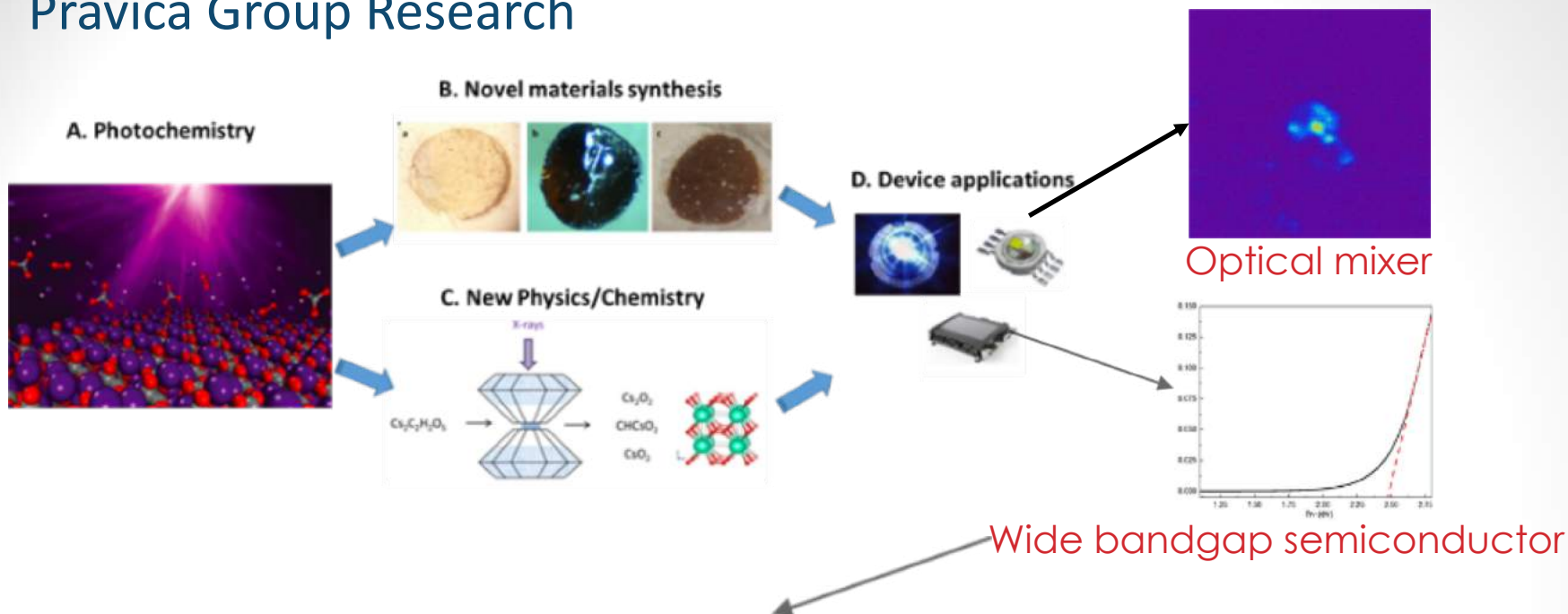
Phone: (702)895-1723

Email: michael.Pravica@unlv.edu

Expertise:

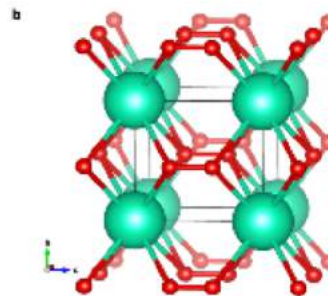
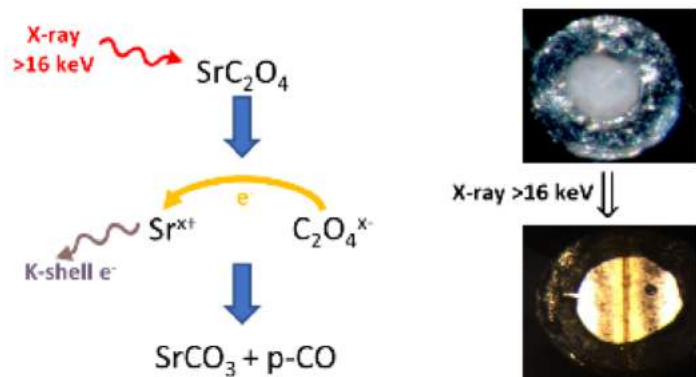
- *Useful Hard X-ray photochemistry*
- High pressure
- Spectroscopy
- *Ion Beam Nuclear Transmutation Doping*

