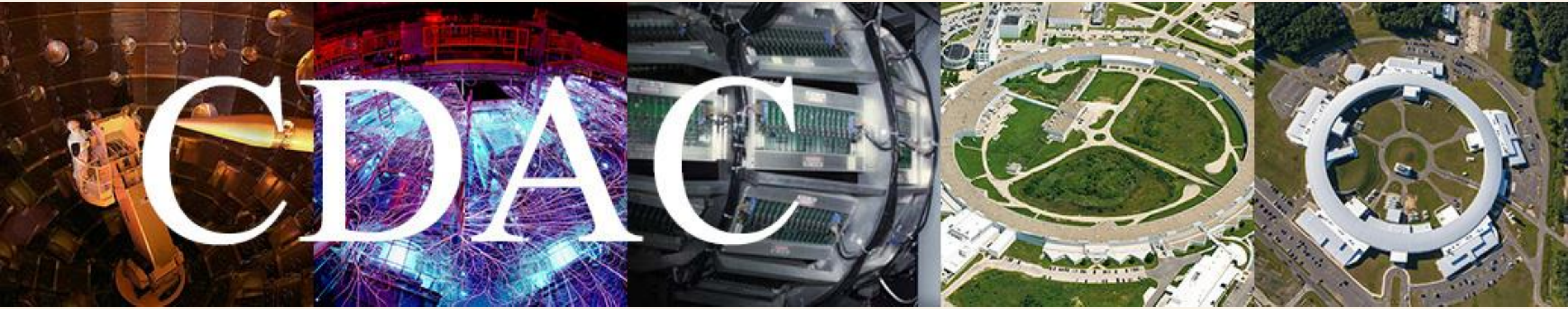


CAPITAL / DOE ALLIANCE CENTER:

A Center of Excellence for High Pressure Science and Technology

Russell J. Hemley

The George Washington University
School of Engineering and Applied Science
Washington, DC 20052

Stewardship Science
Academic Alliances Program

SSAP Symposium, April 12-13, 2017

OUTLINE

1. **Overview**

   MOTIVATION, CENTER STRUCTURE, PERSONNEL

2. **Training**

   EDUCATION, OUTREACH

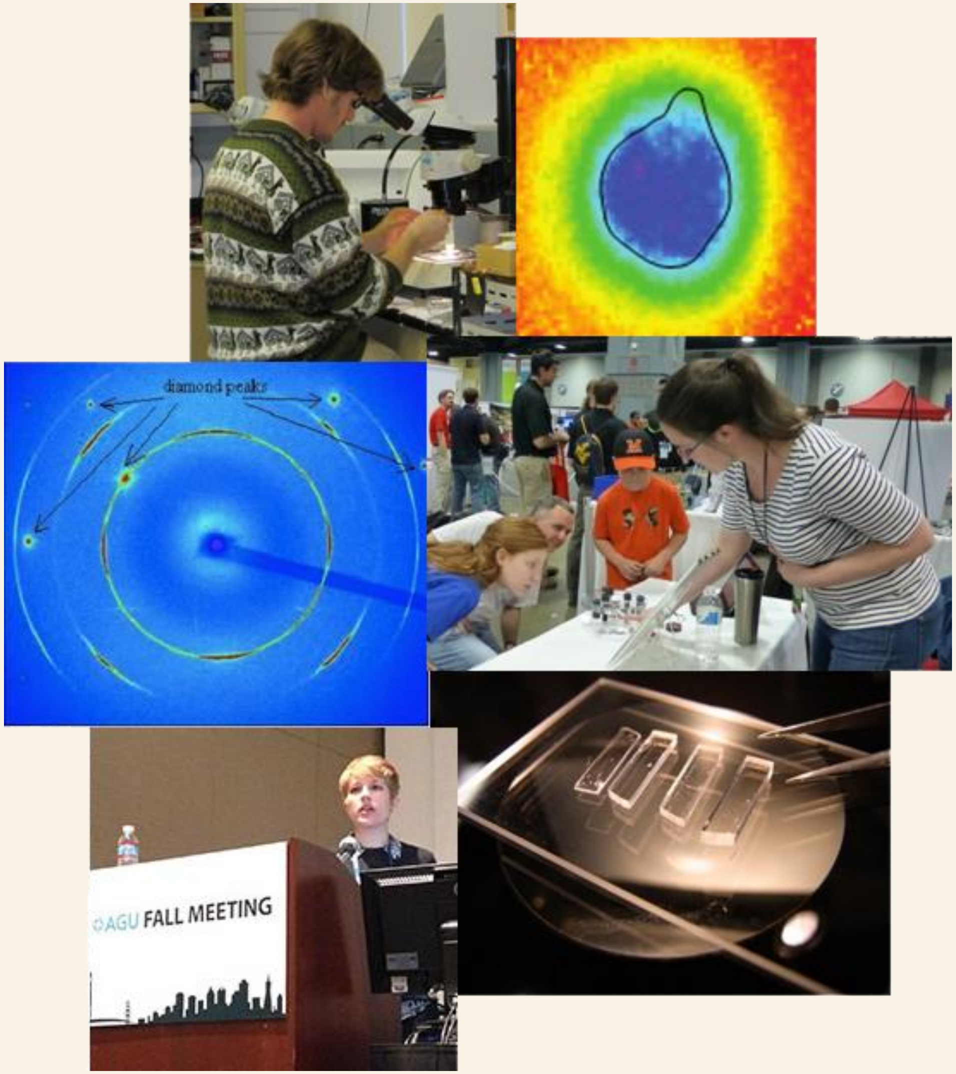
   RESEARCH TRAINING

3. **Selected Science**

   STUDENT AND NNSA LAB PROJECTS

4. **Outlook**

   OPPORTUNITIES

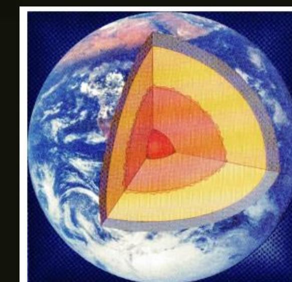


EXTREME ENVIRONMENTS IN THE COSMOS

- Energetic photon/particle flux
- Chemical extremes
- Electromagnetic extremes
- Pressures and temperatures

PRESSURE AS AN EXTREME ENVIRONMENT

Hydrogen gas in intergalactic space
10^{-32} atm



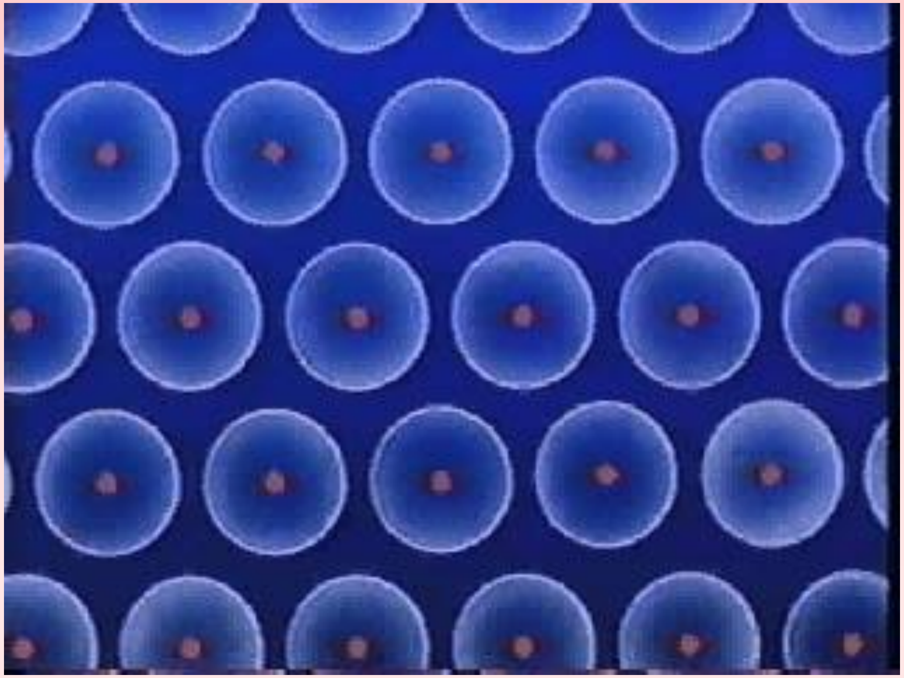
Center of Earth
3.6×10^{6} atm.

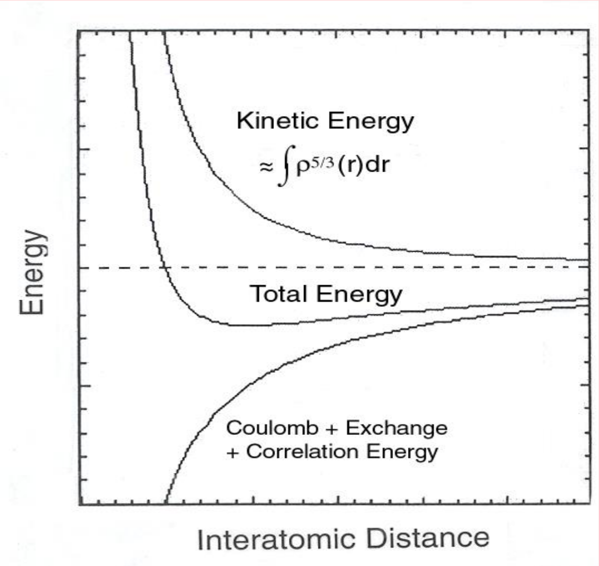
Center of Jupiter -
8×10^{7} atm

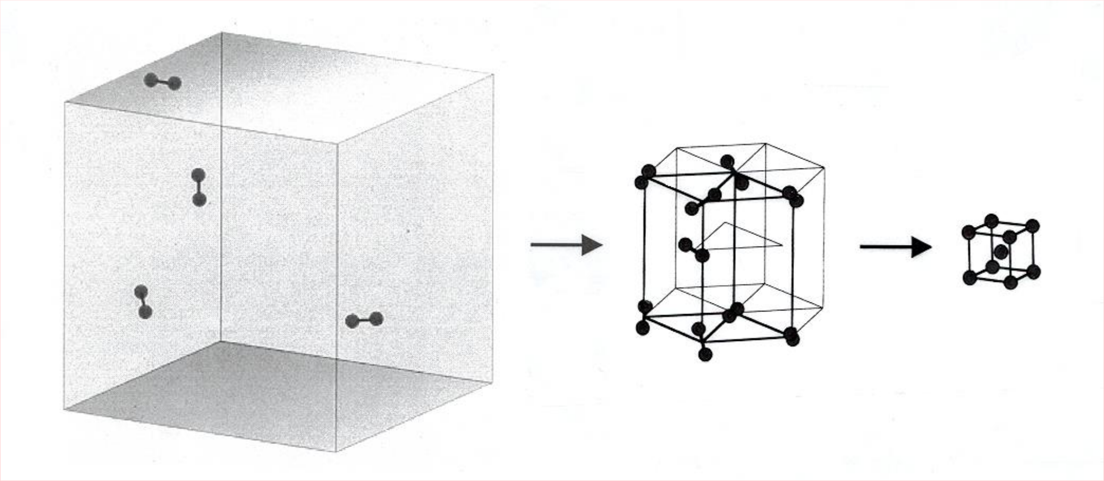
Center of Neutron Star -
10^{28} atm

10^{3} atm $\approx$ kbar
10^{6} atm $\approx$ Mbar
10 kbar = 1 GPa
1 Mbar = 100 GPa

