Advanced Materials: Development & Analysis Research

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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

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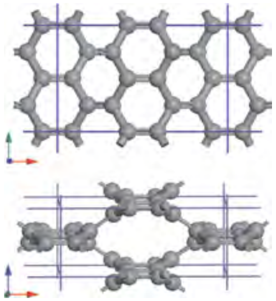
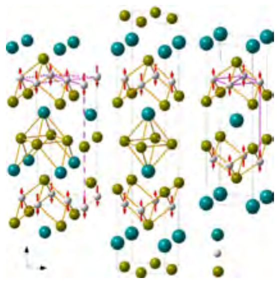
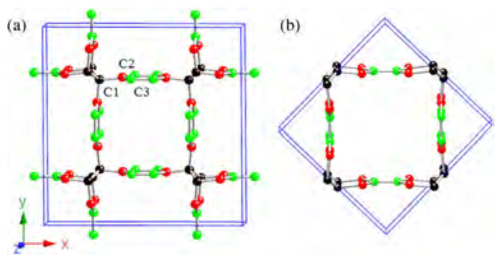


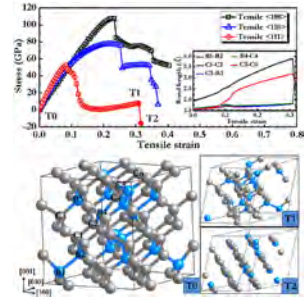
Nodal-ring Dirac semimetal states identified in bco-C_{16} crystal [Wang, Weng, Nie, Fang, Kawazoe, Chen, ***Phys. Rev. Lett.*** 116, 195501 (2016)].



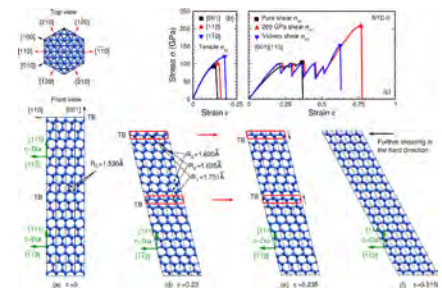
Magnetic Dirac materials $CaMnBi_2$ and $SrMnBi_2$ [Zhang, et al., ***Nature Commun.*** 7, 13833 (2016)].



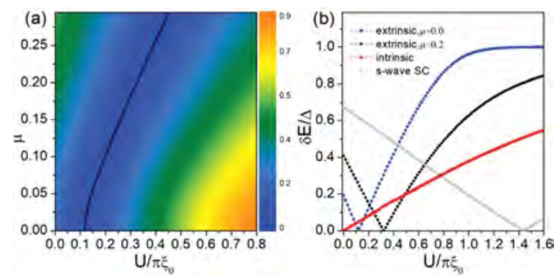
Nodal-net Dirac semimetal states in a graphene network structure [Wang, Nie, Weng, Kawazoe, Chen, ***Phys. Rev. Lett.*** 120, 026402 (2018)].



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

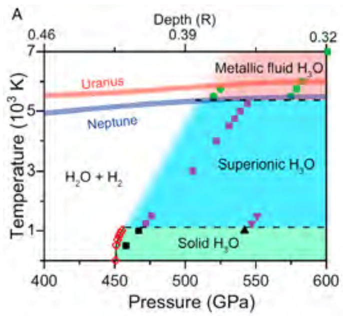


Extreme mechanics of nanotwinned diamond [Li, Sun, Chen, ***Phys. Rev. Lett.*** 117, 116103 (2016)].

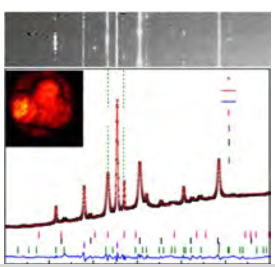


Kondo physics in 2D topological superconductors [Wang, et al., ***Phys. Rev. Lett.*** 122, 087001 (2019)].

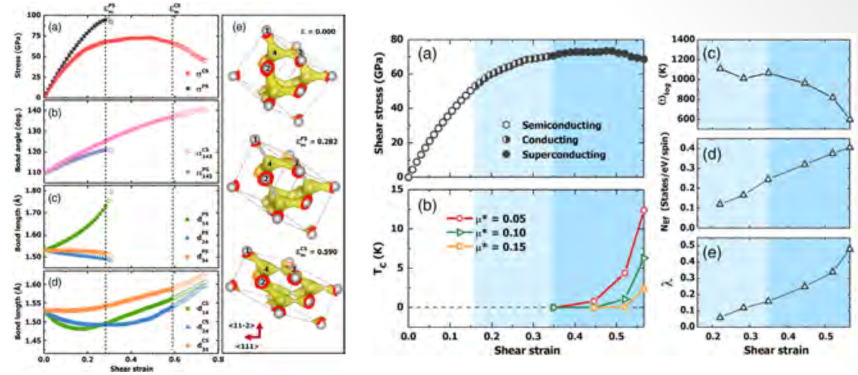
Helium-bearing compound FeO_2He predicted to stabilize at deep-Earth conditions [Zhang, et al., ***Phys. Rev. Lett.*** <u>121</u>, 255703 (2018)].



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



Pressure-stabilized divalent ozonide CaO_3 and its
impact on Earth's oxygen cycles [Wang, et al., ***Nature Commun.*** <u>11</u>, 4702 (2020)].



Metallization and superconductivity in diamond [Liu, et al., ***Phys. Rev. Lett.*** <u>123</u>, 195504 (2019); ***Phys. Rev. Lett.*** <u>124</u>, 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.*** <u>115</u>, 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.*** <u>119</u>, 115503 (2017).

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

Electronic and Magnetic Properties at High Pressure

Dr. Andrew Cornelius
Department of Physics & Astronomy
Phone (702) 895-1727

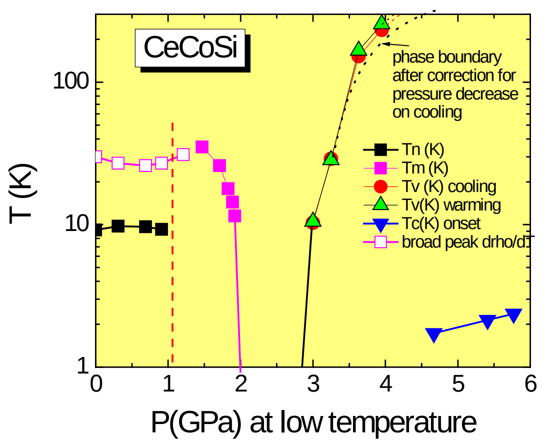
Expertise:

- Experimental high pressure measurements
- Magnetism
- Superconductivity

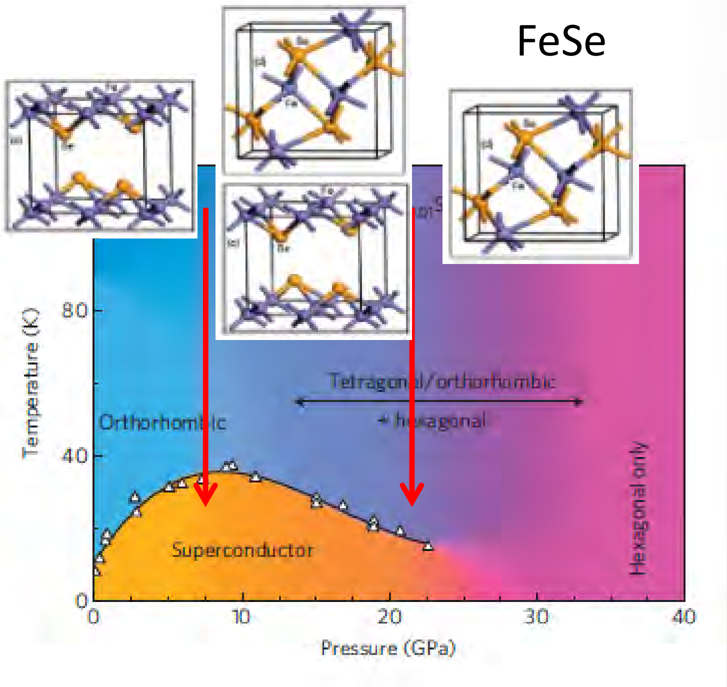
Superconductivity

Quantum Design PPMS at UNLV

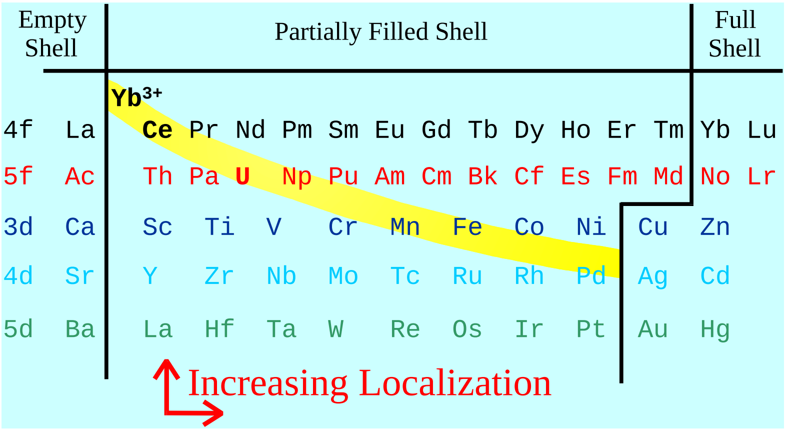
- Measurements from 0.3 K to 400 K
    - Heat capacity, electric and thermal transport, and AC/DC magnetization
- Pressure cells to measure electrical properties (clamp to 3 GPa and diamond anvil cell to >100 GPa)