Pravica Group Research



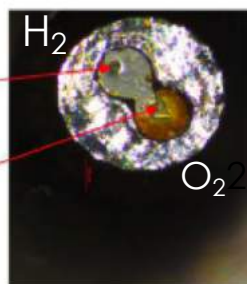
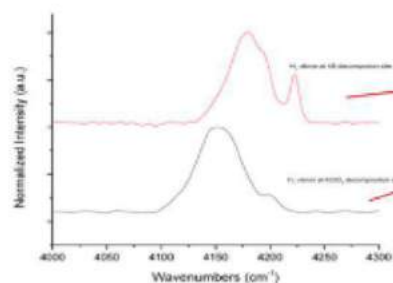
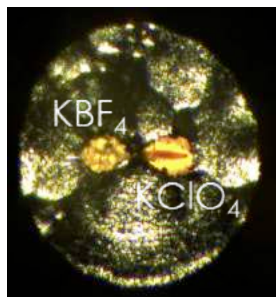
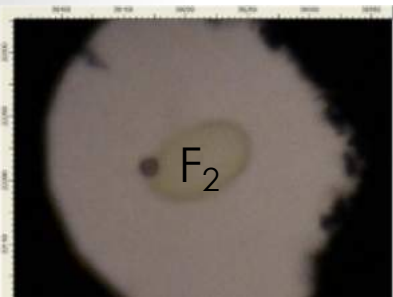
Radiation-hardened sensors/direct energy conversion devices for EXTREME CONDITIONS or tuned solar materials

Useful hard x-ray photochemistry



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

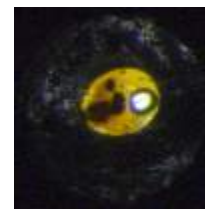
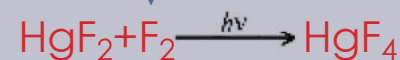
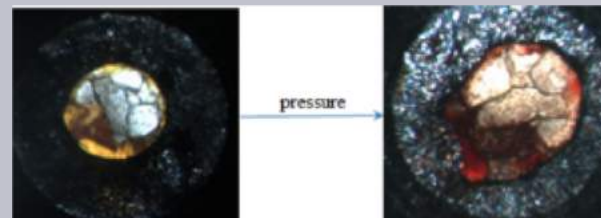
High Pressure Fluorine Chemistry



5 GPa

Molecular mixtures at high pressure

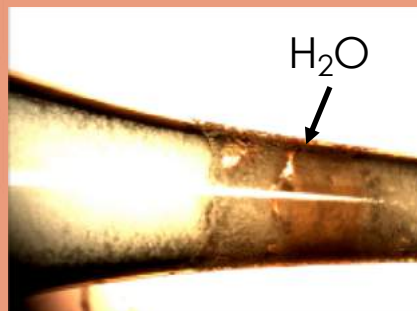
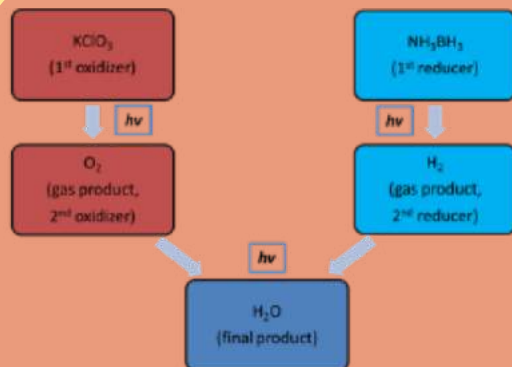
Inner shell chemistry at high pressure



UV-irradiation
produced N₂
bubble



UV irradiation facility



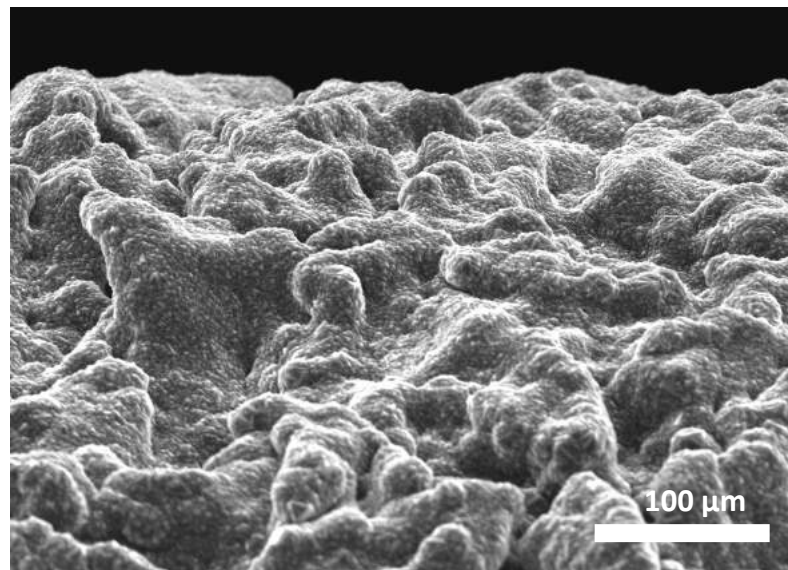
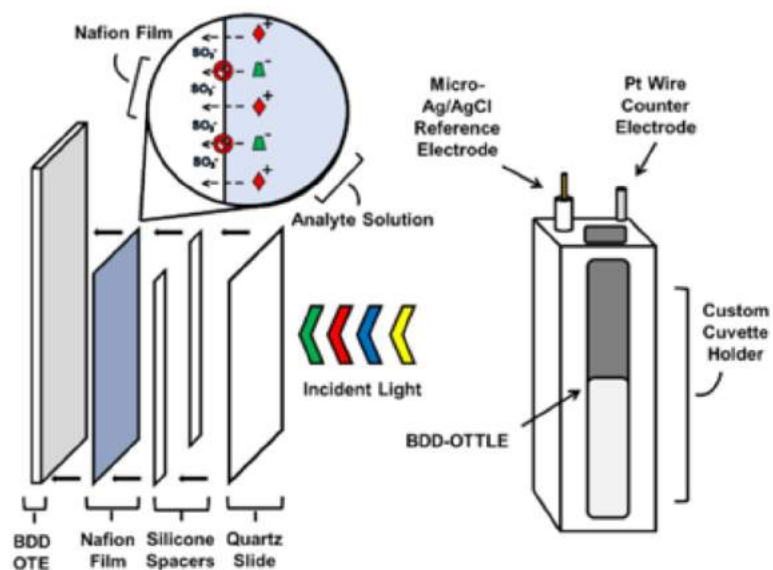
X-ray induced combustion