Compressing Atoms and Molecules







>100's GPa (to ~TPa)

~ eV energies

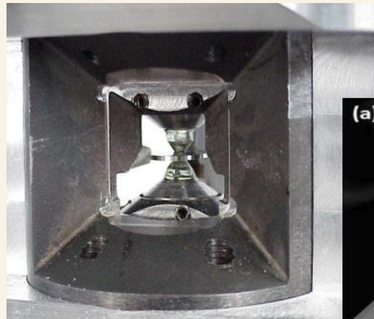
valence electrons

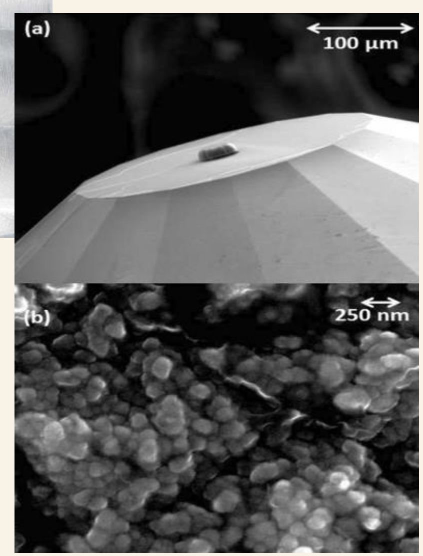
>100's Mbars (1 Gbar)

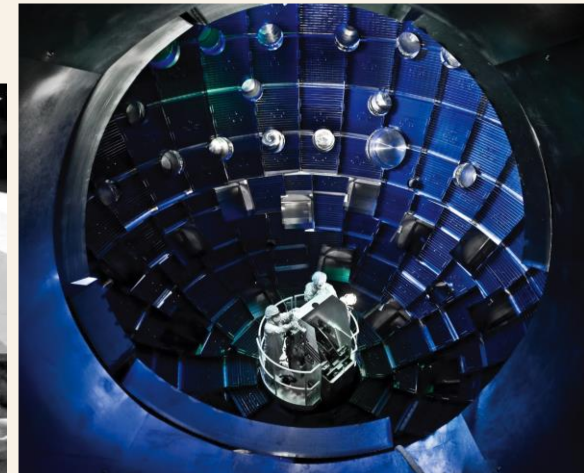
~ keV energies

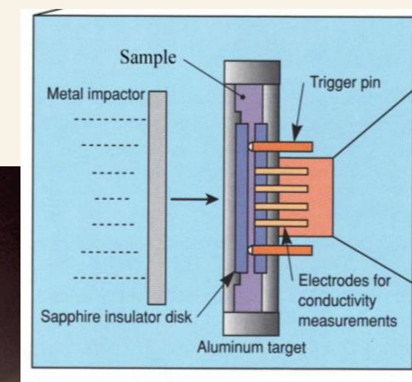
core electrons

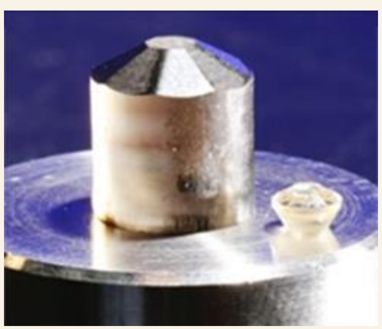
New tools have opened a new world on materials behavior under extreme *P-T* conditions

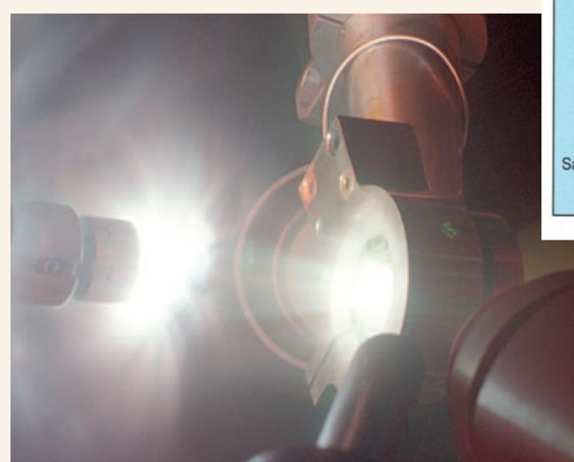








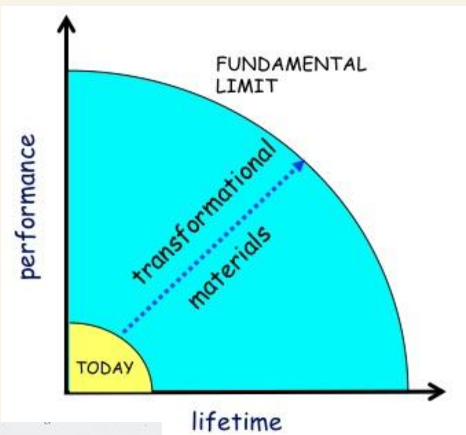


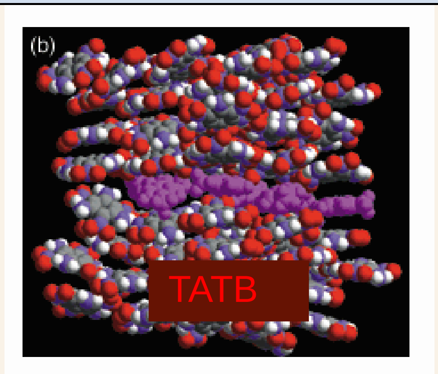


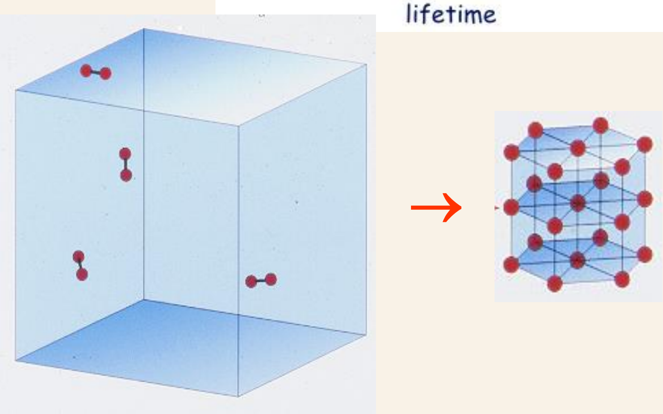
Center Goals

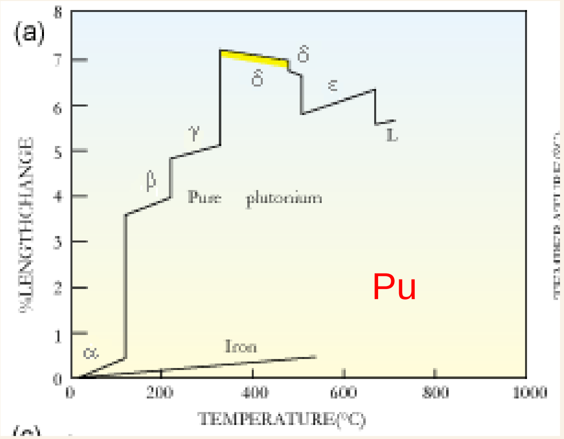
Mission

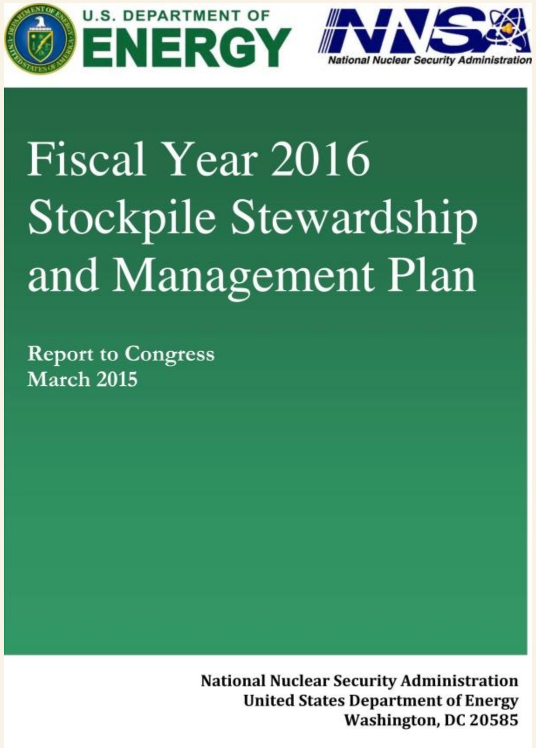
Develop techniques and training to examine the full complement of high *P-T* materials problems essential for stewardship science










U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

Fiscal Year 2016 Stockpile Stewardship and Management Plan

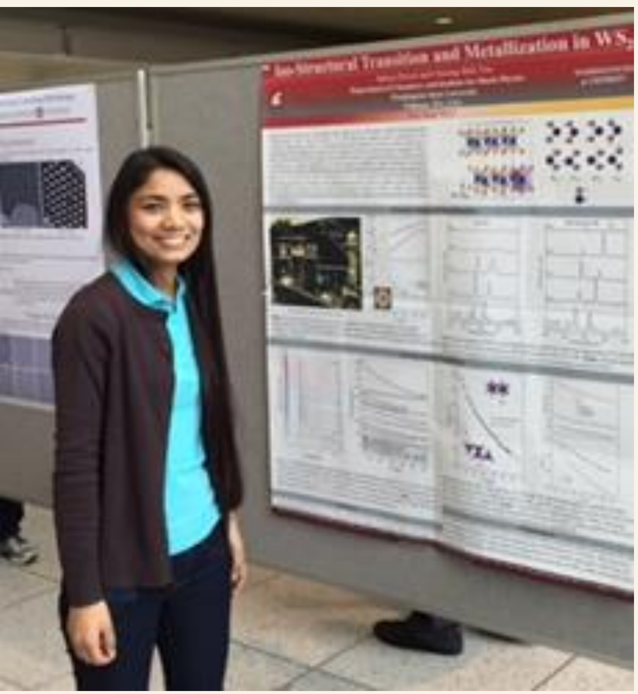
Report to Congress
March 2015

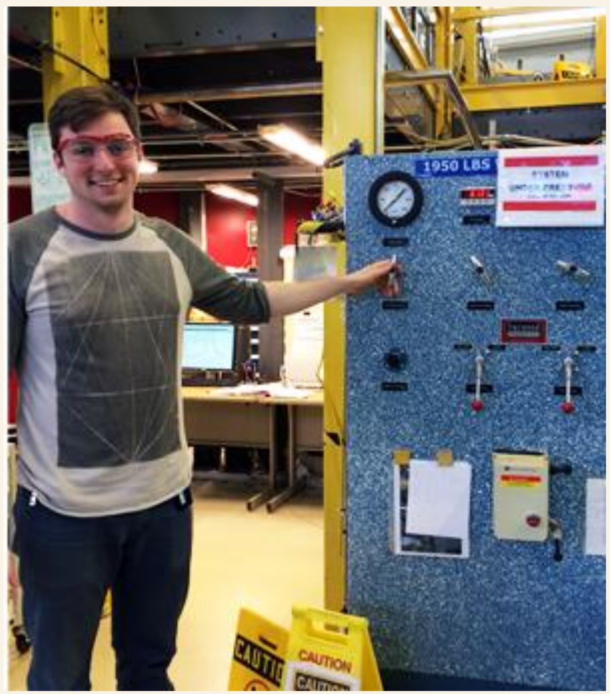
National Nuclear Security Administration
United States Department of Energy
Washington, DC 20585