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

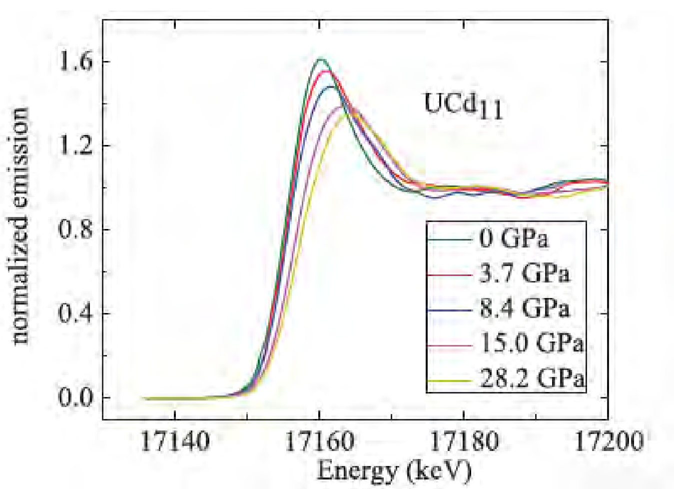


Correlated-Electron Systems

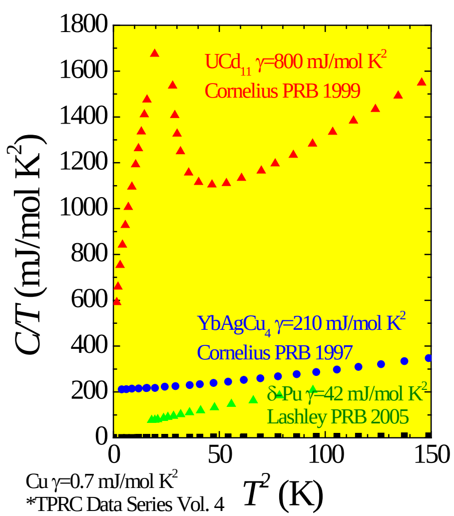


Modified periodic table

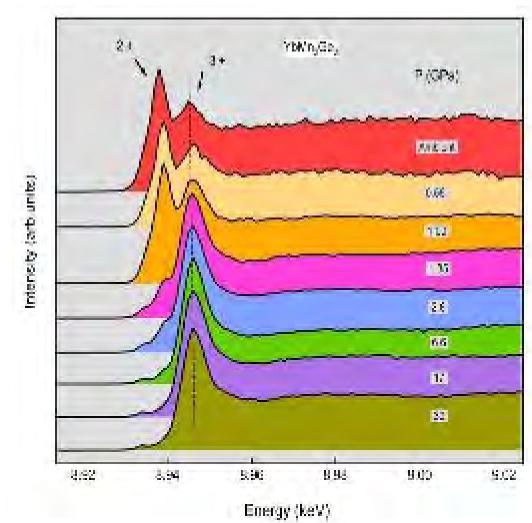
- Going from localized to delocalized electrons one often finds strong electron-electron correlations
- Correlated electron systems can yield interesting behavior: fluctuating valence, superconductivity, non-Fermi liquid, heavy fermion and many more



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

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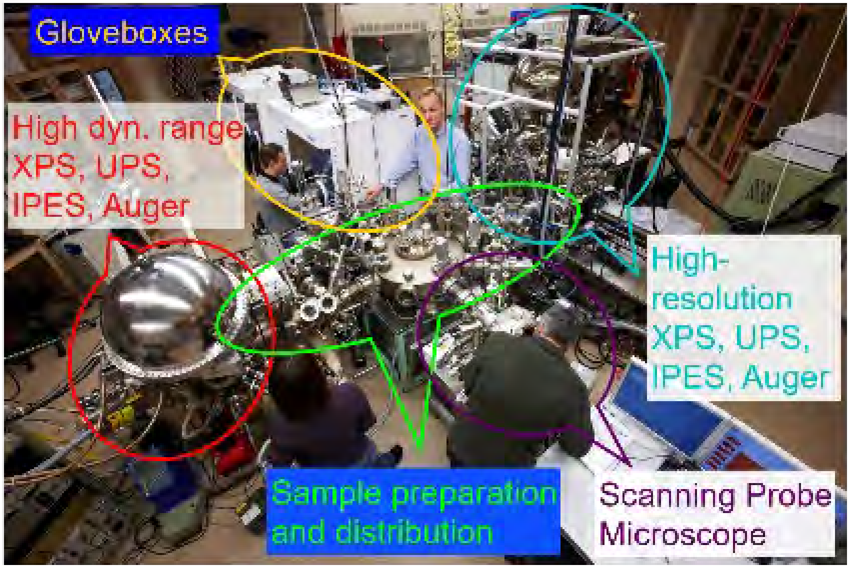
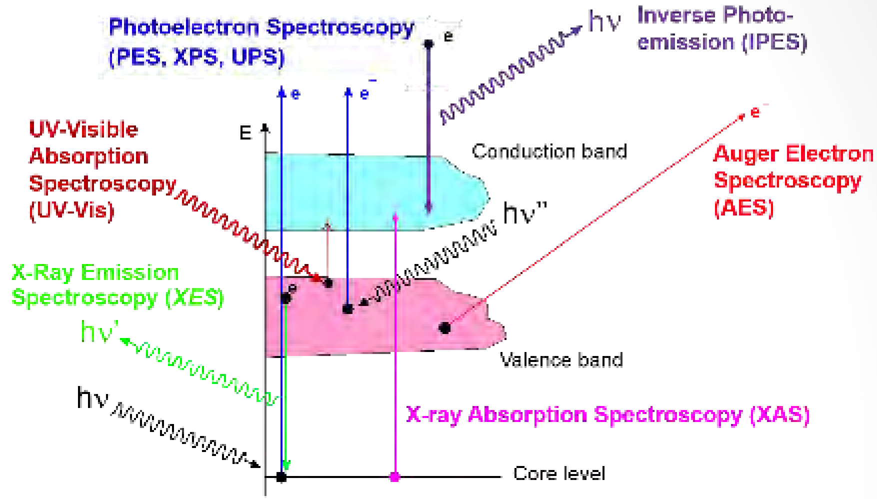
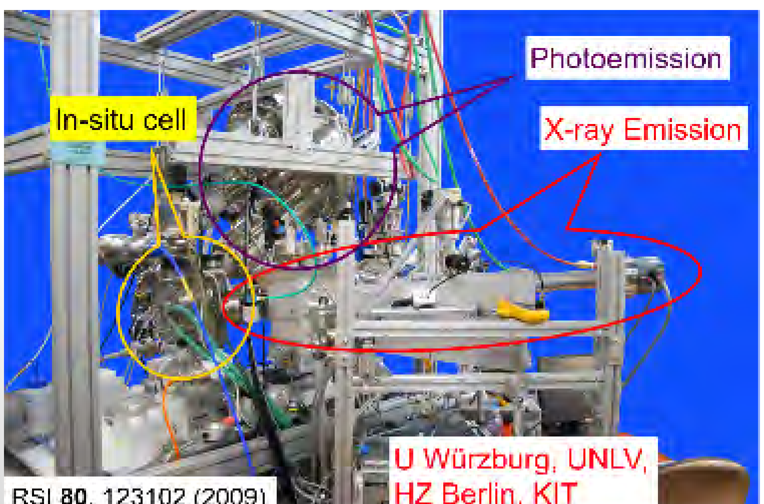
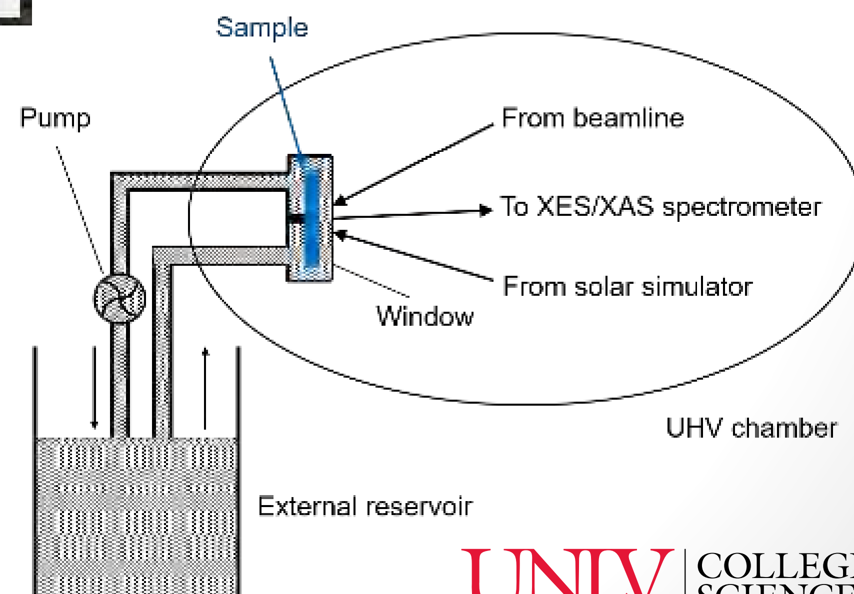
Surface and Interface Characterization





SALSA: Solid And Liquid Spectroscopic Analysis





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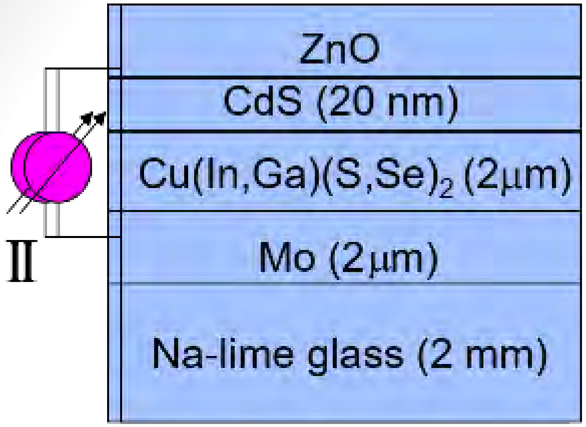
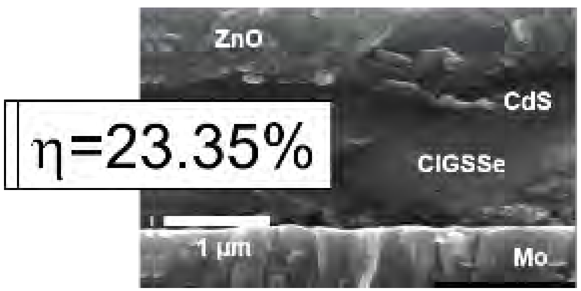
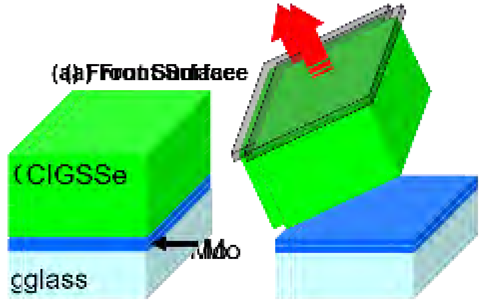
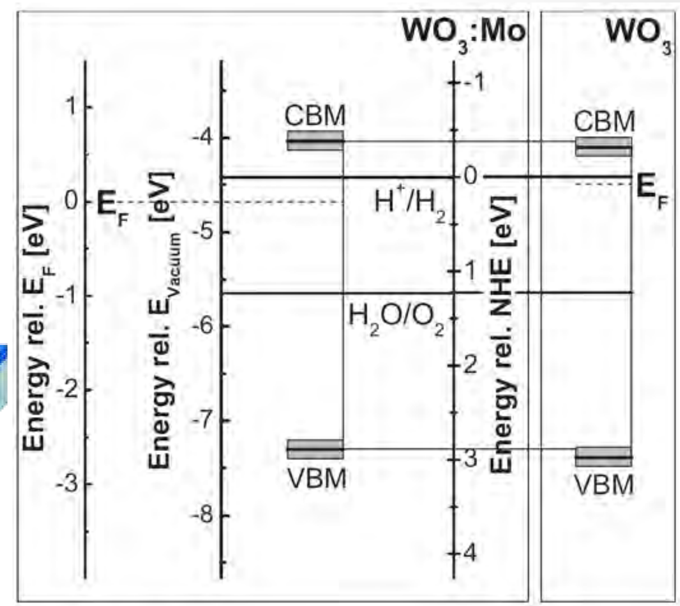
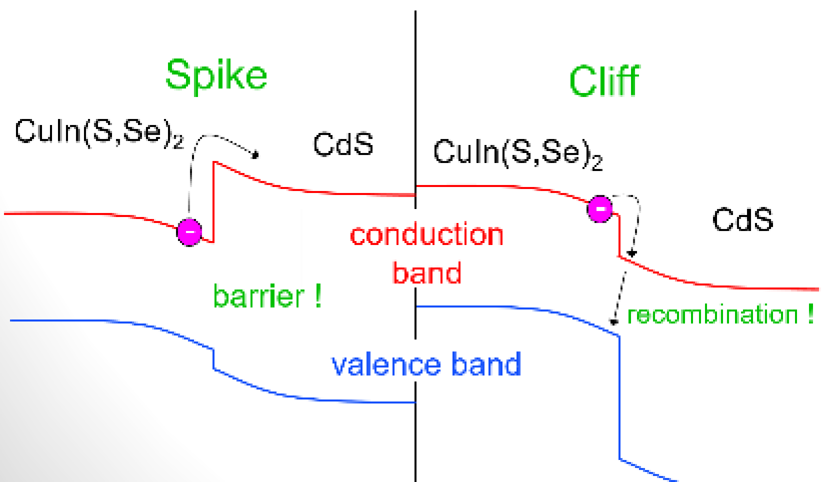
Materials for Energy Conversion