Large Volume Press
For pressure-induced chemistry

Electrochemistry and Spectroelectrochemistry in molten salts for the development of the molten salt nuclear reactor

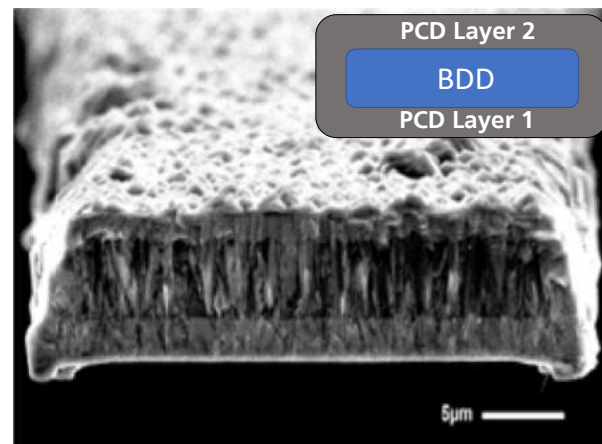
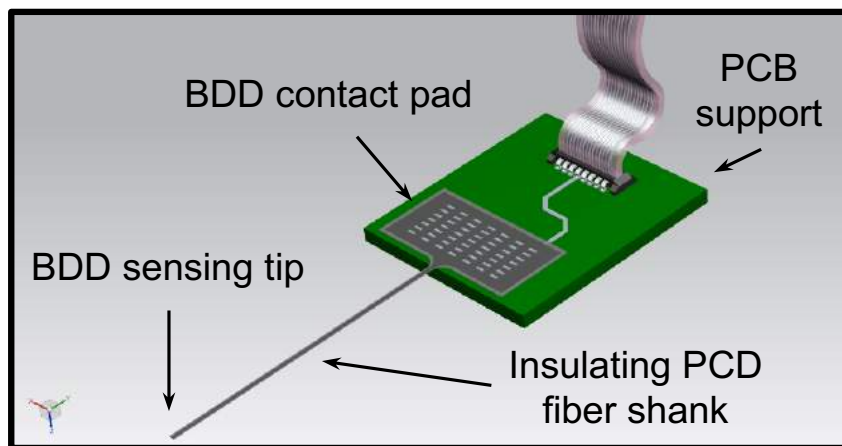
- Fundamental redox and thermodynamic properties of nuclear fuel can be gained using electrochemistry and spectroelectrochemistry.
- Diamond electrodes are specifically amenable to use as the sensing material due to its robustness and tunable properties



SEM image of diamond film

Detection of clinically- and environmentally-relevant analytes with electrochemical sensors

- The all-diamond microfiber electrodes are a supremely biocompatible electrode. With the advantageous properties of diamond electrodes, the suite of potential analytes is expanded.
- The conductive BDD core is covered along the shank with undoped diamond, thereby making the device non-reactive.
- The batch-fabricated nature of these devices make them attractive compared to others.



Publication track record

“Polymer-coated Boron Doped Diamond Optically Transparent Electrodes for Spectroelectrochemistry” C.A Rusinek, M. Becker, R. Rechenberg, D. Zhao, K. Ojo, N. Kaval, and W.R. Heineman. *Electroanalysis*, 2016, 28, 2228-2236.

“Fabrication and characterization of boron doped diamond microelectrode arrays of varied geometry” C.A Rusinek, M. F. Becker, R. Rechenberg, T. Schuelke, *Electrochemistry Communications*, 2016, 73, 10-14

“Large-scale, All Polycrystalline Diamond Structures Transferred on Flexible Parylene-C Films for Neurotransmitter Sensing” B. Fan, Y. Zhu, R. Rechenberg, C.A Rusinek, M.F. Becker, W. Li, *Lab-on-a-Chip*, 2017, 17, 3159-3167.

“Isatin Detection using an All Boron-doped Diamond 3-in-1 Sensing Platform” M. Ensich, V.Y. Maldonado, G. M. Swain, R. Rechenberg, M.F. Becker, T. Schuelke, C.A Rusinek, *Analytical Chemistry*, 2018, 90, 1951-1958.