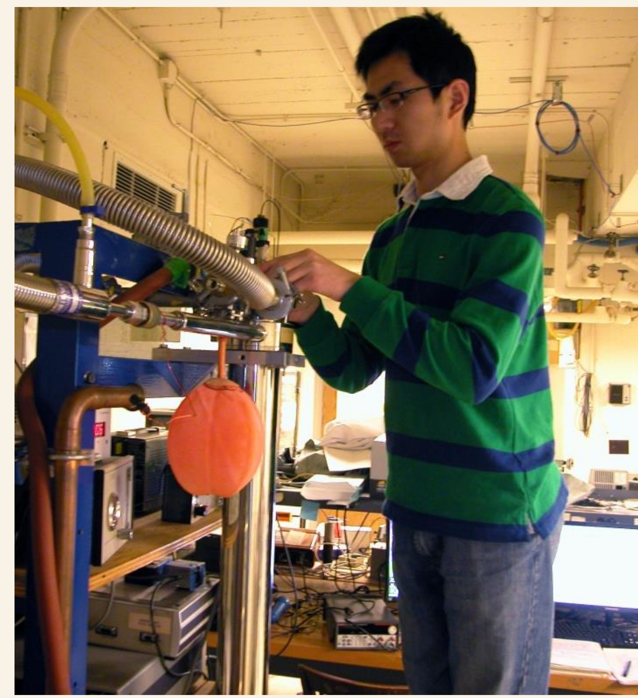
Center Goals

Mission

Develop techniques and training to examine the full complement of high *P-T* materials problems essential for stewardship science







CDAC

➢ ***Train the next generation***

NNSA

Components of the Center

Academic Partners

CALTECH (Fultz)
GEORGETOWN (Ichiye)
MIGHIGAN STATE (Dorfman)
NORTHWESTERN (Jacobsen)
UNIV. ALABAMA – BIRMINGHAM (Vohra)
UNIV. at BUFFALO (Zurek)
UNIV. CALIF. – BERKELEY (Wenk & Jeanloz)
UNIV. CHICAGO (Heinz)
UNIV. HAWAI'I (Dera)
UNIV. ILLINOIS (Dlott)
UNIV. TENNESSEE (Lang)
UNIV. UTAH (Miyagi)
WASHINGTON UNIV. (Schilling)
WASHINGTON STATE UNIV. (Yoo)

Academic Collaborators

FACILITY USERS

NNSA Laboratory Partners

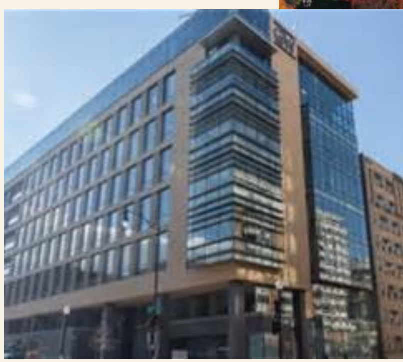
ALL HIGH *P-T* GROUPS AT LLNL, LANL, SNL;
STEERING/ADVISORY COMMITTEE MEMBERS

CDAC

NNSA

CDAC manages and coordinates activities at various facilities for high *P-T* research

CARNEGIE INSTITUTION



GEORGE WASHINGTON UNIVERSITY

- **CDAC DC facilities**

  High P-T technology
  Spectroscopy labs
  Diffraction and microanalysis
  Computational resources
  CVD diamond/materials growth
  Sample preparation

- **CDAC Headquarters**

Steve Gramsch
Coordinator/
Research Scientist

Morgan Phillips
Administrator

Maddury Somayazulu
Senior Lab Manager/
General high pressure

Muhtar Ahart
Ferroelectrics,
Polymeric Materials

Ivan Naumov
Theory and
Computation

Chang-sheng Zha
Hydrogen/
Molecular Systems

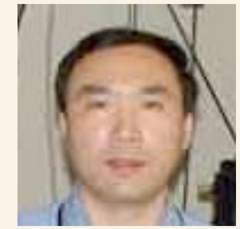
- **Manage facilities**
- **Student mentoring**
- **Visitor training**
- **Technique development**

Kadek Hemawan
CVD, Synthesis

CDAC manages and coordinates activities at major facilities for high *P-T* research

- **High *P-T* synchrotron IR beamline at BNL (NSLS-U2A)**
- **Major component of CDAC**
- **Academic and NNSA Lab users (*e.g.*, LANL, SNL, LLNL)**

NSLS-II

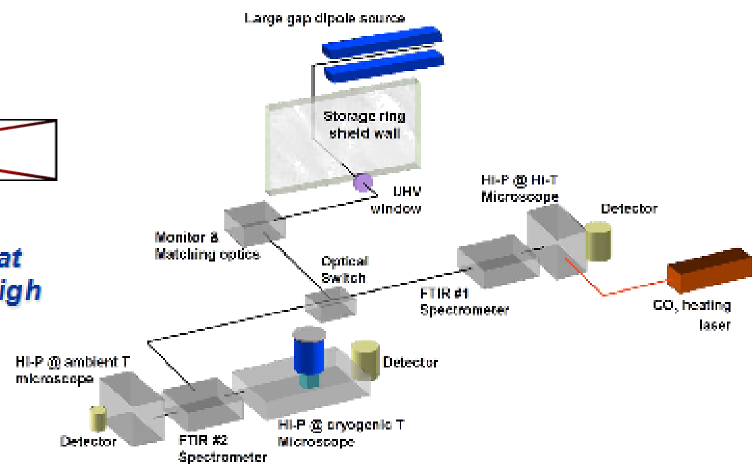


Zhenxian Liu

Floor layout of FIS/MET infrared beamlines at NSLS II

COMPRES

Large-gap IR Beamline at NSLS-II: Endstation for High P-T Devices

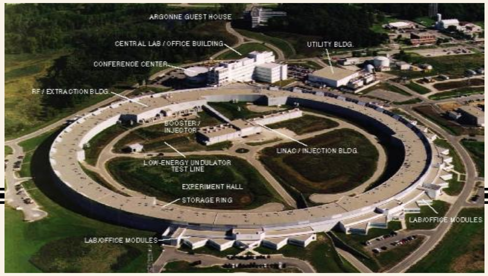


- **Frontier Infrared Spectroscopy (FIS) beamline to be completed in 2017**
- **Improved perform. (stability, far-IR)**
- **New opportunities for NNSA Labs and SSAAP**

CDAC

NNSA

CDAC facilitates high *P-T* experiments at HPCAT at APS



HPCAT HIGH PRESSURE COLLABORATIVE ACCESS TEAM
at the Advanced Photon Source
GEOPHYSICAL LABORATORY, Carnegie Institution of Washington

- **HPCAT (Sector 16) launched in 1998**
- **Dedicated high-pressure facility**
  - Physics, chemistry, materials
  - Advanced techniques
  - Programmatic work (NNSA Labs)
- **Training and education**
  - More than 60% users are students and post-docs
- **Enhanced capabilities**
- **2012 Trilab (LLNL, LANL, SNL)**
- **Upgrades of APS and HPCAT**

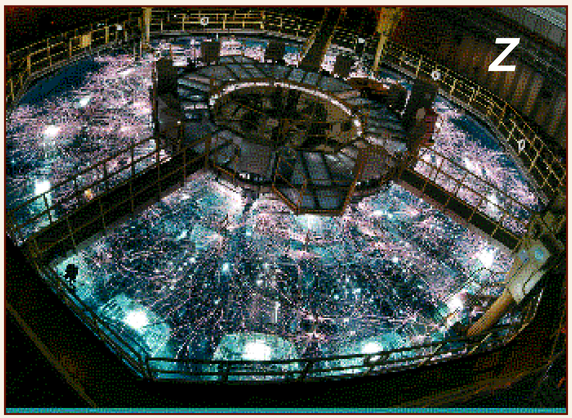
- 9 hutches
- 4 independently operating stations
- support laboratories

Guoyin Shen
HPCAT Director

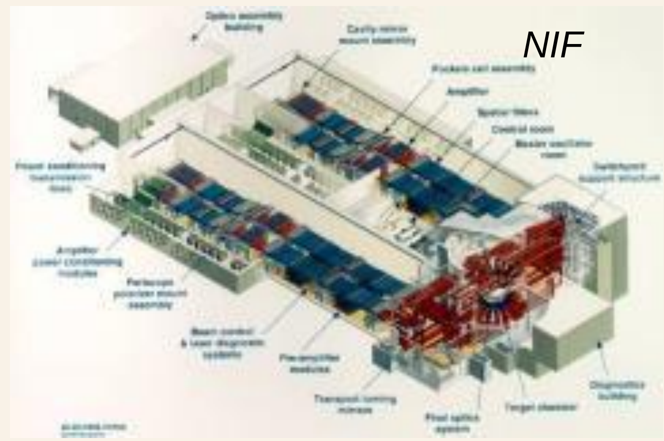
Operations 100% Funded by DOE/NNSA

CDAC supports and promotes research activities at other major DOE facilities

- **Technique development/support for NNSA Lab facilities**



- **CDAC co-leads NIF Discovery Science Campaigns**



1. **Hydrogen 'PPT' Fluid Transition**
2. **Fe Melting 2 TPa in 'habitable' exoplanets**
3. **Hydrogen near melting to TPa pressures**

Neutron diffraction to 100 GPa

[Boehler *et al.*, *High Pres. Res.* (2014)]

CDAC HIGHLIGHTS 2016-2017:

Education, training and outreach

2. TRAINING

- **Supported 17 PhD students – 5 PhDs awarded**
- **56 total PhDs awarded with CDAC support**
- **4 early career scientists join DOE/NNSA labs/HQ**
  - Max Murialdo (Caltech) to LLNL
  - Will Shaw (Illinois) to LLNL
  - Joshua Townsend (Northwestern) to SNL
  - Andrew Shamp (Buffalo) to NNSA HQ
- **CDAC/HPCAT/Lab collaborations**
  - 580+ collaborators/coauthors from 150+ institutions
- **Presentations at major national meetings**
  - AGU – Fall 2016: 29 abstracts; APS – March 2017: 31 abstracts
- **Student and Faculty Awards**
  - Yi Hu (Univ. Hawai'i Bullard Fellowship)
  - Sakun Duwal (NASA; WSU Golding Scholarship; WSU Seminar Award)
  - Will Bassett (APS GSCCM Early Career Award)
  - Erin Nissen (NNSA Fellowship)
  - Lowell Miyagi (NSF CAREER grant)
  - Brent Fultz (Neutron Scattering Society of America Fellow)
  - Russell Hemley (Marker Lecturer, PSU; Sack Lecturer, Cornell; S&T Lecturer, SNL)