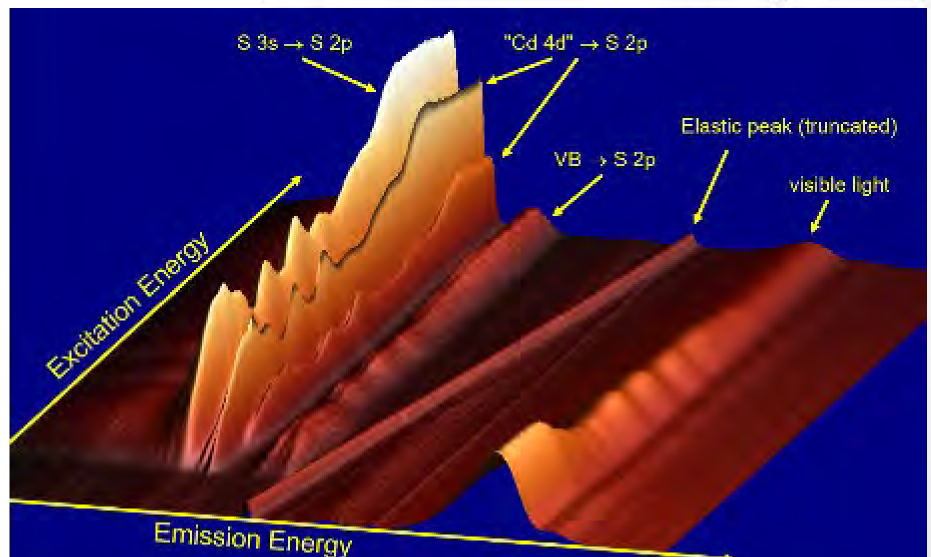










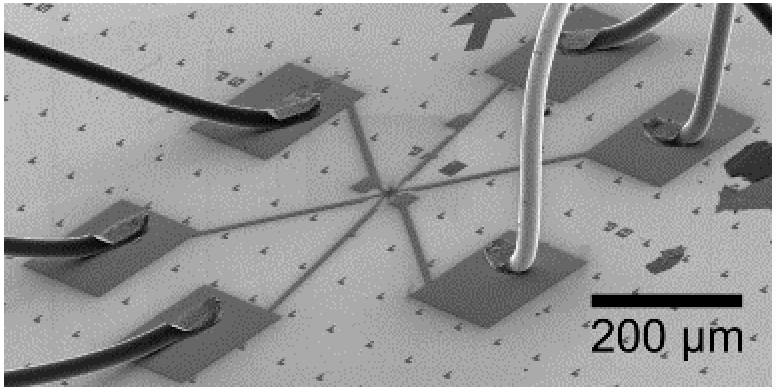


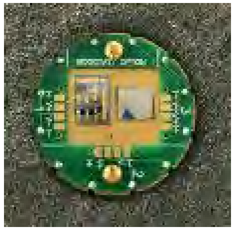
Island – Quantum computing, quantum sensing

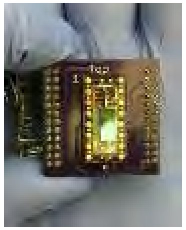
The Nanoscale Physics Group @ UNLV

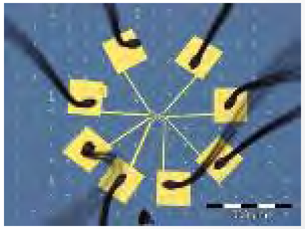
Areas of Research

- 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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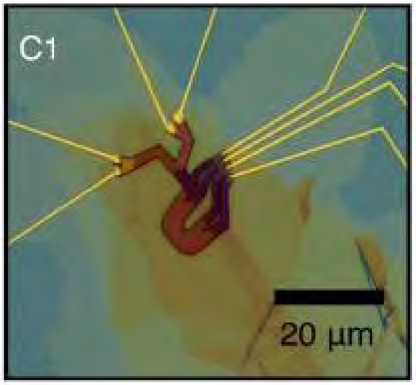
Island's Lab website

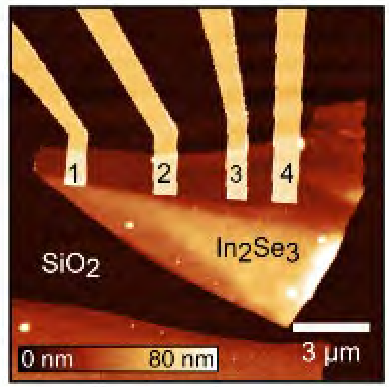
Island – Quantum computing, quantum sensing

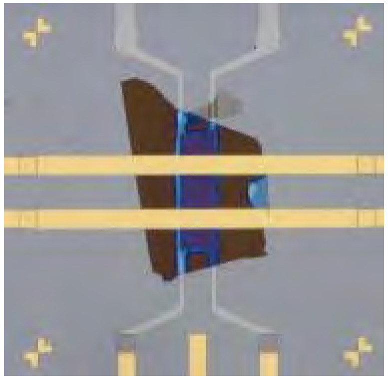
Quantum computing: Topological phases for fault-tolerant, universal quantum computing.

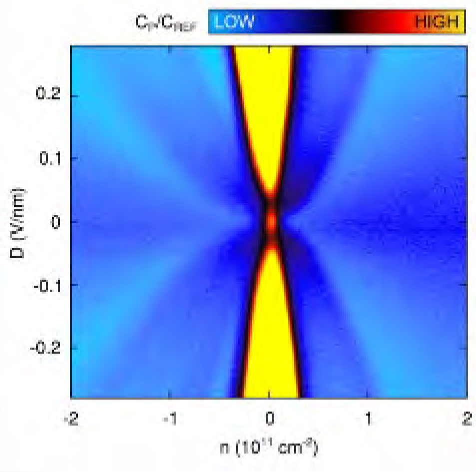
Industry-disruptive photodetectors: Ultra-sensitive phototransistors designed with 2D materials and heterostructures.

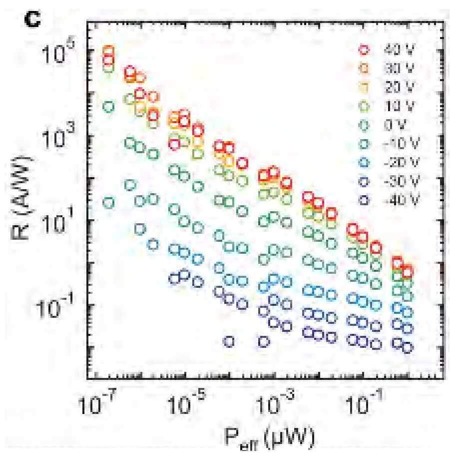
Transient phases of driven systems: Non-equilibrium response of pumped nanomaterials below the diffraction limit.

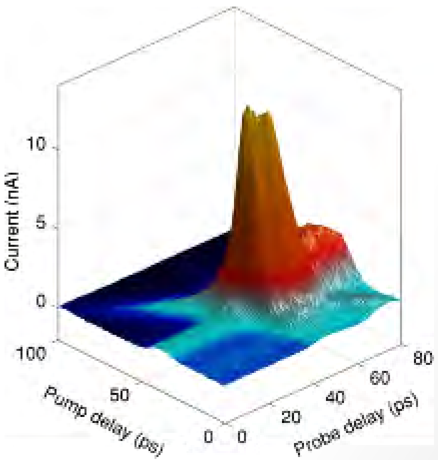












Island, J. O., et al. *Nature* **571** (2019): 85–89.

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)

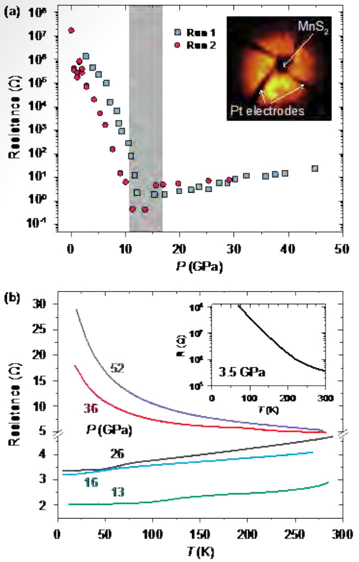
Environmental instability of few-layer black phosphorus
J.O. Island, G.A. Steele. H.S.J. van der Zant, and A. Castellanos-Gomez, 2D Materials, **2**, 011002 (2015). (arXiv)

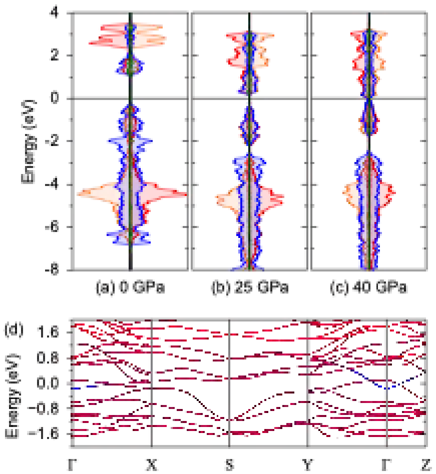
Ultrahigh photoresponse of few-layer TiS3 nanoribbon transistors
J.O. Island, M. Buscema, M. Barawi, J.M. Clamagirand. J.R. Ares, C. Sanchez, I.J. Ferrer, G.A. Steele, H.S. J van der Zant, and A. Castellanos-Gomez, Advanced Optical Materials, **2**, 641 (2014). (arXiv)

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)