“Analysis of Ag(I) Biocide in Water Samples using Anodic Stripping Voltammetry with a Boron-doped Diamond Disk Electrode” V.Y. Maldonado, P.J. Espinoza, C.A Rusinek, G.M. Swain, *Analytical Chemistry*, 2018, 90 (11), 6477–6485.

“All Diamond Microfiber Electrodes for Neuroelectrochemistry” C.A Rusinek, Y. Guo, R. Rechenberg, E. Purcell, C. McKinney, M.F Becker, W. Li, *Journal of the Electrochemical Society*, 2018, 165 (12), G3087-G3092.

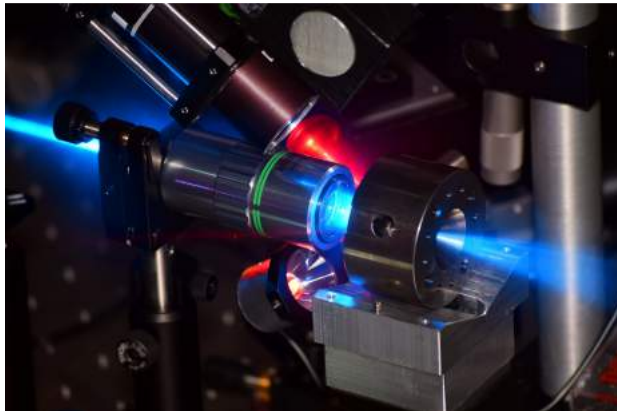
“Indium Tin Oxide Film Characteristics for Cathodic Stripping Voltammetry” M. Ensich, B. Wehring, G.D Landis, M.F Becker, T. Schuelke, C.A Rusinek, *ACS Applied Materials and Interfaces*, 2019, 11 (18), 16991-17000.

“Determination of Lead with a Copper-Based Electrochemical Sensor” W. Kang, X. Pei, C.A Rusinek, A Bange, E.N Haynes, W.R Heineman, I. Papautsky. *Analytical Chemistry*, 2017, 89, 3345-3352.

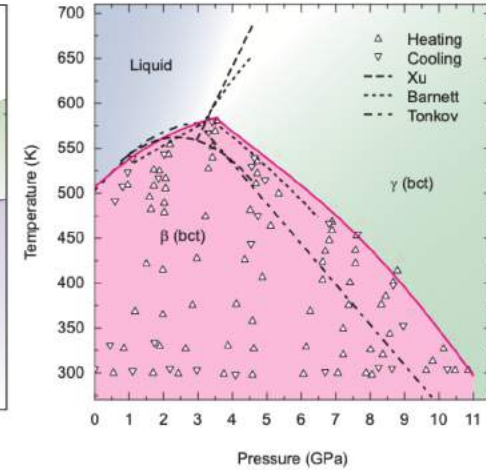
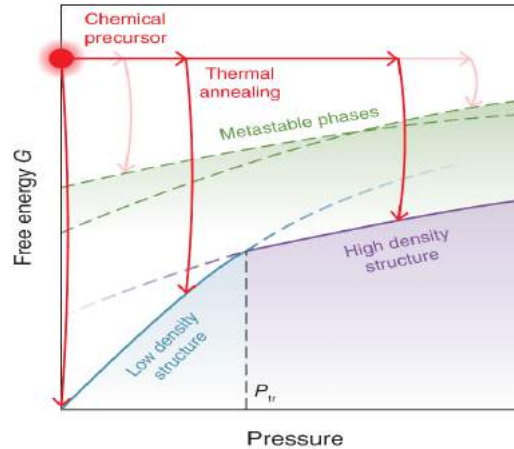
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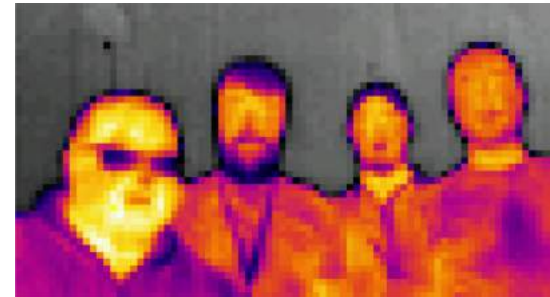
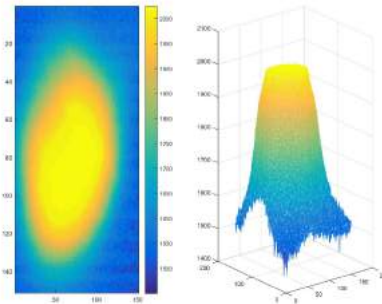
Salamat Group – Collaboration with MSTs