Max Murialdo (LLNL)

Will Shaw (LLNL)

Joshua Townsend (SNL)

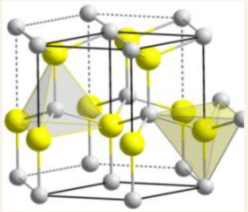
Andrew Shamp (NNSA HQ)

Educational Enrichment at NNSA Labs

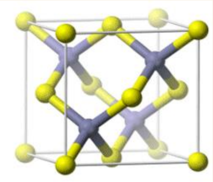
Jane Herriman
California Institute of Technology

LLNL
CCMS Summer Institute
Summer 2016-Present
E. Schwegler X. Andrade, E. Draeger
Ehrenfest Molecular Dynamics
With the Qb@ll Code

Phonon thermodynamics of GaN and related materials



wurtzite



zincblende

Andrew Shamp
University at Buffalo

LLNL
Quantum Simulations
Summer 2014

NNSA Fellow (June 2017)

Eloisa Zepeda-Alarcón
UC – Berkeley

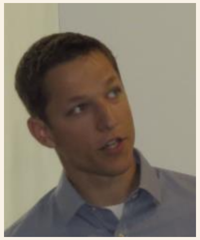
LANL
Materials Science in Radiation and Dynamics Extremes
Summer 2014

LLNL Postdoc (Jan. 2018)

John Lazarz
Northwestern University

LANL - Shock and Detonation Physics
Fall 2014 + September 2015 – December 2016

LANL Postdoc (Jan. 2018)



A broad range of fundamental problems in high *P-T* science is being investigated

3. SCIENCE

- *STRUCTURES AND PHASE RELATIONS*
- *EQUATIONS OF STATE*
- *ELASTICITY, RHEOLOGY, STRENGTH*
- *ELECTRON AND PHONON DYNAMICS*
- *TRANSPORT PROPERTIES*
- *EXTREME CONDITIONS CHEMISTRY*

DIVERSE MATERIALS

- High Z metals
- Molecular
- Systems
- Low-Z gases
- High explosives
- Polymers
- Composites

…

2016-2017: 199 Publications (including in press)

- 27 Student papers (16 Student First Author Papers)

Since 2003: 1790+ Publications

(250+ Student Publications)

- 96 Phys. Rev. Lett., 87 Nature, 25 Science, 83 PNAS

CDAC

NNSA

CDAC HIGHLIGHTS 2015-2016:

Student / Postdoc Presentations

3. SCIENCE

22 posters at this meeting

Muhtar Ahart (Carnegie) - *Sound velocity and energy dispersive x-ray diffraction measurements of B4C and Si-doped B4C at high P-T conditions*

William Bassett (Illinois) - *Shock initiation of explosives under the microscope*

Tiange Bi (Buffalo) - *Superconducting phases of phosphorus hydride under pressure: Stabilization via mobile molecular hydrogen*

Benjamin Brugman (Michigan State) - *Strength of solid krypton and xenon to 94 GPa*

Bethany Chidester (Chicago) - *Phase behavior and equations of state of the actinide oxides*

Samantha Clark (Northwestern) - *Creating binary CuBi compounds at high pressure*

Samantha Couper (Utah) - *High temperature deformation and slip systems in $NaNiF_3$ perovskite and post-perovskite*

Sakun Duwal (Washington State) - *Phase diagram and photochemistry of H_2S and H_2^+S under pressure*

Zachary Geballe (Carnegie) - *Fast electrical heating experiments on PdHx and H_2O at high pressures*

Kadek Hemawan (Carnegie) - *Encapsulated electrodes on diamond anvils for high pressure experiments*

Jane Herriman (Carnegie) - *Thermodynamic properties of GaN: evolution with temperature and pressure in the wurtzite and zincblende phases*

John Lazarz (Northwestern) - *Equation of State of Majoritic Garnet up to 25 GPa*

Feng Lin (Utah) - *Modeling lattice strain and texture evolution in post-perovskite type minerals: implications for slip systems activity*

Samuel Moore (UAB) - *Two-stage nanocrystalline diamond micro-anvils for studies on materials under extreme conditions*

Erin Nissen (Illinois) - *Dynamics of shock compressed water*

Raul Palomares (Tennessee) - *Characterizing the effects of dense electronic excitation in CeO_2 and ThO_2*

Andrew Shamp (Buffalo) - *Theoretical studies of the principle Hugoniot and solid state properties of boron carbide in extreme conditions*

Hannah Shelton (Hawai'i) - *Noble gas transport by amphiboles: In situ structural analysis of neon within ferroactinolite*

Jing Song (Washington University) - *Magnetic ordering at anomalously high temperatures in Nd and Dy under extreme pressure*

James Walsh (Northwestern) - *High-pressure synthesis of unprecedented intermetallic compounds*

Fred Yang (Caltech) - *Magnon-phonon interaction in Pd_3Fe*

Eloisa Zepeda-Alarcon (Berkeley) - *Texture development in two-phase mineral aggregates: Modeling plastic deformation with finite element methods*

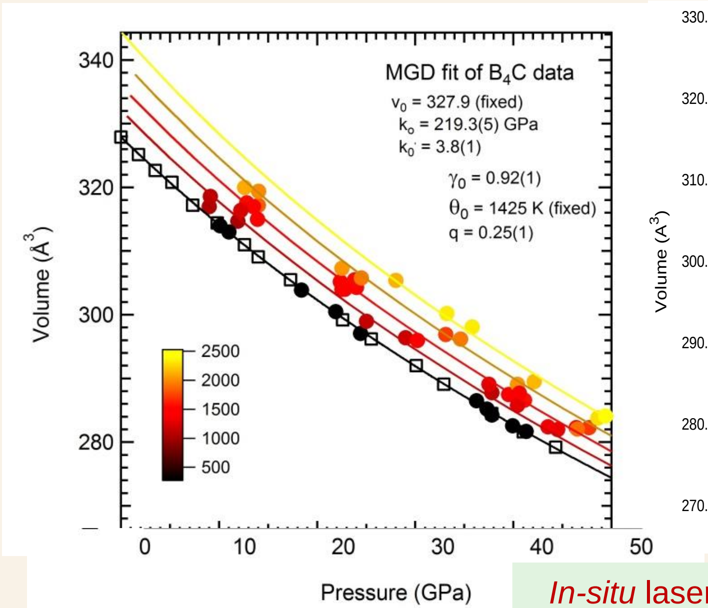
Selected Examples

1. *Structures and EOS*
2. *New Materials*
3. *High Tc Superconductors*
4. *Dense Hydrogen*

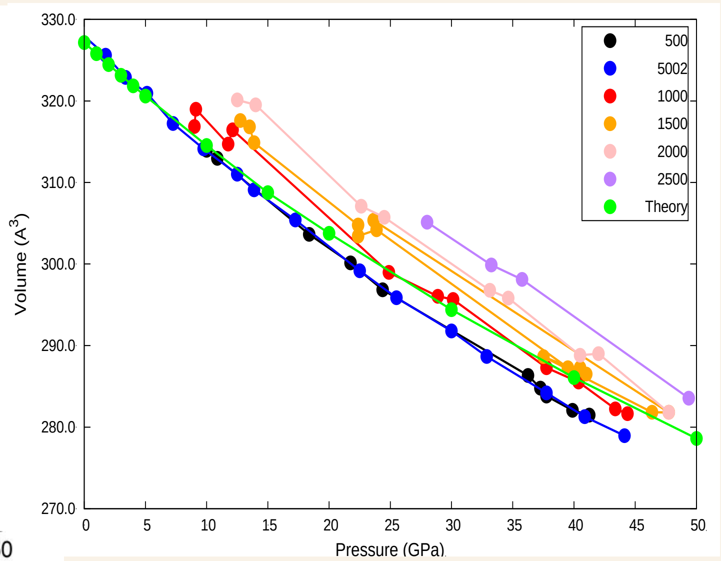
P-V-T EOS of B_4C from static and shock compression

3. SCIENCE

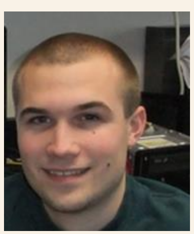
Static

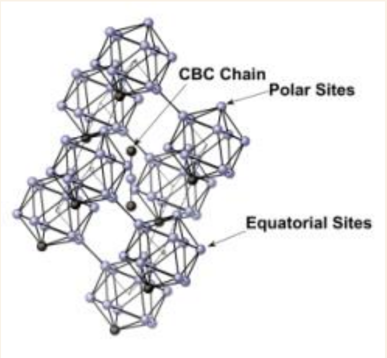


Theory



In-situ laser heating
at HPCAT 16ID-B





Andrew Shamp **Eva Zurek** **M. Somayazulu** **Muhtar Ahart**

CDAC

Buffalo-HPCAT-LLNL-Carnegie

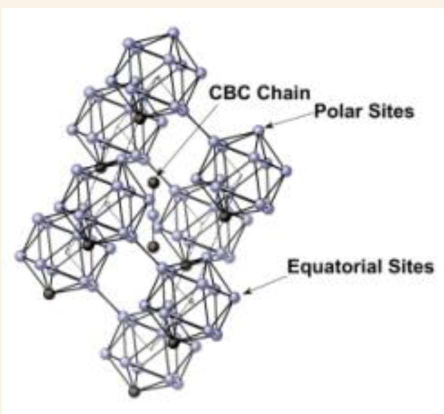
NNSA

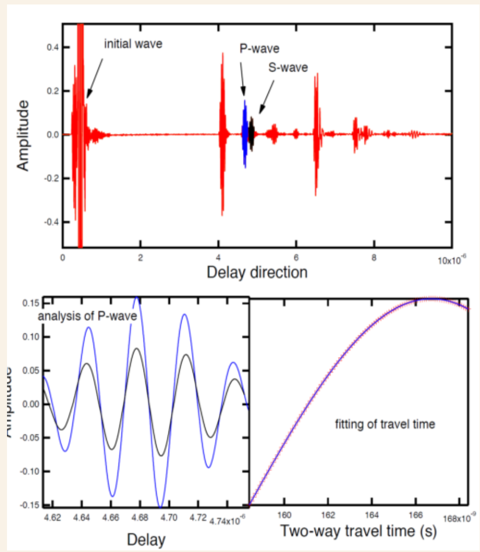
High P-T sound velocity and structure of B_4C and Si-doped B_4C

3. SCIENCE

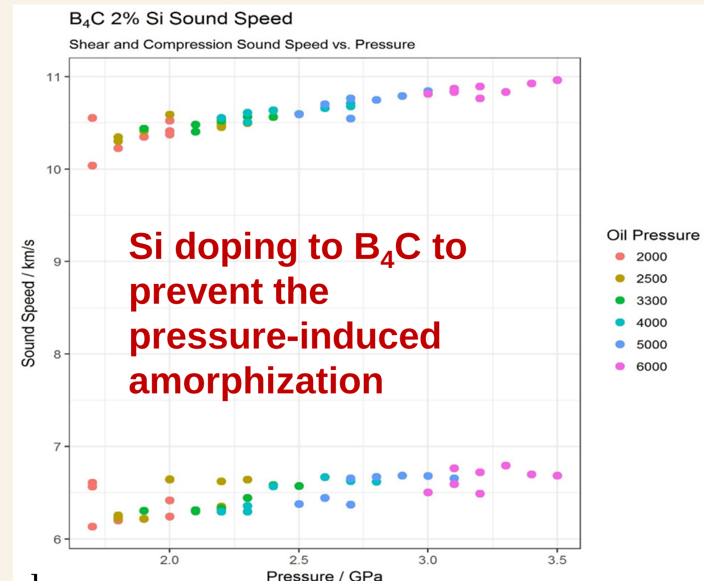
Boron Carbide: high melting point, high stability, outstanding hardness, low density, resistance to wear; and results in a range of applications from neutron control rods in fast breeder reactors, to light body armor, etc.