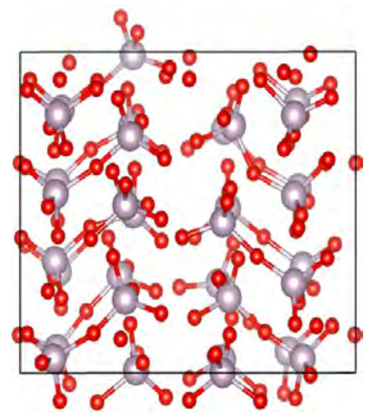
Precise and reversible band gap tuning In single-layer MoSe2 by uniaxial strain
J.O. Island, A. Kuc, E.U. Diependaal, H.S.J. van der Zant, T. Heine, and A. Castellanos- Gomez, Nanoscale, **8,** 2589 (2016). (arXiv)

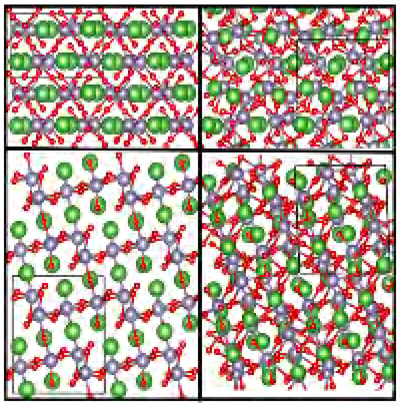
Island's Lab website



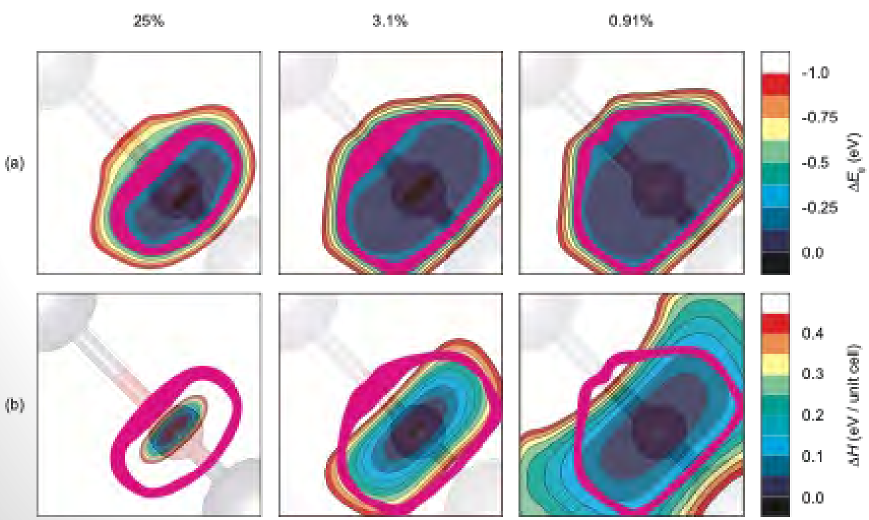


We primarily perform electronic structure simulations to understand pressure driven phenomenon particularly related to correlated electron systems and changes in bonding.



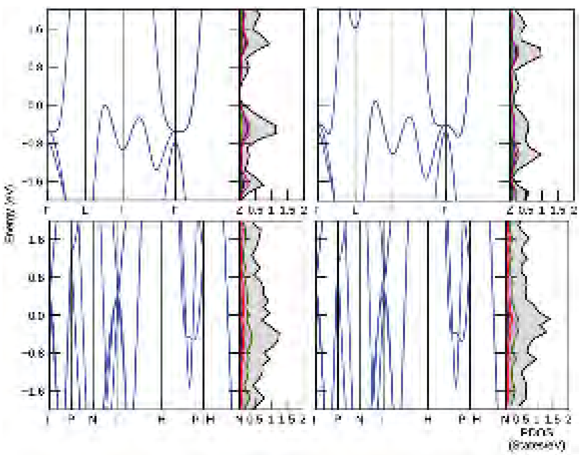


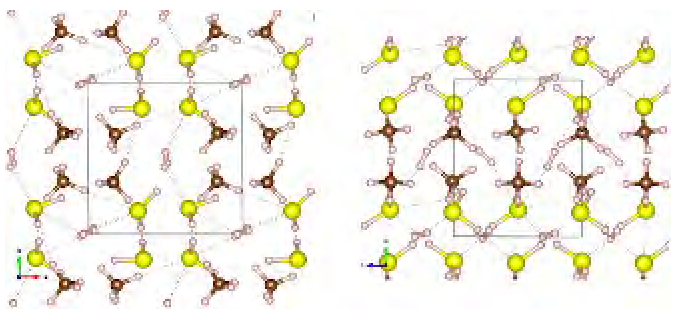
This includes molecular dynamics to understand the thermal behavior of materials and melts,

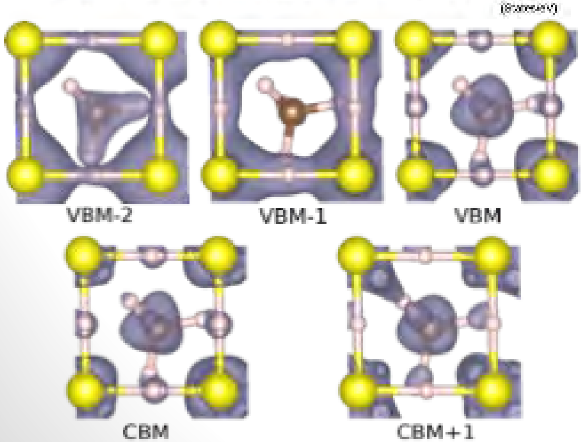


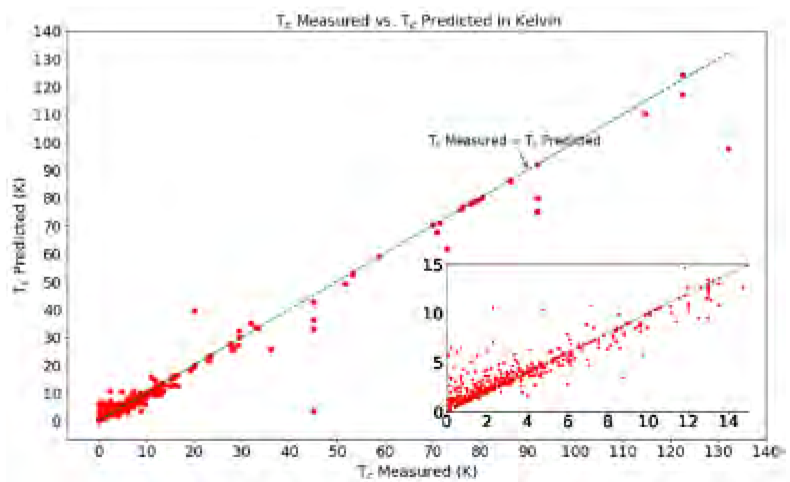
as well as crystal structure prediction and the electronic response to pressure driven perturbations in crystalline lattices.

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.







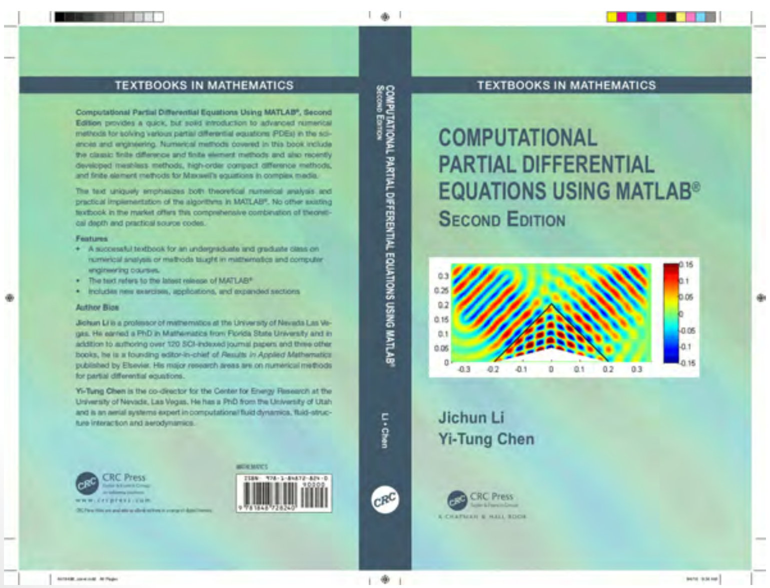


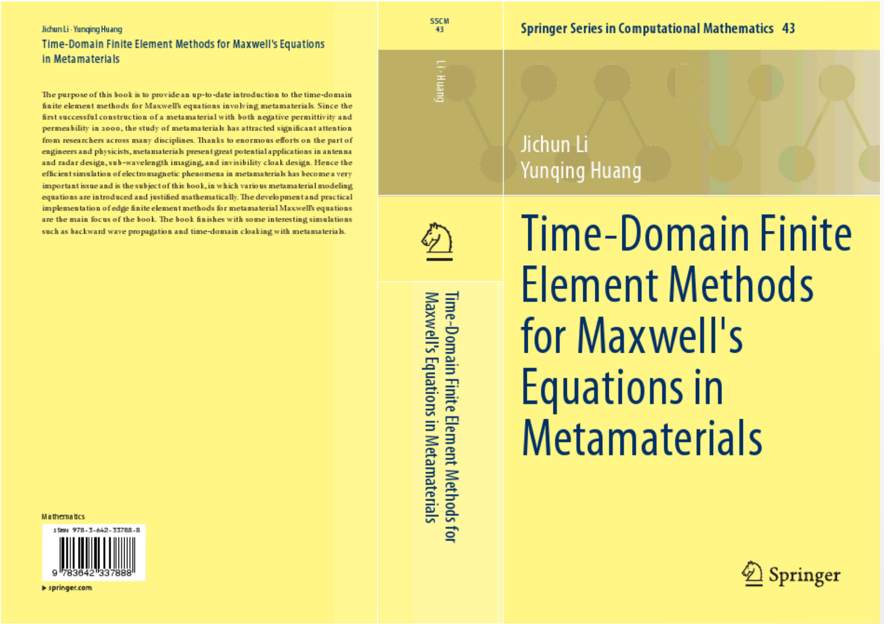
Scientific Computing and Mathematical Modeling

Dr. Jichun Li
Department of Mathematical Sciences
Phone: (702)895-0365
Email: jichun.li@unlv.edu

Expertise:

Computational Electromagnetics
Numerical Methods for PDEs
Mathematical Modeling





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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.