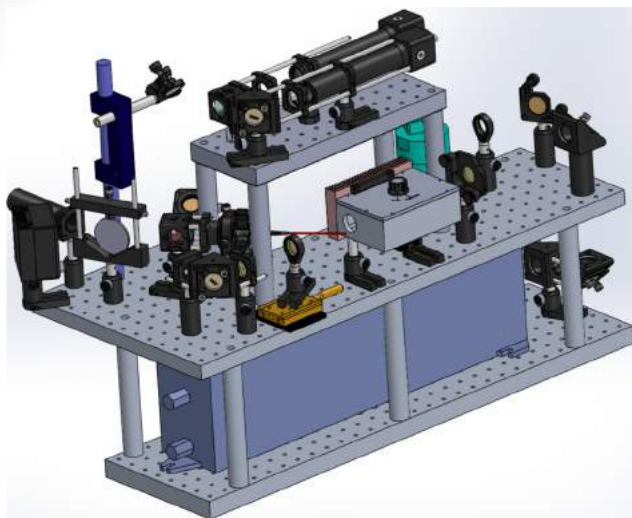
Metrology – accurate mapping of P, V, T



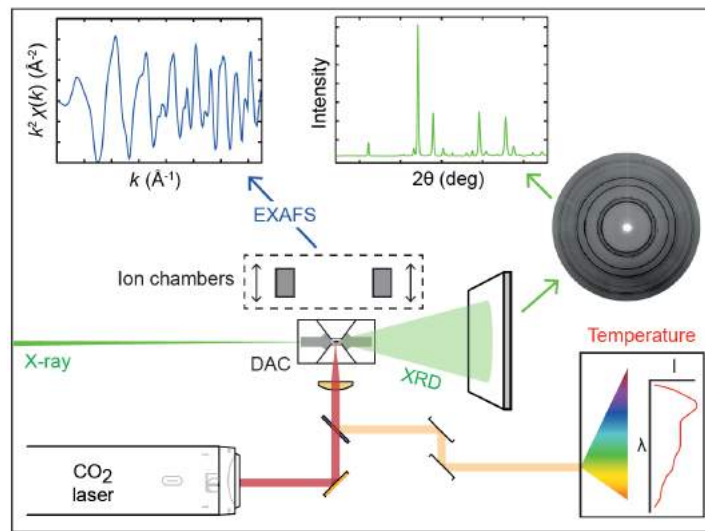
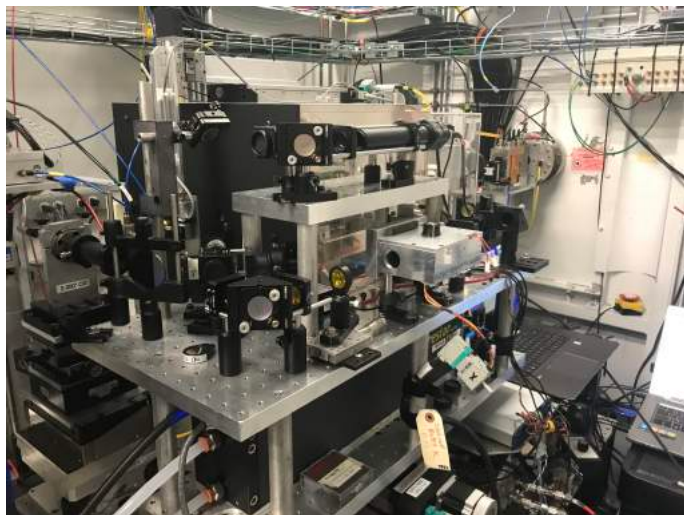
High temperature modelling – understanding emissivity under extreme conditions



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: $\text{La}_2\text{Sn}_2\text{O}_7$ 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 CaCO_3 at lower mantle pressures [Physical Review M 2, 013605 \(2018\)](#)
- (5) D. Smith, J. S. Smith, C. Childs, E. Rod, R. Hrubciak, 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 \(2014\)](#)

[Google Scholar: Ashkan Salamat](#)

Materials Compression & Strain

Dr. Oliver Tschauner

Research Professor

Department of Geoscience

Phone: 702-895-3137

Email: olivert@physics.unlv.edu

Expertise:

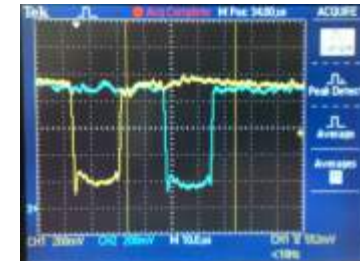
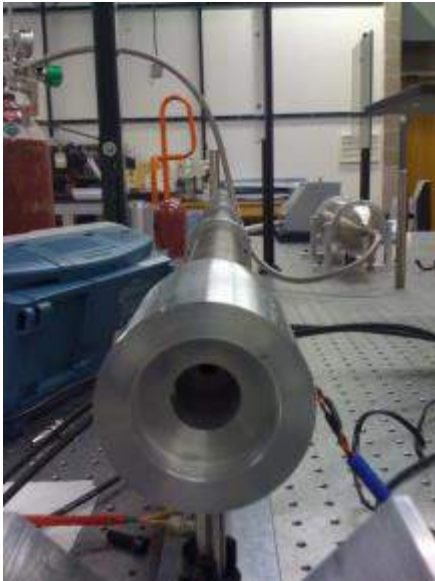
- Dynamic compression
- Crystal structure analysis
- Minerology

Dynamic Compression

Shockwave Lab:

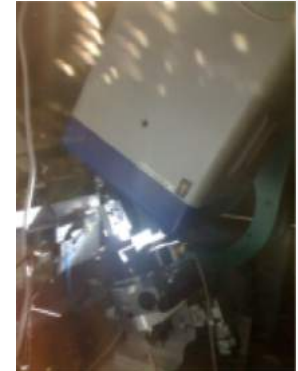
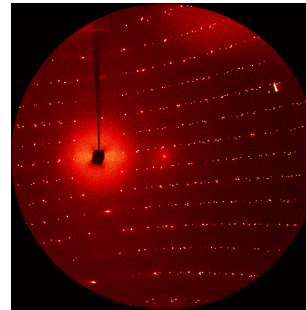
Compressed He gas, single-stage guns, vertical gun

- Velocimeter, impedance match calculation of sample shock pressure
- Recovery Experiments
- Advantage of advanced structural and chemical characterization at synchrotrons

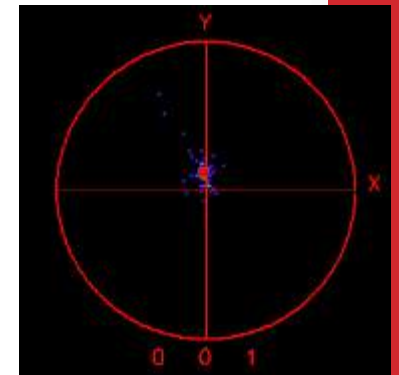
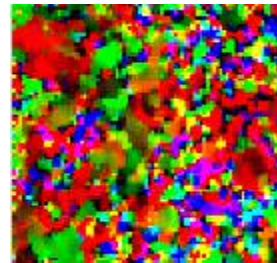


Microscale analysis: Structure, Strain, HE materials

A. Microscale Structure
analysis HPCAT



B. Dynamic compression
strain mapping
Laue XRD



C. HE materials
EOS
HPCAT, LLNL



Explore New Physics Beyond the Standard Model

Dr. Yan Zhou

Department of Physics and Astronomy

Phone: 702-895-3084

Email: yan.zhou@unlv.edu

Expertise

- Precision measurements
- Quantum information processing
- Cold and ultracold molecules
- High-resolution spectroscopy

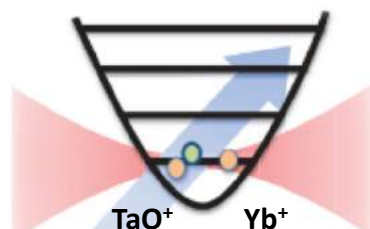
Exploring new physics beyond the Standard Model using ultracold molecular ions and highly-charged ions

Trap



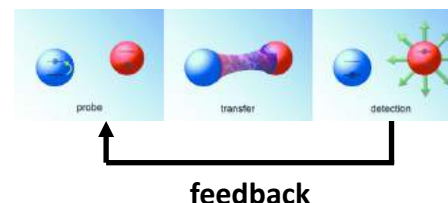
Nature, 417, 709 (2002)

Sympathetic cooling

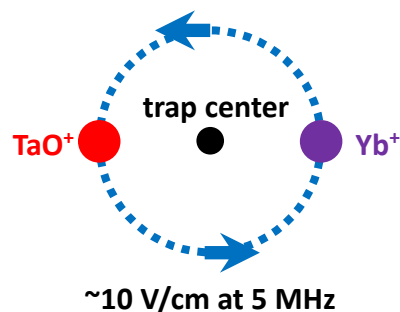


State readout & control

Quantum Logic scheme



Bias E-field



Bias B-field

$$H_{Zeeman} = m_F \mu_B B_{rot}$$

$$H_{Berry} = m_F \omega_{rot} \langle \alpha \rangle$$



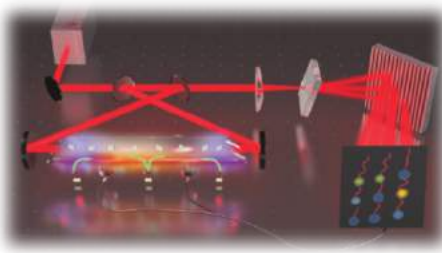
Universal platform

- $^{232}\text{ThF}^+$ for eEDM
- $^{229}\text{ThF}^+$ for NMQM
- $^{181}\text{TaO}^+$ for NMQM
- $^{179}\text{HfO}^+$ for NSD-PV
- All can be for Axion

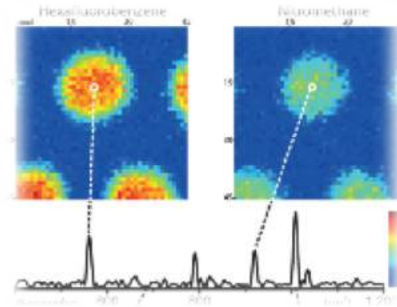
...