Rhombohedral
R-3m





Ultrasonic spectrum at 3 GPa and 1073 K. Lower panel shows the analyzed travel time for P-wave.



Pressure dependencies of velocities for Si 2% doped B4C at various temperatures

Jennifer Ciezak Gustav Borstad Muhtar Ahart

ARL-Carnegie-GWU

CDAC NNSA

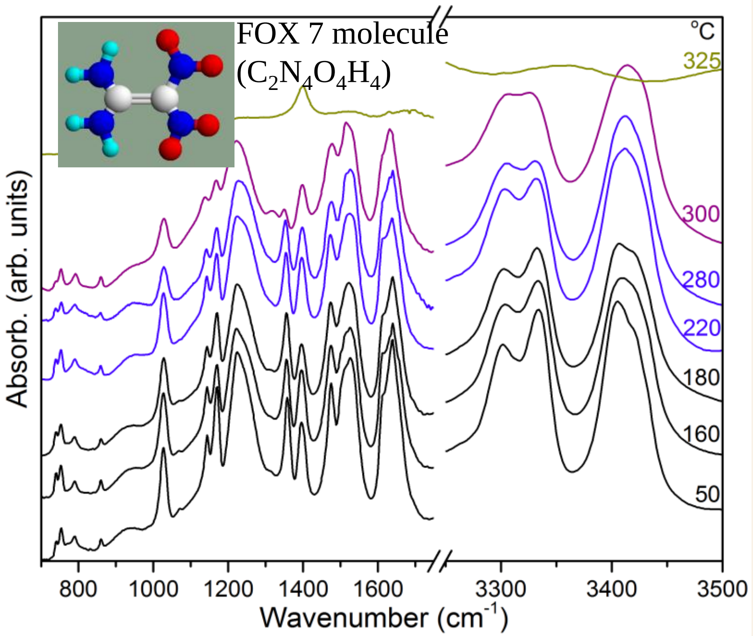
Synchrotron IR studies of energetic materials at high *P-T* conditions

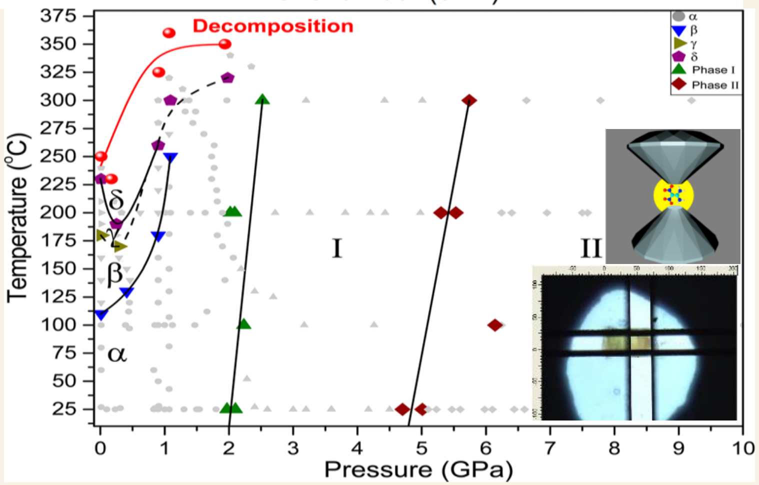
3. SCIENCE

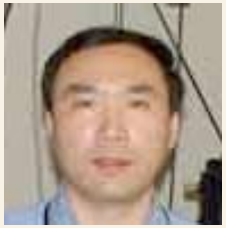
Detailing the complex phase diagram of FOX 7 ($C_2N_4O_4H_4$), an insensitive high power explosive using externally heated DAC combined with synchrotron IR techniques. This study will stimulate additional work on insensitive high explosives.

- In-situ techniques for direct phase determination, IR measurements along with molecular dynamics simulations, were employed to explore the nature of the unusual phase boundaries.
- Resolving multiple solid-solid transitions and determining onsets of decomposition is crucial for further improving our understanding of the behavior of energetic materials.

[M. Bishop, N Velisavljevic, R Chellappa, Y Vohra, *J. Phys. Chem. A* (2015); M Bishop, R Chellappa, Z Liu, D Preston, M. Sandstrom, D Dattelbaum, Y Vohra, N Velisavljevic, *J Phys Chem* (2014)]



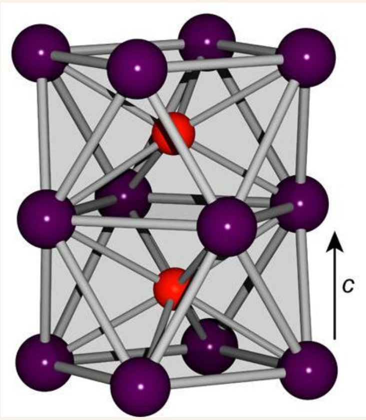




Zhenxian Liu

UAB-Carnegie-LANL

High pressure yields new materials



Discovery of $FeBi_2$

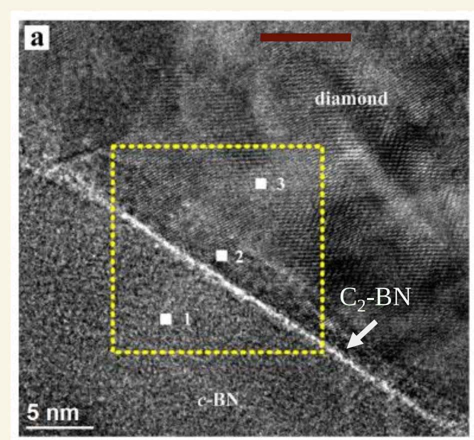
- $FeBi_2$: First chemical bond between Fe and Bi
- 30 GPa / 1800 K

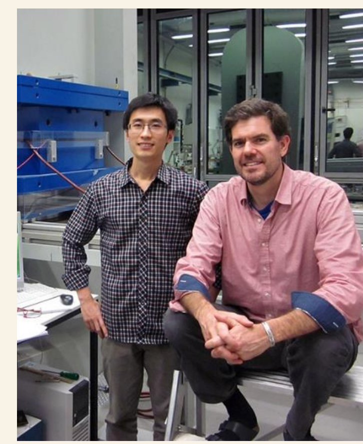
[J. Walsh, S. Clarke et al. *ACS Cent. Sci.* (2016)]

James Walsh, Samantha Clarke (Northwestern)

Ultrahard Stitching in C_2-BN Composite

- Nanotwinned composite of diamond and cBN
- B-C-N solid solution instead of grain boundaries
- ultrahard, Hv = 85 GPa
- p-type seminconductor
- high thermal stability (T_{OX} ~1200K)





Xioabing Liu, Steve Jacobsen)Northwestern)

CDAC

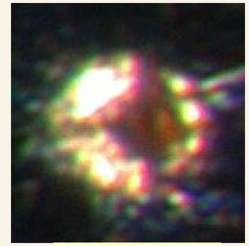
[X. Liu *et al*. *Sci. Rep* (2016)]

NNSA

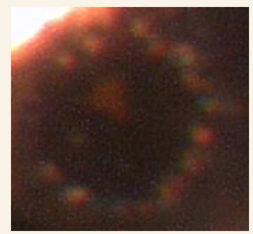
Synthesis of novel compounds: xenon nitride at high *P-T* conditions

3. SCIENCE

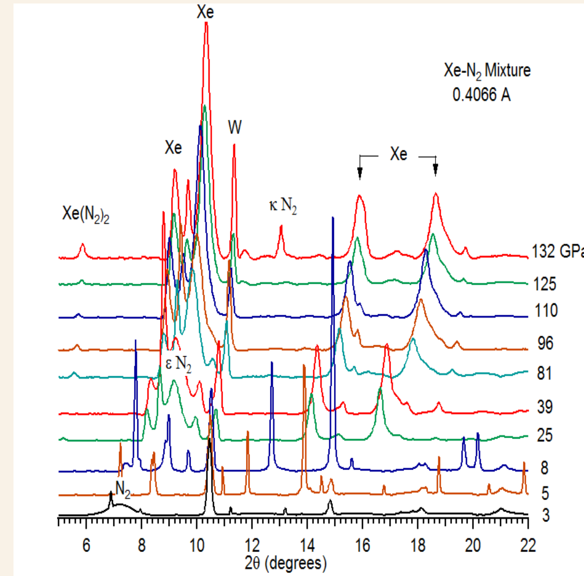
- Mixtures of Xe and N_2 compressed in a DAC form a cubic and bct, vdW compound $Xe(N_2)_2$
- $Xe(N_2)_2$ becomes opaque and black at pressures above 120 GPa where it couples to a YLF laser.
- Pulsed and CW heating yields a monoclinic phase identified as similar to the theoretically predicted Xe_3N_4
- Raman, FTIR spectroscopy indicates presence of linear N_4 units rather than ring-like N_6 units

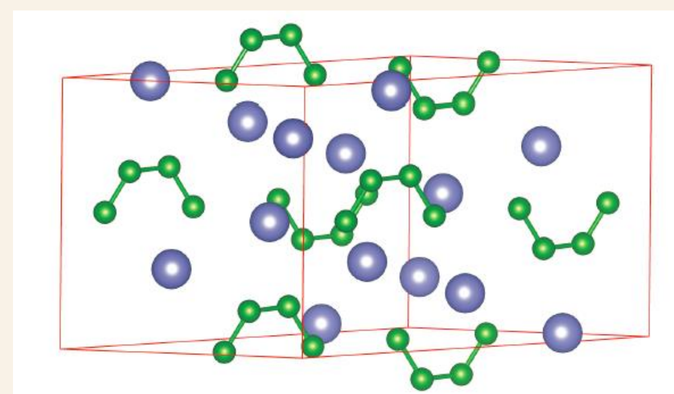


12 GPa



132 GPa





M. Somayazulu

Yue Meng

Dana Dattelbaum

[M. Somayazulu et al., *in preparation*]