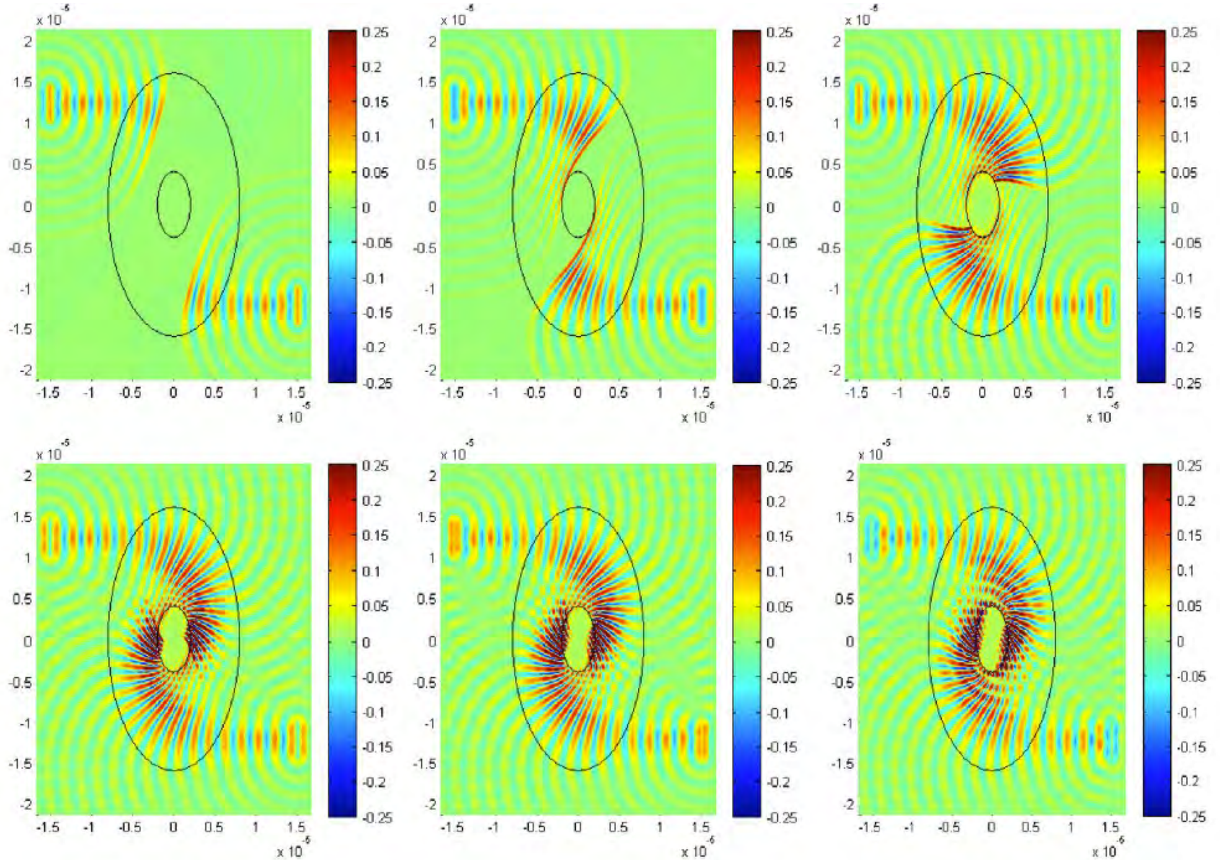
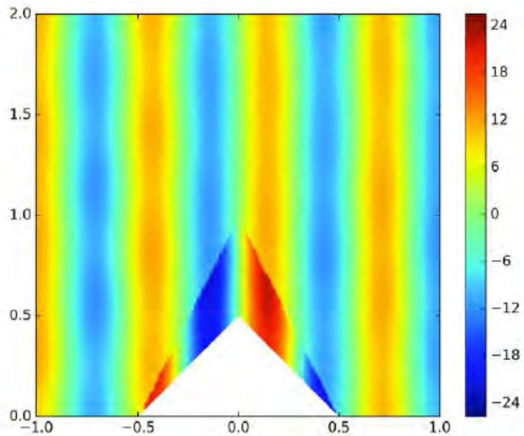
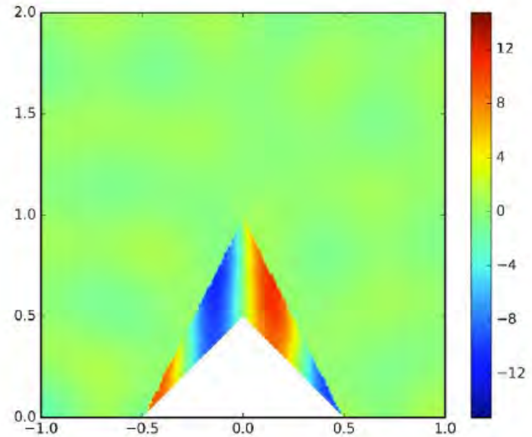


Fig. 4.5. Example 2. Magnetic fields H_z at various time steps for the elliptical OBHs simulation. Top left: 1600 steps. Top middle: 2400 steps. Top right: 3600 steps. Bottom left: 4800 steps. Bottom middle: 5200 steps. Bottom right: 8000 steps.

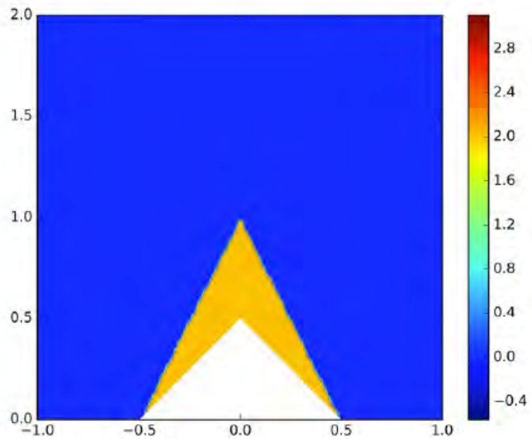
Jichun Li et al (Optimal control for electromagnetic cloaking metamaterial design): Computer and Mathematics with Applications 79 (2020) 1165-1176.



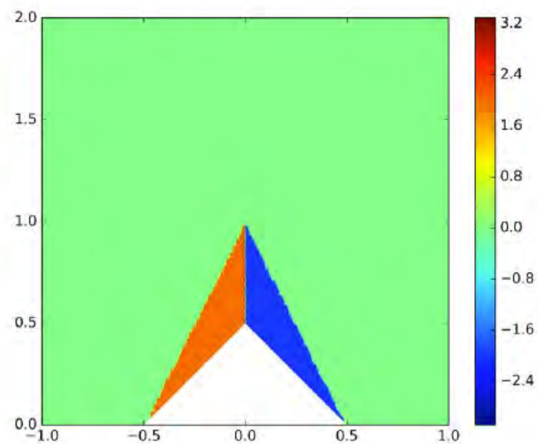
(a) $\nabla_h \times \boldsymbol{E}_h$



(b) $\nabla_h \times (\boldsymbol{E}_h - \boldsymbol{E}_w)$



(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 $\max \epsilon_2 = 2.02687675$

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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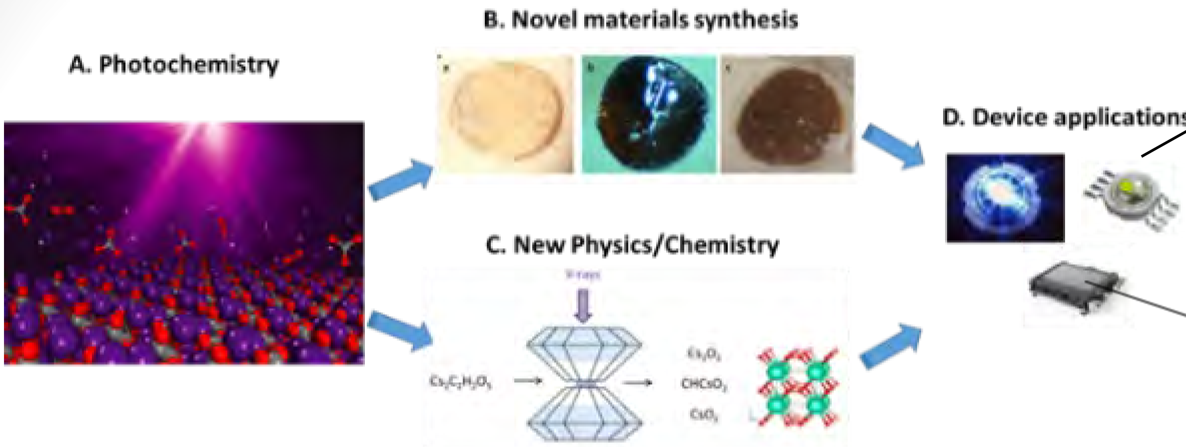
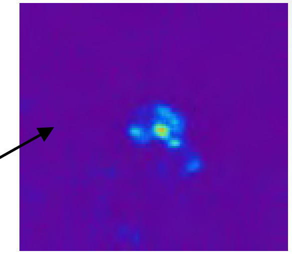
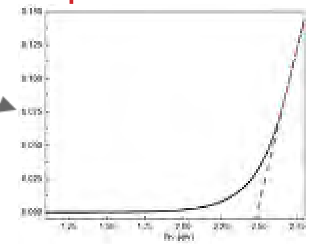
Pravica Group Research





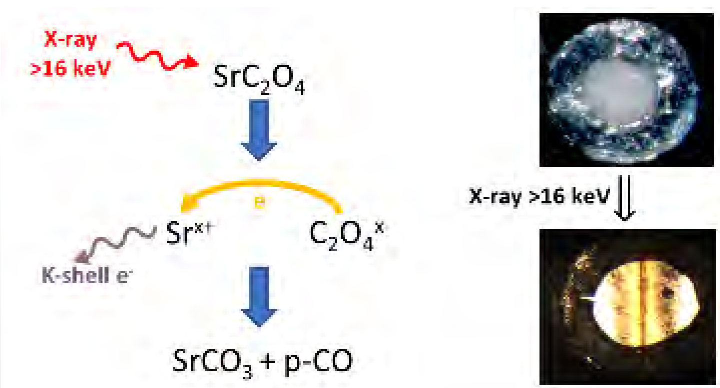
Optical mixer

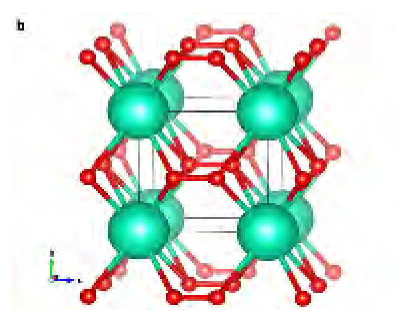


Wide bandgap semiconductor

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

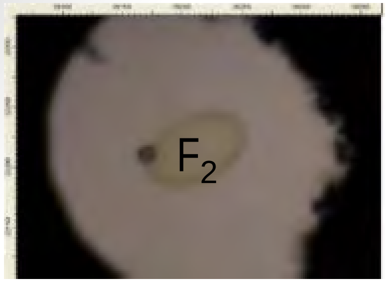
Useful hard x-ray photochemistry

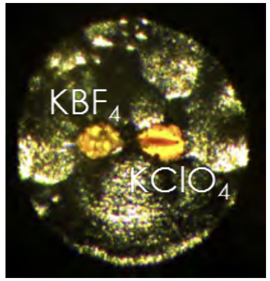




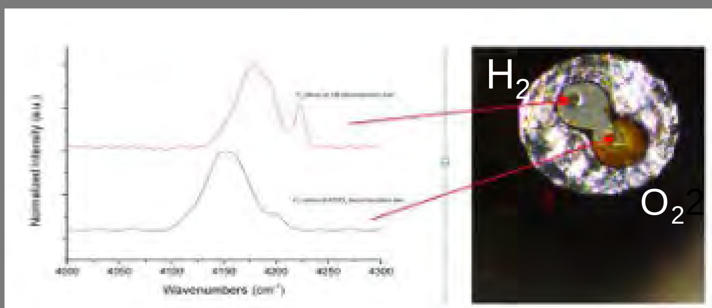
Novel structures of known materials produced With hard x-rays and high pressure (e.g. CsO_2)