New technology and new applications based on optical frequency comb

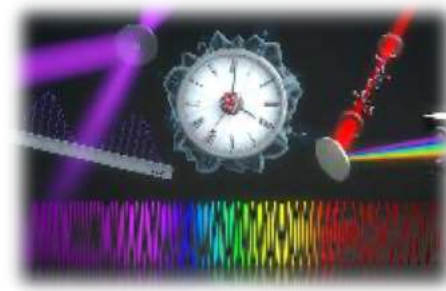
high resolution spectroscopy



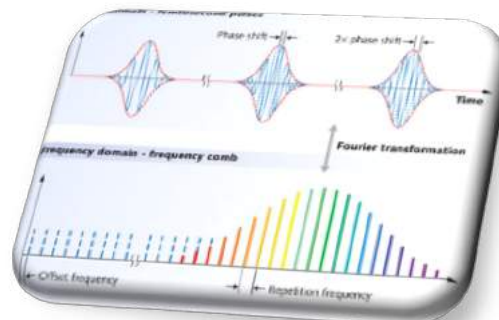
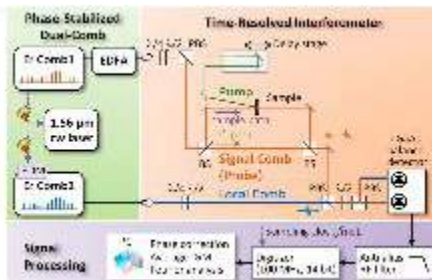
nonlinear spectroscopy



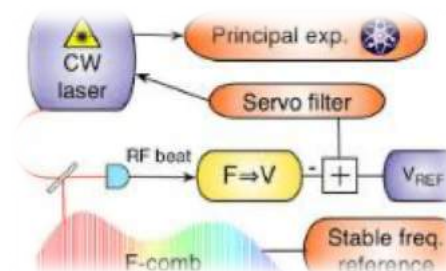
Atomic clock



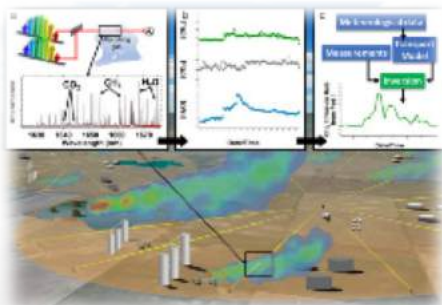
ultrafast spectroscopy



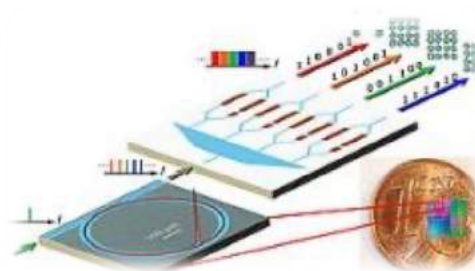
Laser stabilization



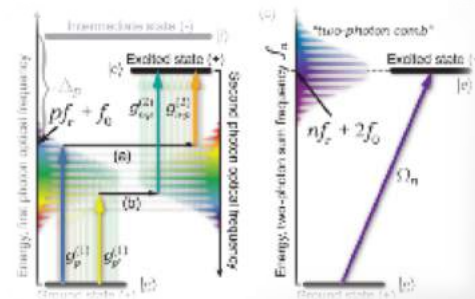
Tracing detection



Communication

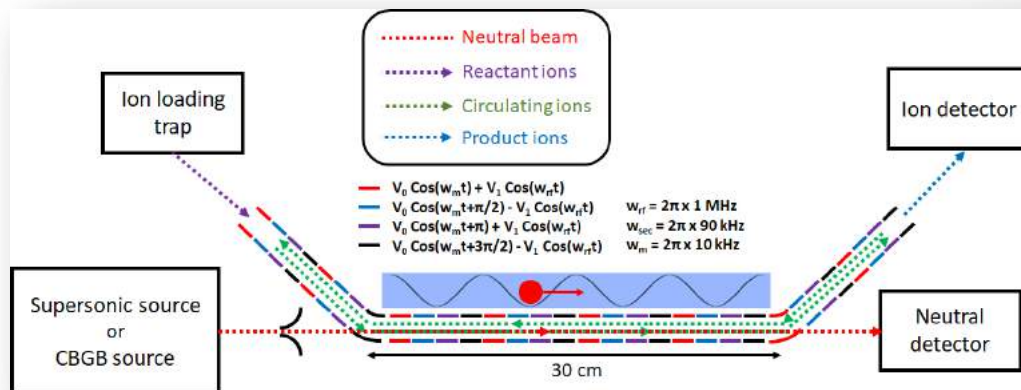
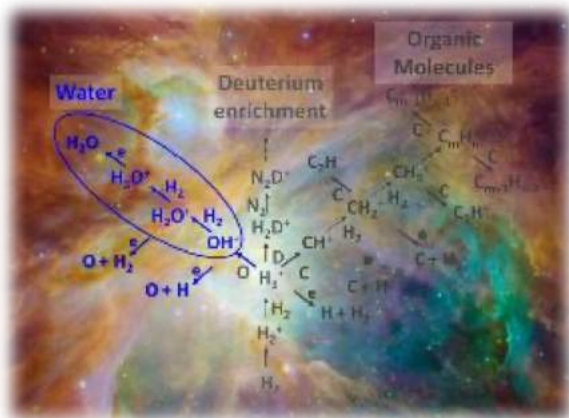


Laser cooling



Figures are from multiple references

Revealing mechanisms of universe evolutions by studying cold ion-radical reactions



- Chain reactions
- Radiative association
- Tunneling resonances
- Collisional resonances
- Discrepancies of reaction dynamics between chemical physics labs and astronomical observatories