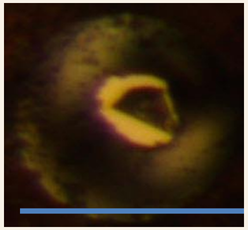
CDAC

Carnegie-GWU-LANL-HPCAT

NNSA

Synthesis and compression of PdH_x and PdD_x to megabar pressures

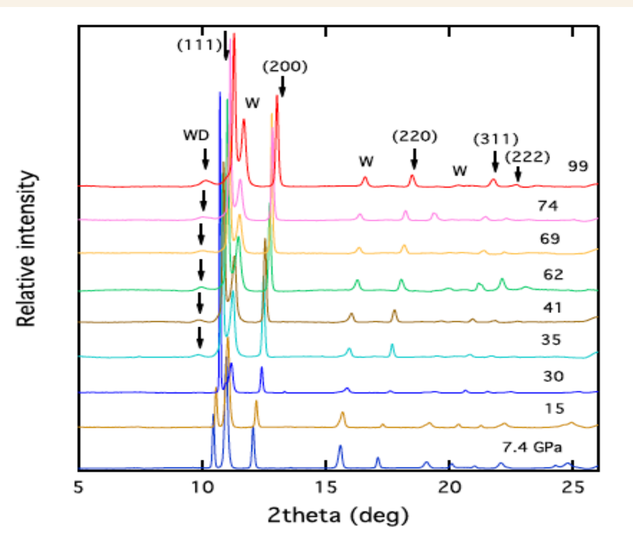
3. SCIENCE



100 microns

Pd Foil / Deuterium at 10 GPa at 300 K

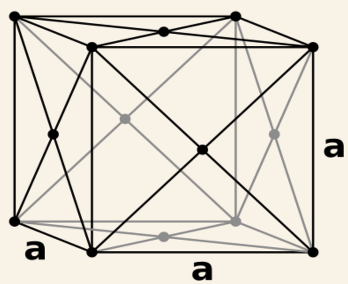
- **High-pressure behavior of PdH(D), a known superconductor?**
- **PdH_x where x > 1 is predicted to have a much higher T_c.**
- **Can we create PdH_x or PdD_x where x > 1 under pressure ?**



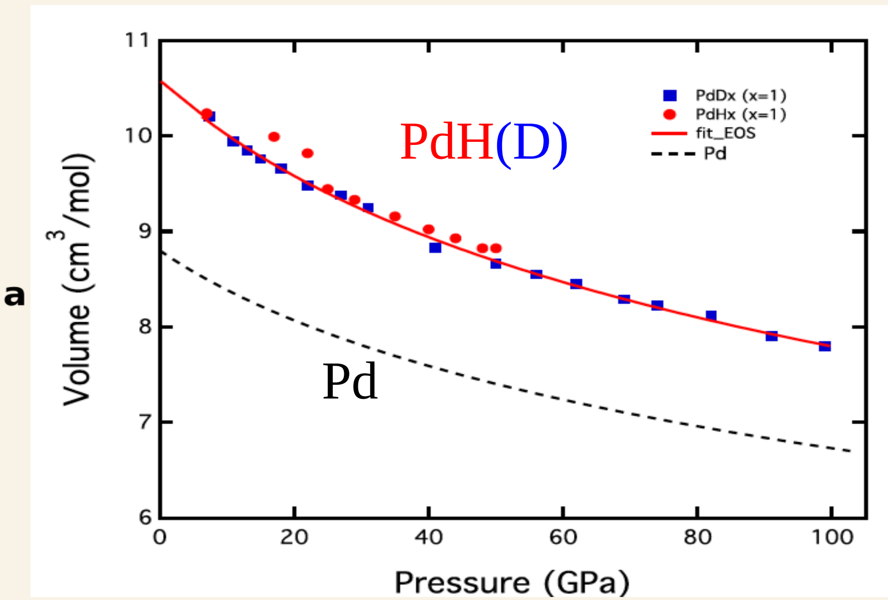
Diffraction patterns of PdD_x show th at PdD persists up to 100 GPa

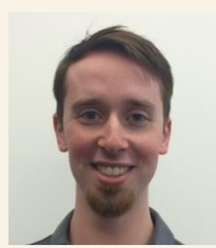
[Ahart *et al., in preparation*]

Structure



FCC Pd and PdHx





Keenan Brownsberger

Muhtar Ahart

- **Synthesis of PdD_x and Pd H_x with x=1**
- **No structural transitions obs erved up to 100 GPa**

CDAC

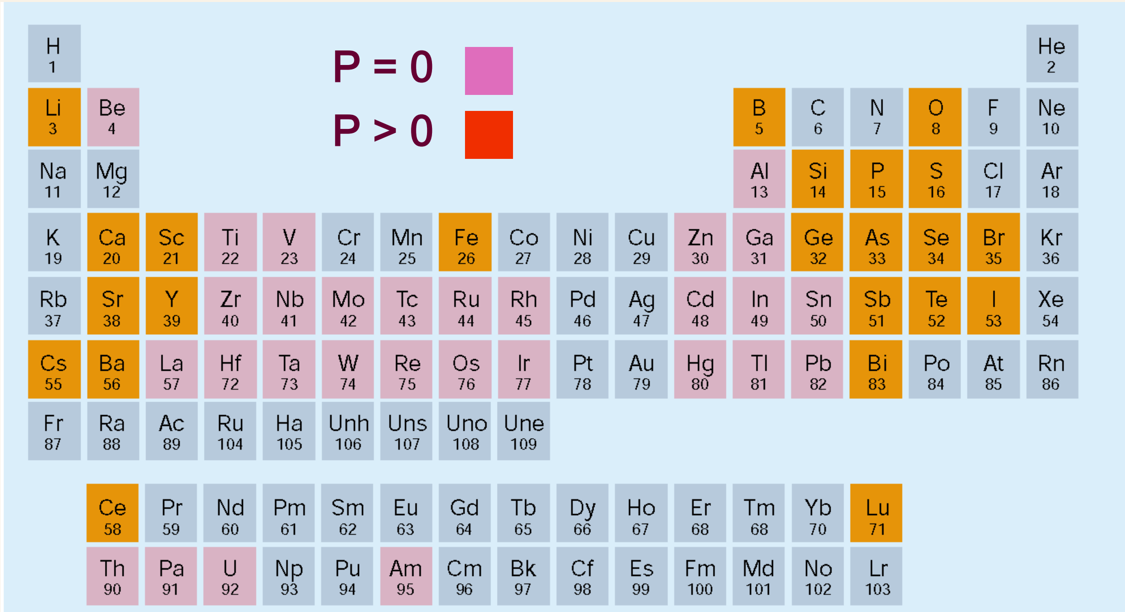
Whitworth-Carnegie

NNSA

High-Pressure Superconductivity

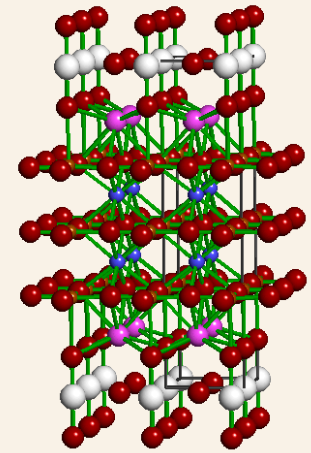
SUPERCONDUCTING ELEMENTS

23 produced under pressure; e.g., O, S, B, Fe, Li, Ca



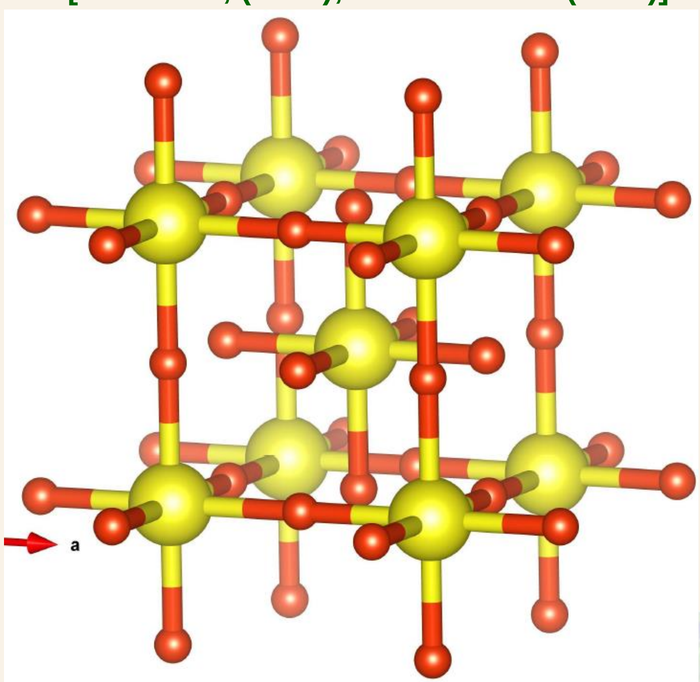
$HgBa_2Ca_2Cu_3O_{8+\delta}$

T_c = 164 K (30 GPa)



[Gao *et al*., (1994); Lokshin *et al.* (2002)]

'H_3S'



- ***Still higher T_c?***
- ***Other 'superhydrides'?***
- ***Recoverable phases?***

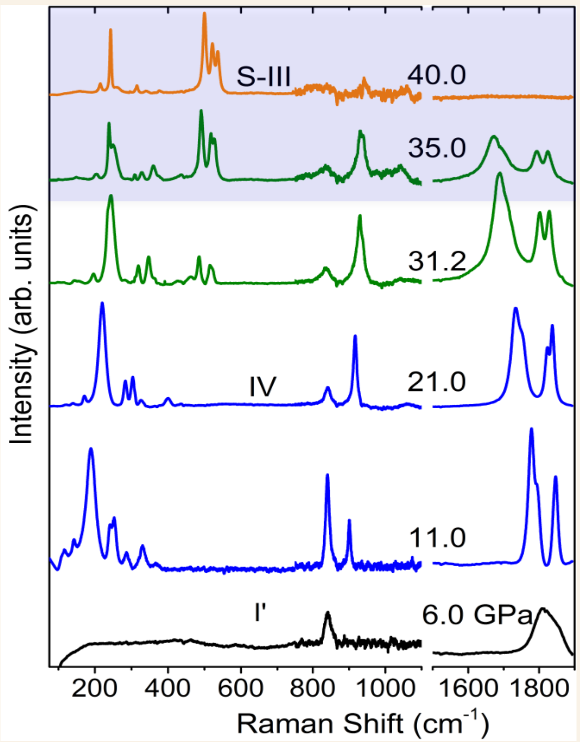
T_c = 203 K (200 GPa)

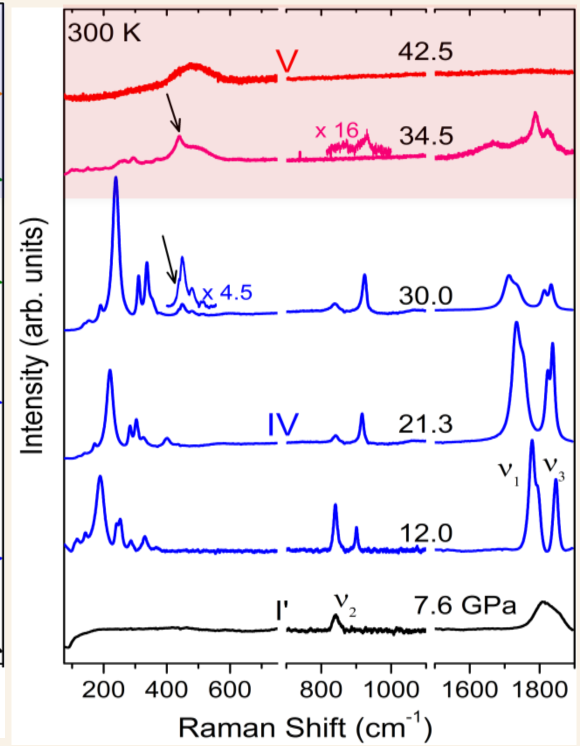
[Drozdov et al., *Nature* (2015)]