High Pressure Fluorine Chemistry



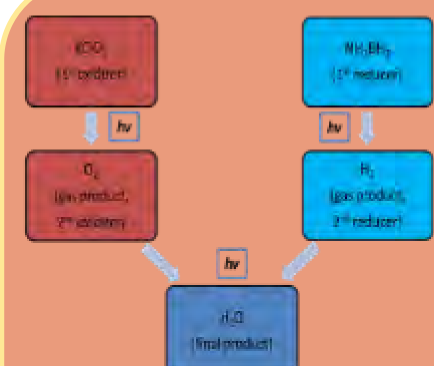


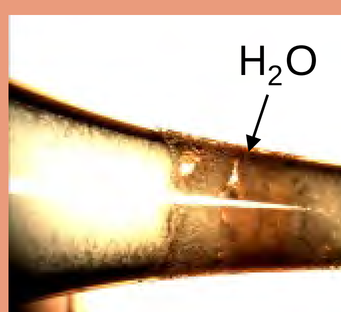
$$2F_2 + O_2 \xrightarrow{h\nu} 2OF_2 \text{ @ 3 GPa}$$



5 GPa

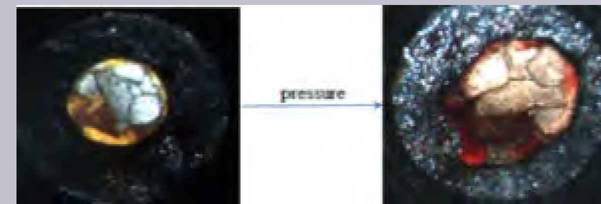
Molecular mixtures at high pressure





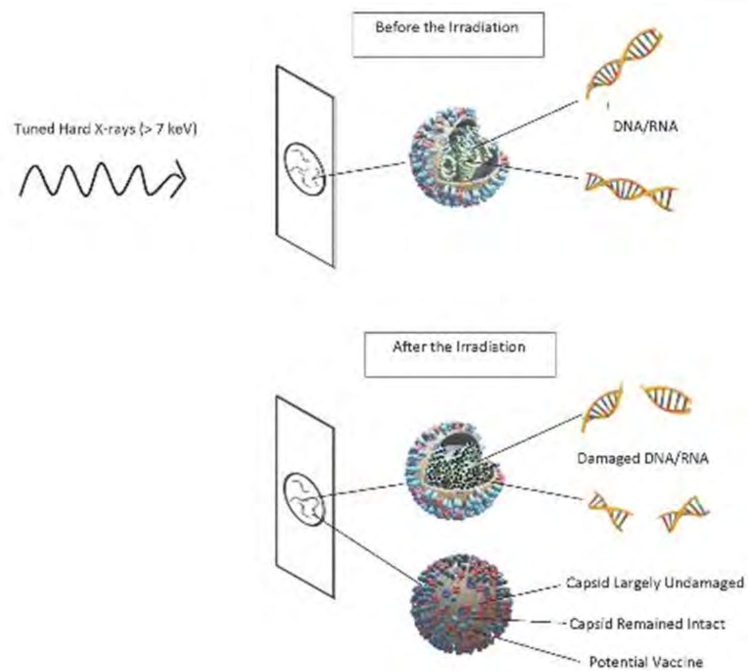
X-ray induced combustion

Inner shell chemistry at high pressure



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

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

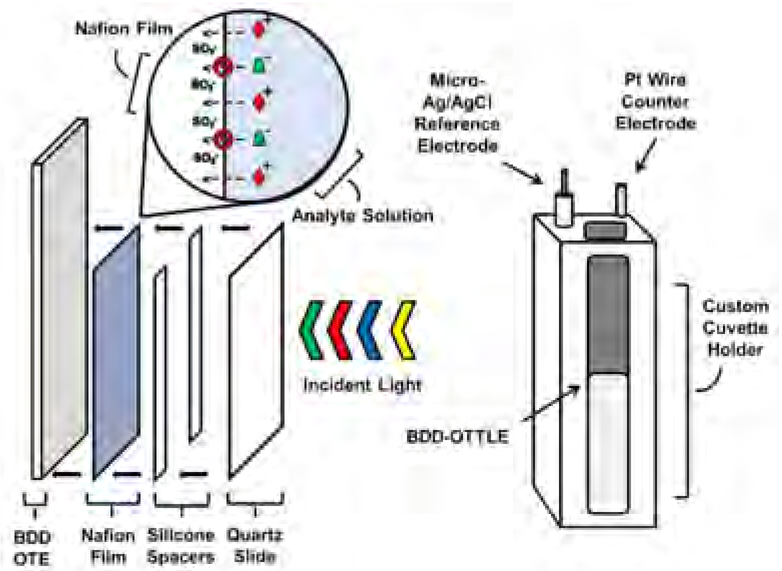


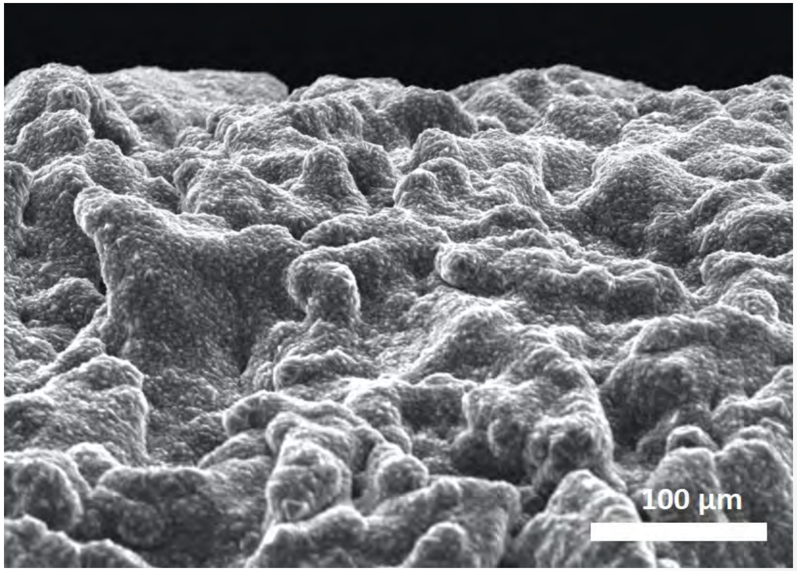
Using tuned hard x-rays to damage viruses to create high quality vaccines by targeting specific molecular groups/bonds that resonantly absorb x-ray energy leading to decomposition chemistry.

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

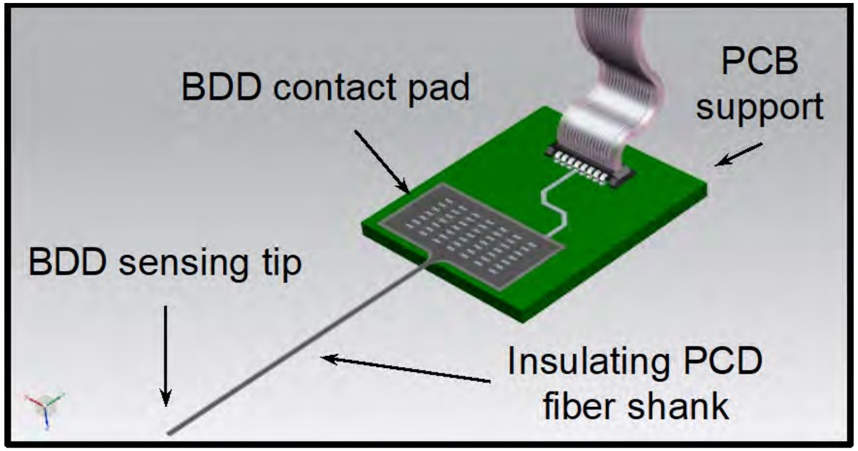


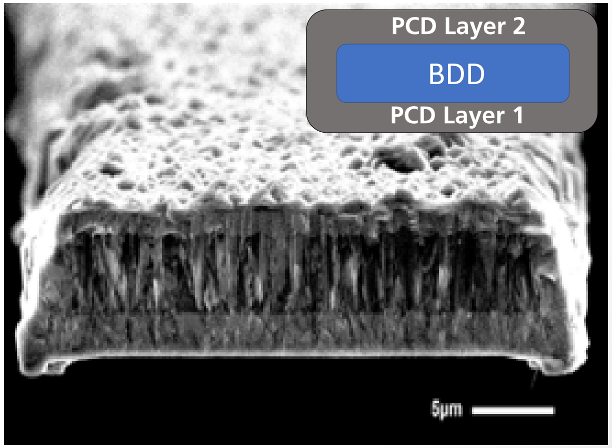


SEM image of diamond film

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 un-doped diamond, there by 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. Ensch, 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.

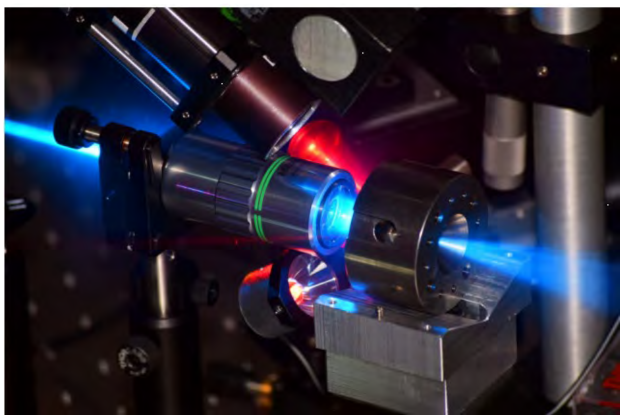
“All Diamond Microfiber Electrodes for Neuroelectrochemistry” C.A Rusinek, Y. Guo, R. Rechenberg, E. Purcell, C. McKinney, M.F Becker, W. Li, Journal of the Electrochemical Society, 2018, 165 (12), G3087-G3092.

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

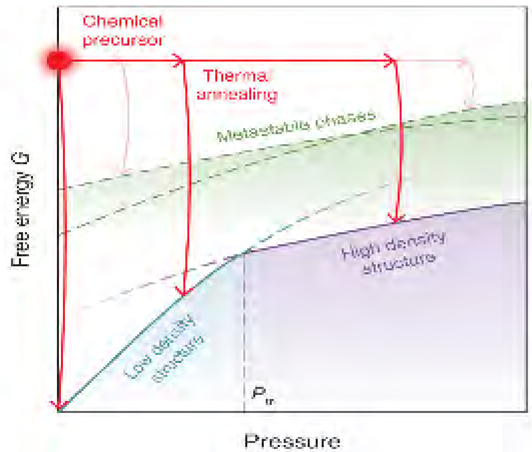
“Detemination of Lead with a Copper-Based Electrochemical Sensor” W. Kang, X. Pei, C.A Rusinek, A Bange, E.N Haynes, W.R Heineman, I. Papautsky. Analytical Chemistry, 2017, 89, 3345-3352.