Parameters	Expected specifications
Interaction arm length	30 cm
Ion beam velocity	0-1000 m/s
Collision energy range	<0.1 meV to >100 meV
Energy resolution	<0.1 meV
Effective reaction duration	1 s
Detection sensitivity	$1 \times 10^{-16} \text{ cm}^{-3} \text{ s}^{-1}$

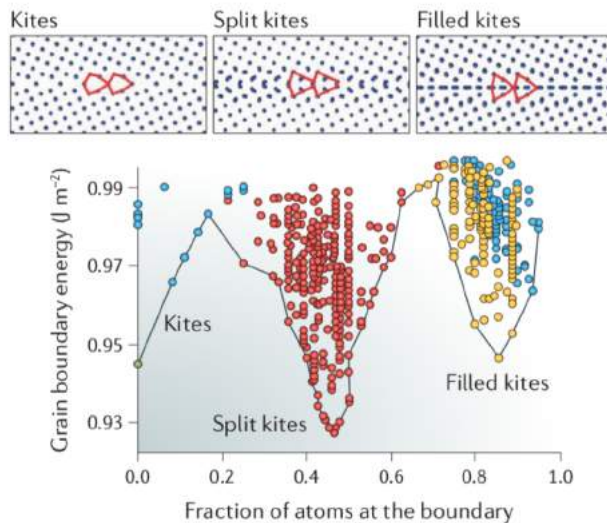
Qiang Zhu (Structure Prediction Aided by Artificial Intelligence)



- Develop **open source codes** (USPEX, PyXtal)



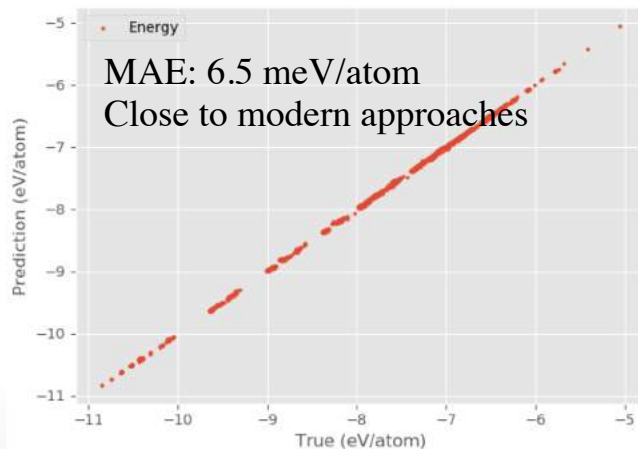
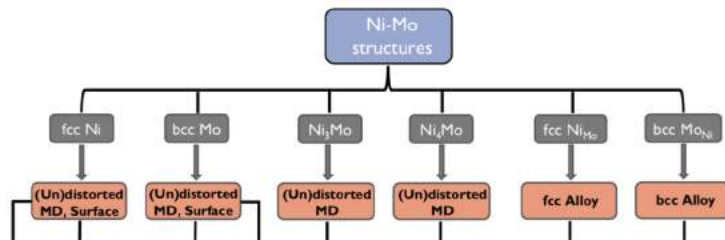
- Predict the atomic structure of materials from **first-principles**



- Applicable to a range of materials (for **both bulk and defects**) under extreme conditions where experimental characterization is limited

Qiang Zhu (Material Informatics & Big Data Analytics)

PyXtal_FF



An example of training force field on Ni-Mo alloys

- Perform high throughput simulations to investigate materials based on target properties
- Publish online database with all computational details
- Develop machine learning interatomic potentials to enable large scale atomistic simulation ([PyXtal_FF](#))

Qiang Zhu (Select Publications)

- Yanxon H, Zagaceta D, Wood B, [Zhu Q*](#), On Transferability of Machine Learning Force Fields: A case study on silicon, arXiv, 2020
- [Zhu Q*](#), Frolov T, Choudhary K, Computational Discovery of Inorganic Electrides from an Automated Screening, Matter, 2019
- Oganov A.R, Pickard C.J., [Zhu Q](#) and Needs R.J., Structure Prediction Drives Materials Discovery, Nature Review Materials, 2019
- [Zhu Q*](#), Samanta A, Li B, Rudd R.E and Frolov T. Predicting Phase Behaviors of Grain Boundaries with Evolutionary Search and Machine Learning, Nature Communication, 2018
- Xu W, [Zhu Q*](#), Hu CT, Structure of Glycine Dihydrate: Its implications to crystallization of glycogen from solution and modification of glycine in space, 2017
- [Zhu Q](#), Shtukenberg A.G. et al, Resorcinol crystallization from the melt: a new ambient phase and new riddles, JACS, 2016
- [Zhu Q*](#), Jung D.Y., Oganov A.R. et al, Stability of xenon oxides at high pressure, Nature Chemistry, 2013
- [Zhu Q*](#), Oganov A.R., Glass C.W., Stokes H, Constrained evolutionary algorithm for structure prediction of molecular crystals: methodology and applications
- Full list is available at <http://scholar.google.com/citations?user=1vO0eS0AAAAJ&hl=en>