Transformations in H_2S

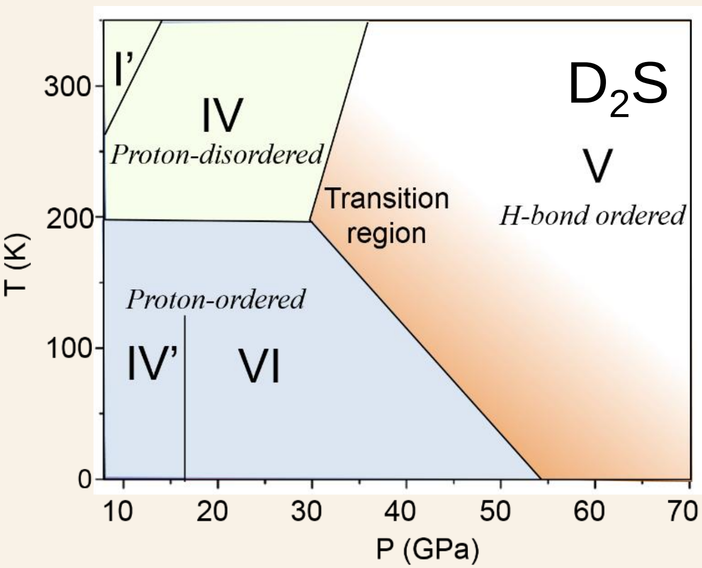
Photo-Decomposition
Under Light

No Photo-Decomposition
Under Dark





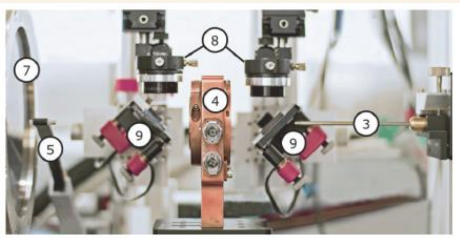
Sakun Duwal
(Washington State)



[S. Duwal and C. S. Yoo. *J. Phys. Chem C* (2016)]

Synthesis of superconducting hydrides megabar pressures

3. SCIENCE

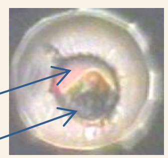


Laser heating set up

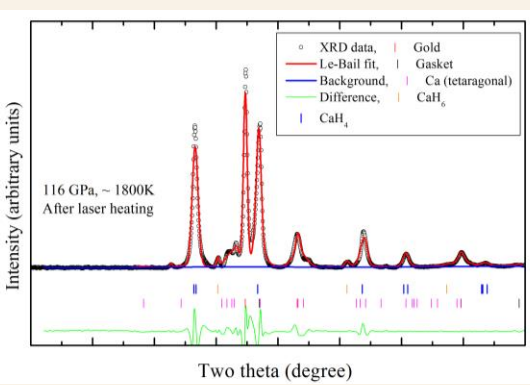
- Laser heating in presence of hydrogen is detrimental for diamond anvils and causes failure
- Pulsed laser heating was adapted for in-situ synthesis of higher hydrides as superconductive material
- Wang et al. (2012) predict that sodalite CaH_6 with T_c~ 235 K

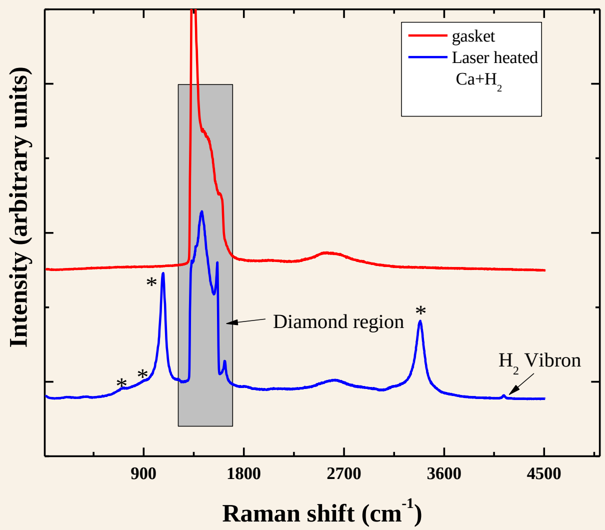
Schematic pulsed heating

H_2 Ca



100 µm

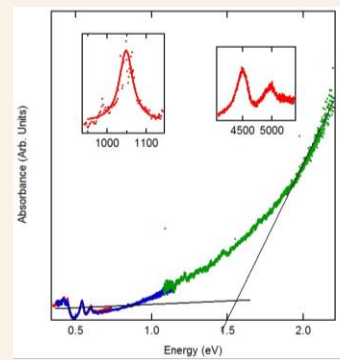




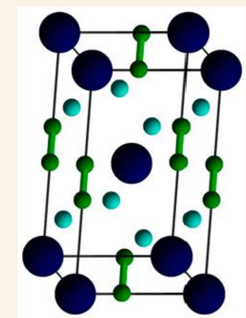
Raman spectra of laser heated $Ca+H_2$ at ~120 GPa

'*' Raman modes for CaH_4

[A. K. Mishra *et al., in press*]

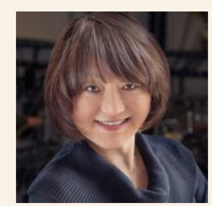


IR absorbance of the band gap



Tetragonal CaH_4

Ajay K Mishra



Yue Meng

Eva Zurek

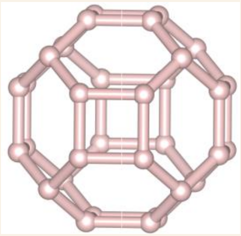
CDAC

Carnegie-GWU-Buffalo-HPCAT

NNSA

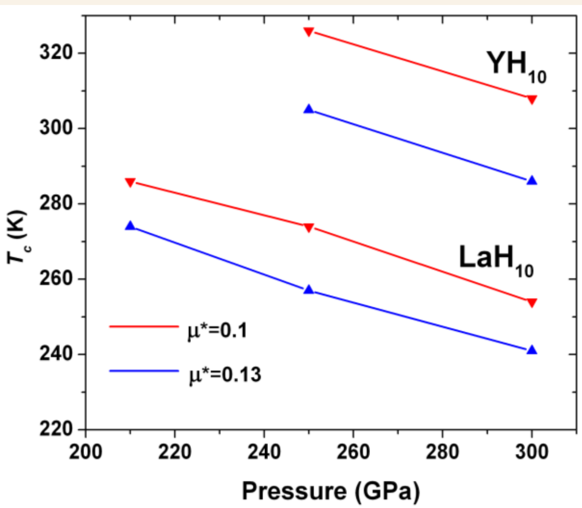
Predicted high T_c superconductivity in compressed lanthanum and yttrium hydrides

3. SCIENCE



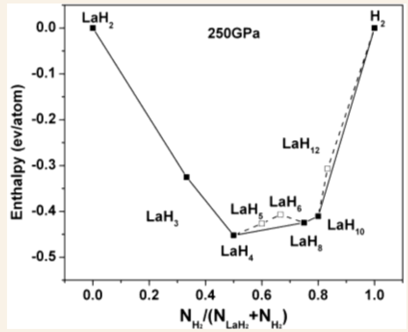
$[4^6 6^{12}]$

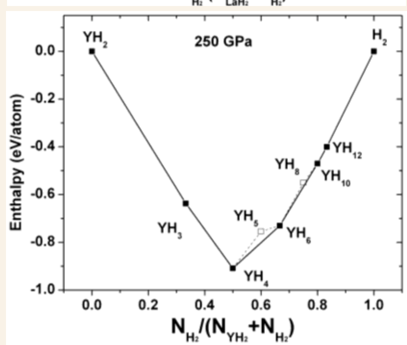
- **Is it possible to predict a room temperature superconductor?**
- **More hydrogen content, the T_c is higher**
- **More valence electrons, the more hydrogen content**

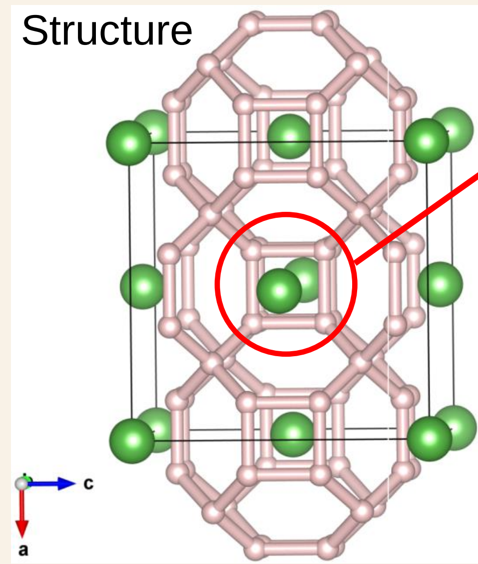


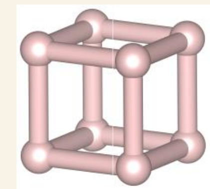
T_c as a function of pressure

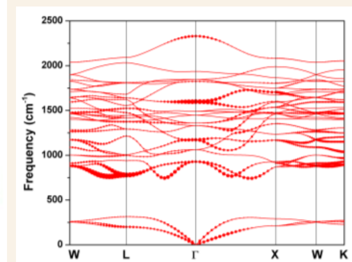
[Liu *et al.*, *PNAS, in press*].