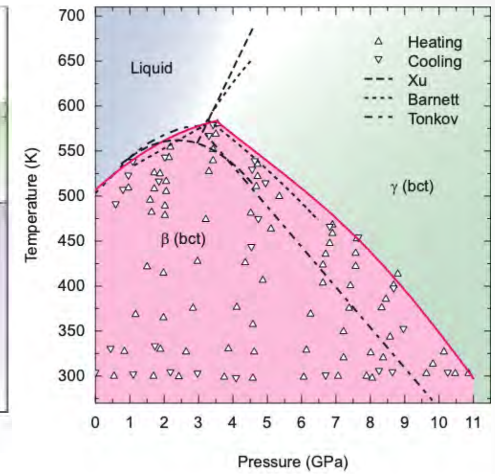
Google Scholar: Google scholar webpage of Dr. Rusinek

Salamat Group – Collaboration with MSTS

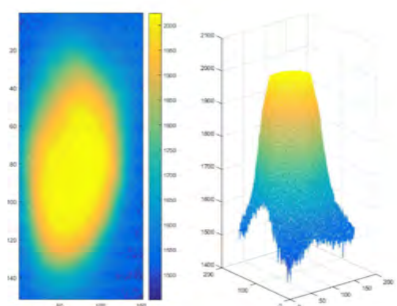


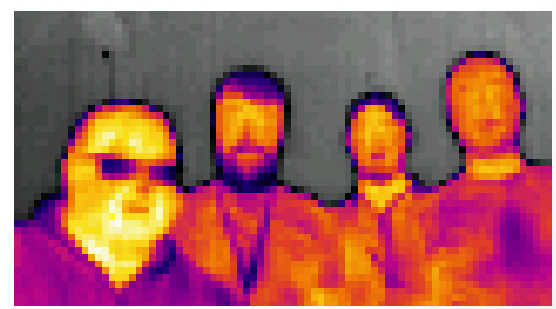
Metrology – accurate mapping of P, V, T





High temperature modelling – understanding emissivity under extreme conditions





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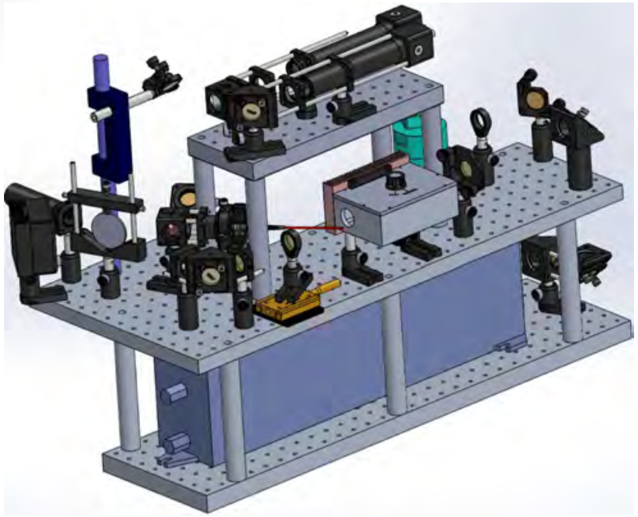
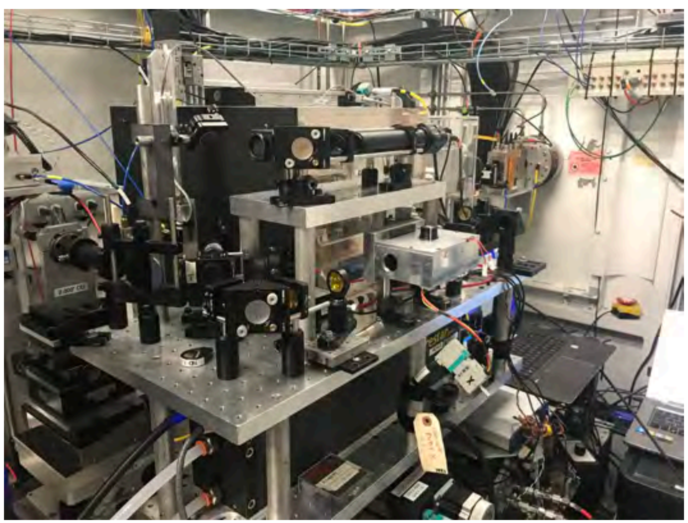
Warm dense matter – probed using EXAFS

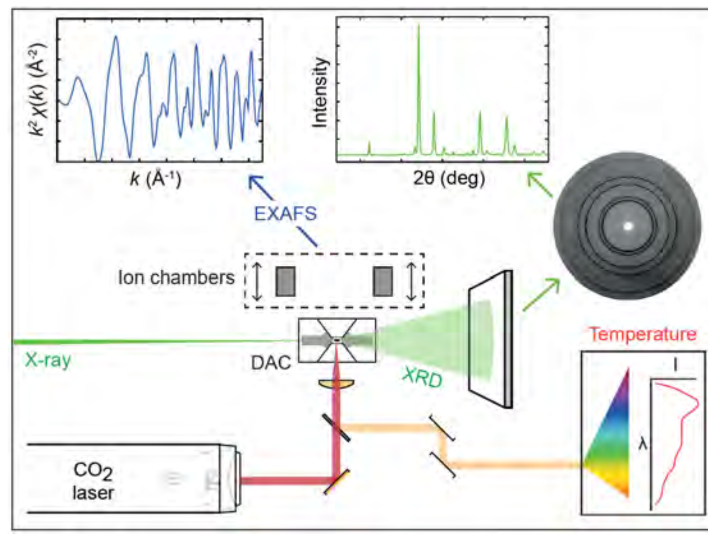


- Development of a CO_2 laser heating
- Direct heating of non-metallic systems in a DAC
- First HTHP EXAFS measurements of insulators

- 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)

Materials Compression & Strain

Dr. Oliver Tschauner
Research Professor
Department of Geoscience
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Expertise:

Dynamic compression
Crystal structure analysis
Minerology

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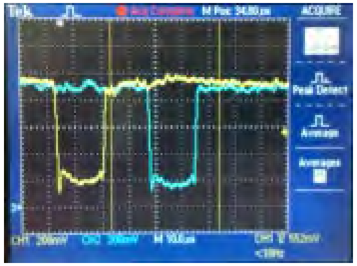
Dynamic Compression

Shockwave Lab:

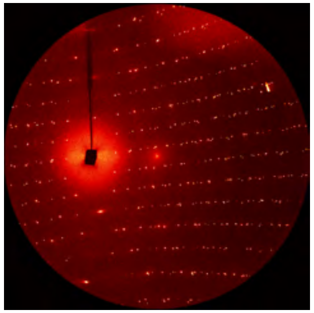
Compressed He gas, single-stage guns, vertical gun

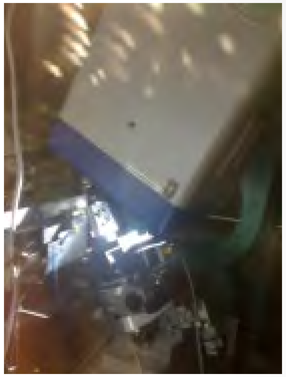
- Velocimeter, impedance match calculation of sample shock pressure
- Recovery Experiments
- Advantage of advanced structural and chemical characterization at synchrotrons



Microscale analysis: Structure, Strain, HE materials

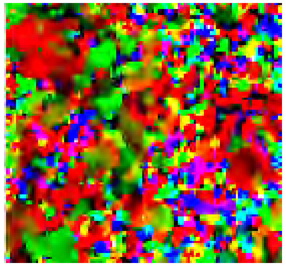
A. Microscale Structure analysis HPCAT

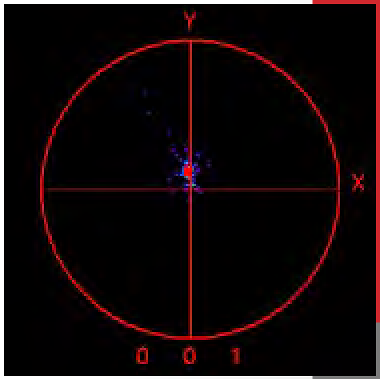




B. Dynamic compression strain mapping

Laue XRD

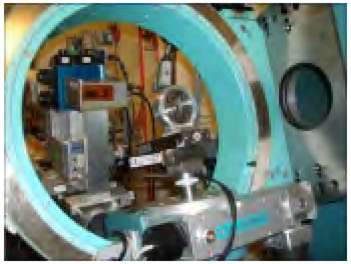




C. HE materials

EOS

HPCAT, LLNL



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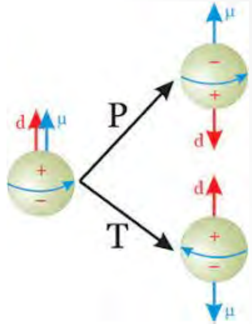
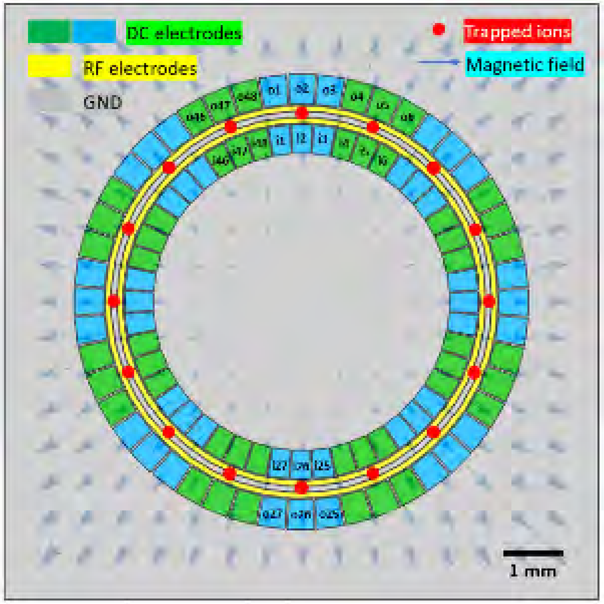
Zhou Group– Precision measurements, quantum computation, and cold chemistry



- Explore new physics beyond the Standard model by precision measurements
- Develop a quantum transducer bridging ion trap and superconducting quantum computers
- Cold and ultracold ion-radical collisions
- Dual optical frequency comb high-resolution and ultrafast spectroscopy



https://www.physics.unlv.edu/~yanzhou/index.html

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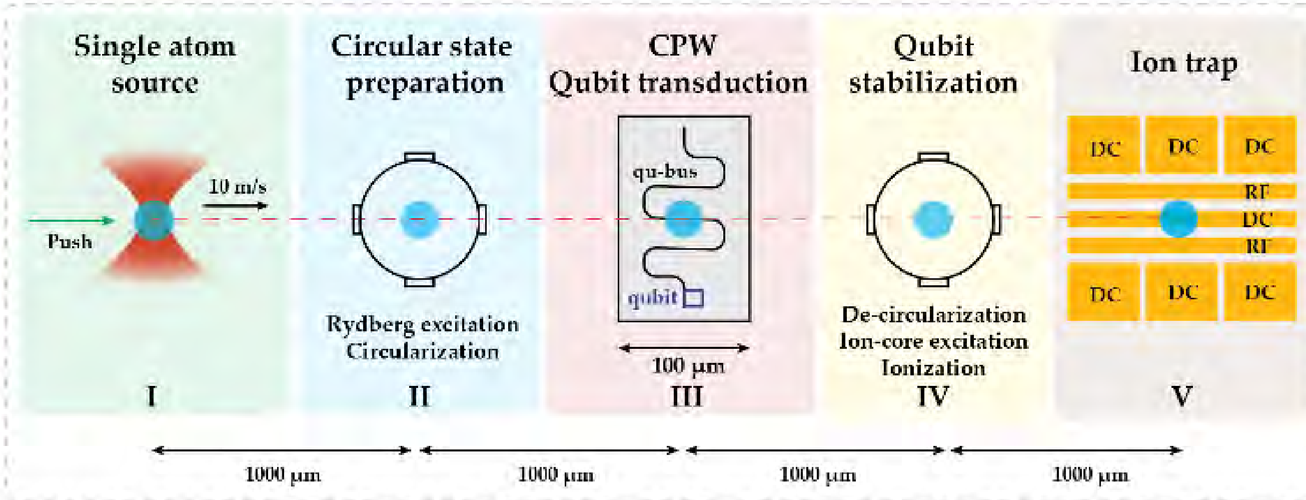
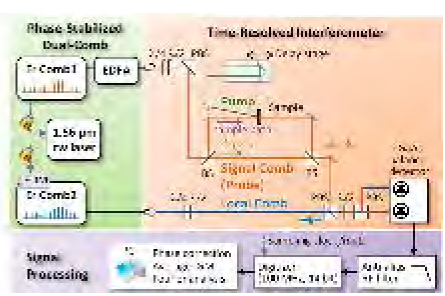
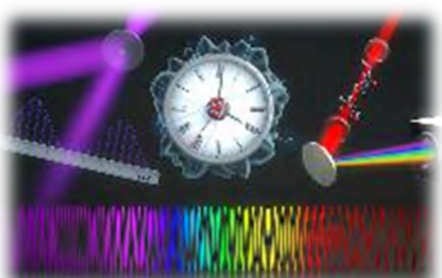
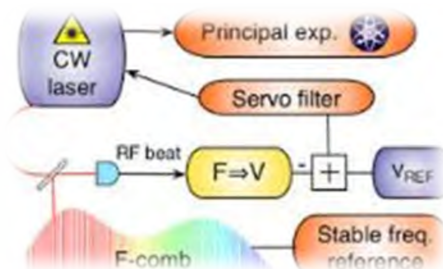
Quantum transducer bridging ion trap and supercoducting quantum computers

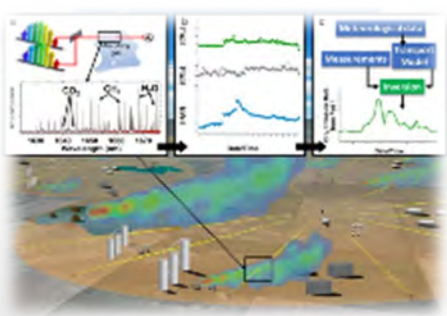


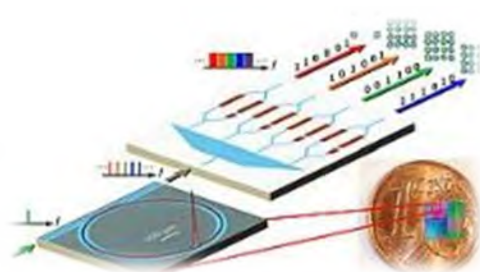
Dual phase stabilized optical frequency combs

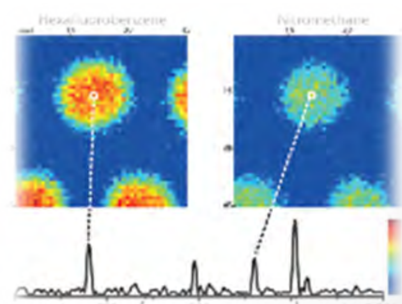




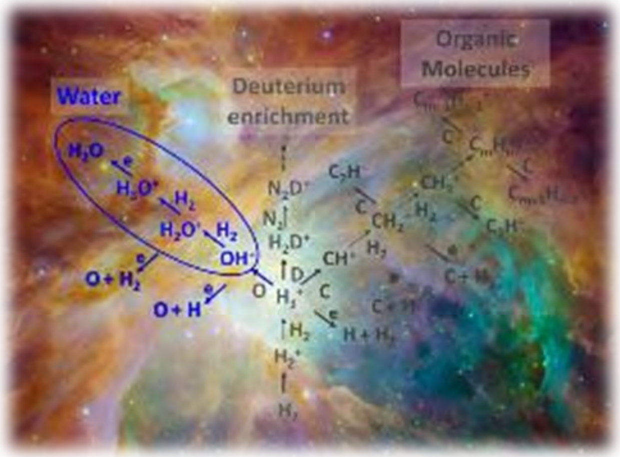




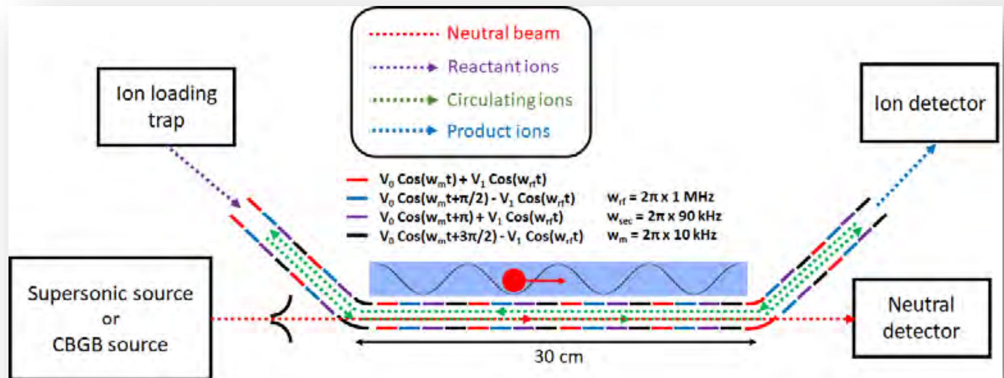


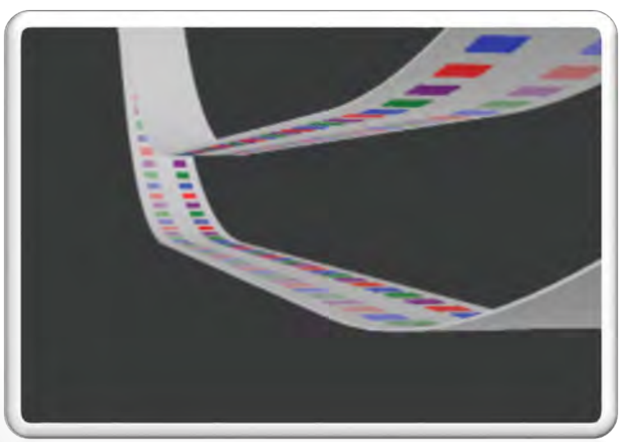


Revealing mechanisms of universe evolutions by studying cold ion-radical reactions



- Chain reactions
- Radiative association
- Tunneling resonances
- Collisional resonances





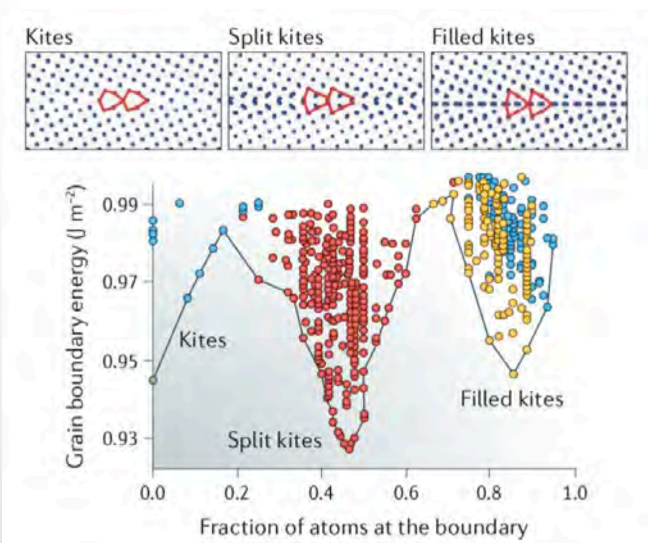
Parameters	Expected specifications
Interaction arm length	30 cm
Ion beam velocity	0-1000 m/s
Collision energy range	<0.1 meV to >100 meV
Energy resolution	<0.1 meV
Effective reaction duration	1 s
Detection sensitivity	1 x 10^{-16} $cm^{-3}s^{-1}$

Qiang Zhu (Structure Prediction Aided by Artificial Intelligence)

USPEX Computational Materials Discovery

PyXtal

- 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



Zhu, et al, Nat. Comm., 2018

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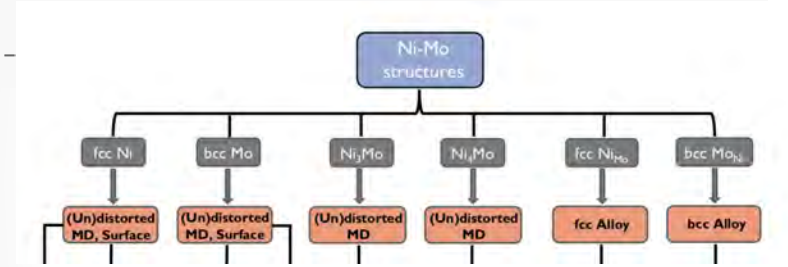
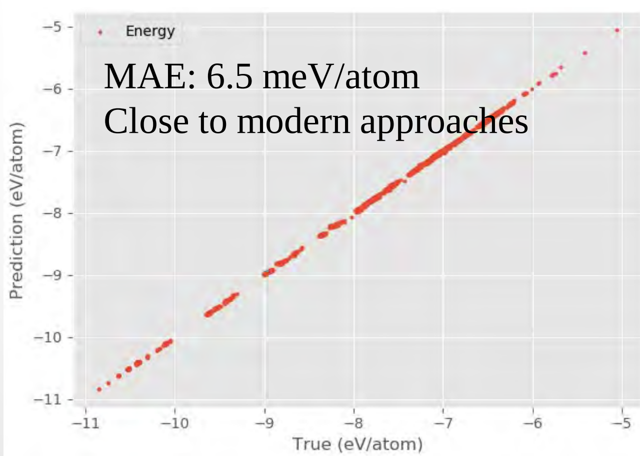
Qiang Zhu (Material Informatics & Big Data Analytics)





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