Dynamically stable

- **LaH_{10} and YH_{10} are predicted to be stable above 200 GPa**

T_c is about 300 K at 250 GPa

Hanyu Liu

Ivan Naumov

Roald Hoffman

N.W. Ashcroft

CDAC

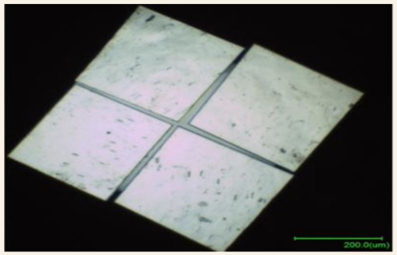
Carnegie-Cornell-GWU

NNSA

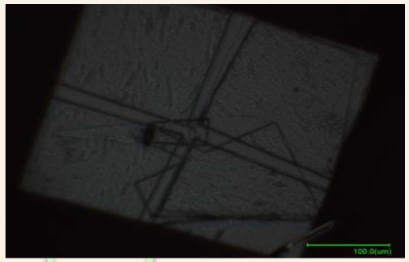
Encapsulated Electrodes on Diamond Anvils for High Pressure Experiments

3. SCIENCE

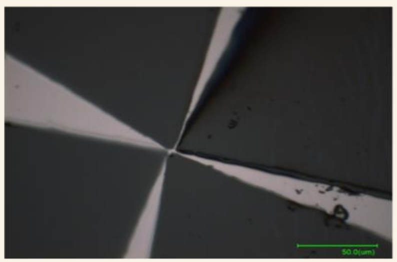
Fabrication of diamond anvils encapsulation



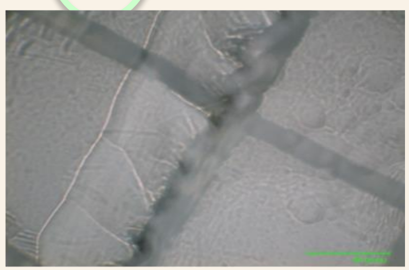
1. masked



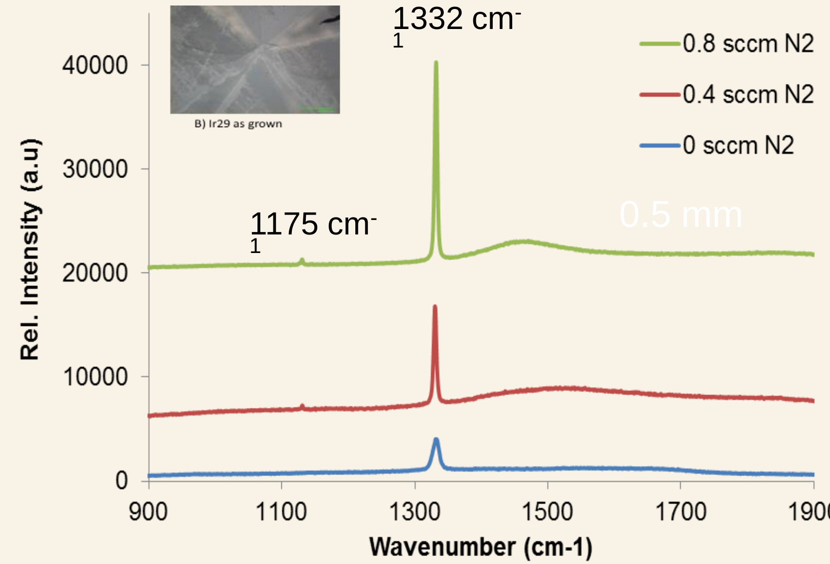
2. etch



3. sputtered



4. CVD growth



Effect of N_2 addition in plasma chemistry

[K. Hemawan *et al., in progress*].

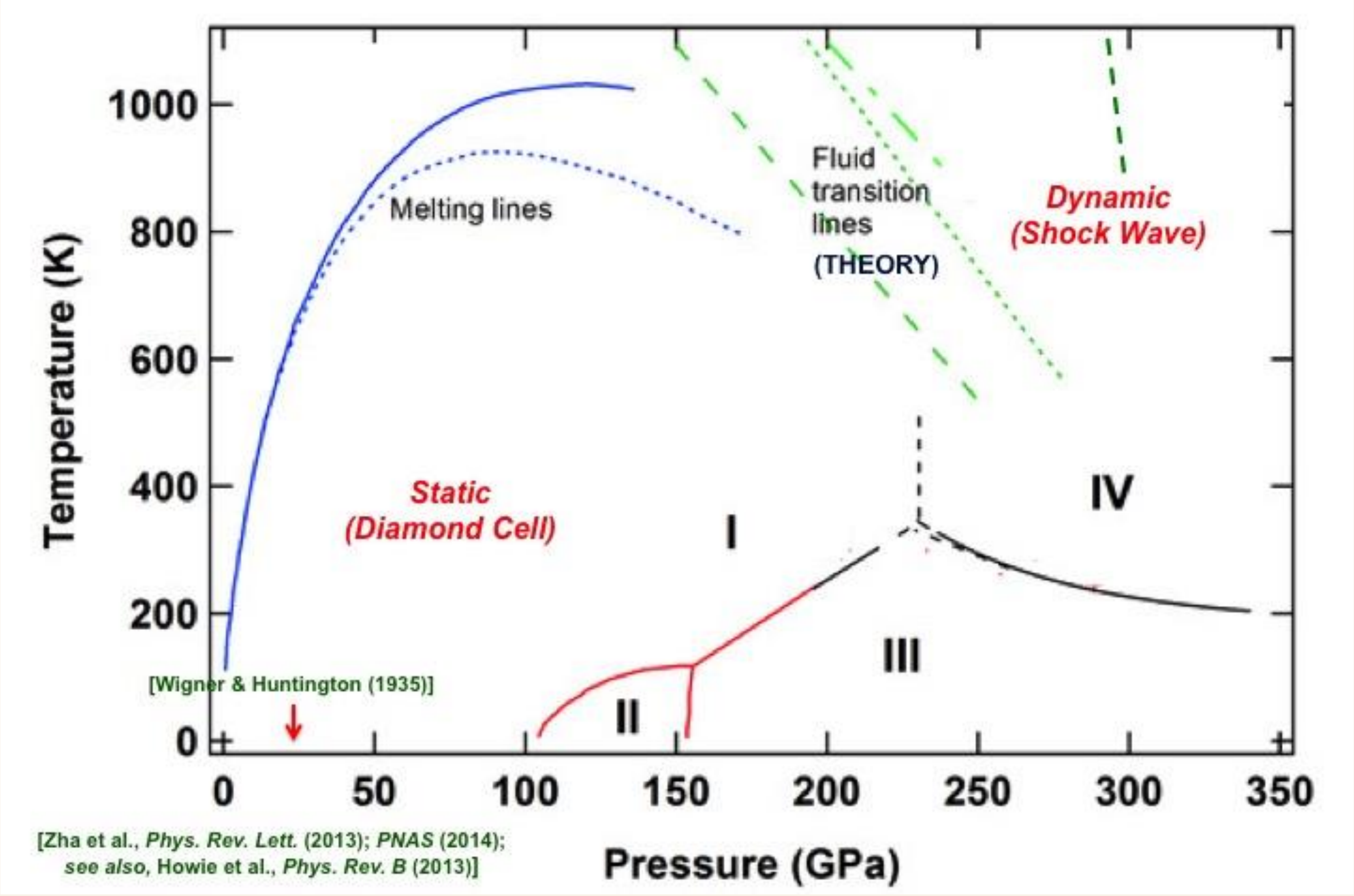
- **Electrical resistance measurements of high-pressure hydrogen or metallic polyhydrides using diamond designer anvils has potential to reveal new superconductors with transition temperatures above 200 K.**
- **The encapsulation is achieved by specific pocket design holder, nitrogen addition, and substrate temperature of 1050 ° C.**

Zack Geballe

Kadek Hemawan

Carnegie

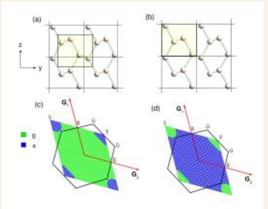
Hydrogen *P-T* Phase Diagram



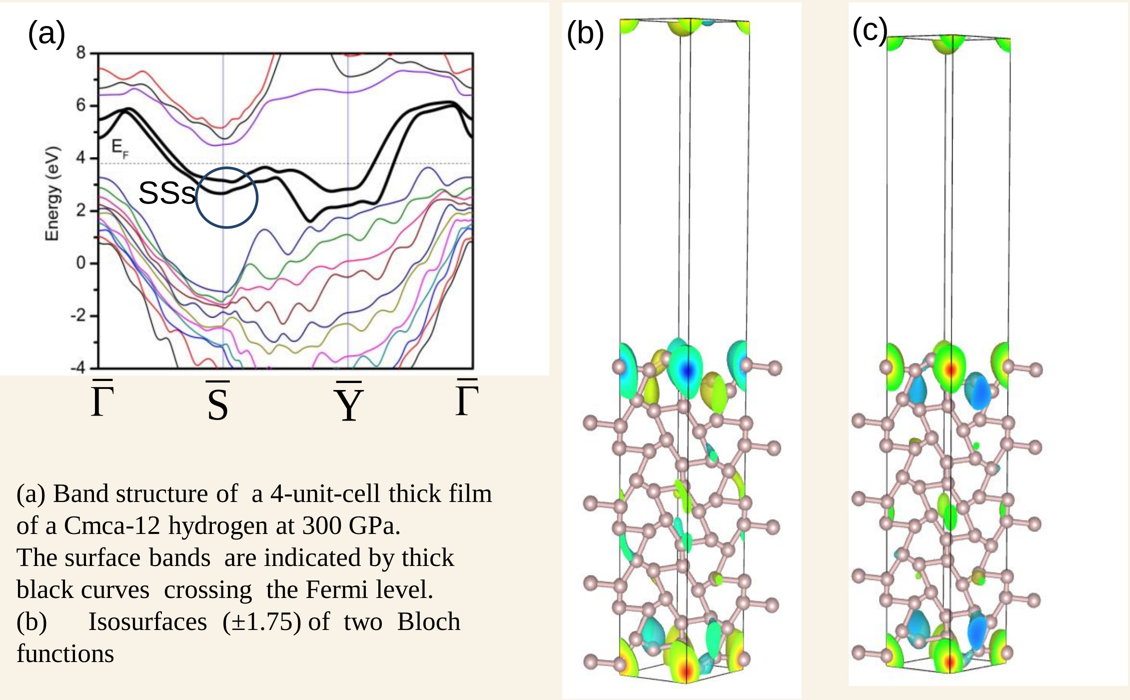
Topological surface states in dense hydrogen and other low-Z elements

3. SCIENCE

- **2D or quasi-2D systems can be potentially good superconductors.**
- **We show that metallic surface states can appear in insulating phases of compressed H, Li, and Na due to topological reasons.**

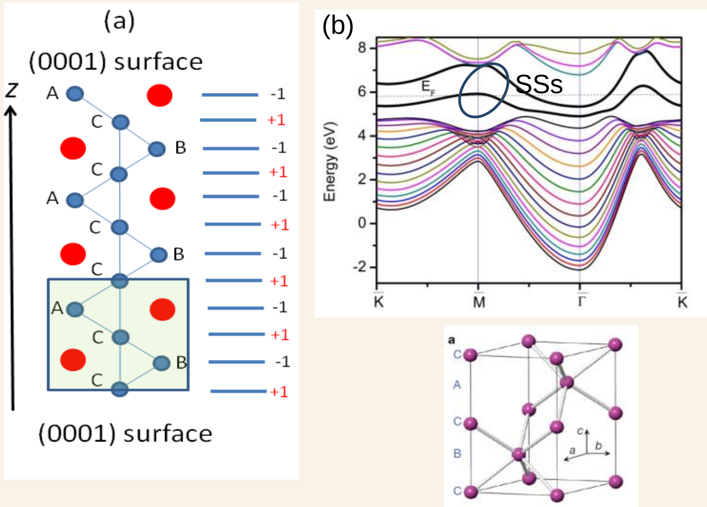


Cmca-12 hydrogen: metallic SSs cover the whole 2D Brillouin zone (1)



(a) Band structure of a 4-unit-cell thick film of a Cmca-12 hydrogen at 300 GPa. The surface bands are indicated by thick black curves crossing the Fermi level.
(b) Isosurfaces (±1.75) of two Bloch functions

Elemental high-pressure electride Na-hP4: 2D electron gas on polar surfaces (2)



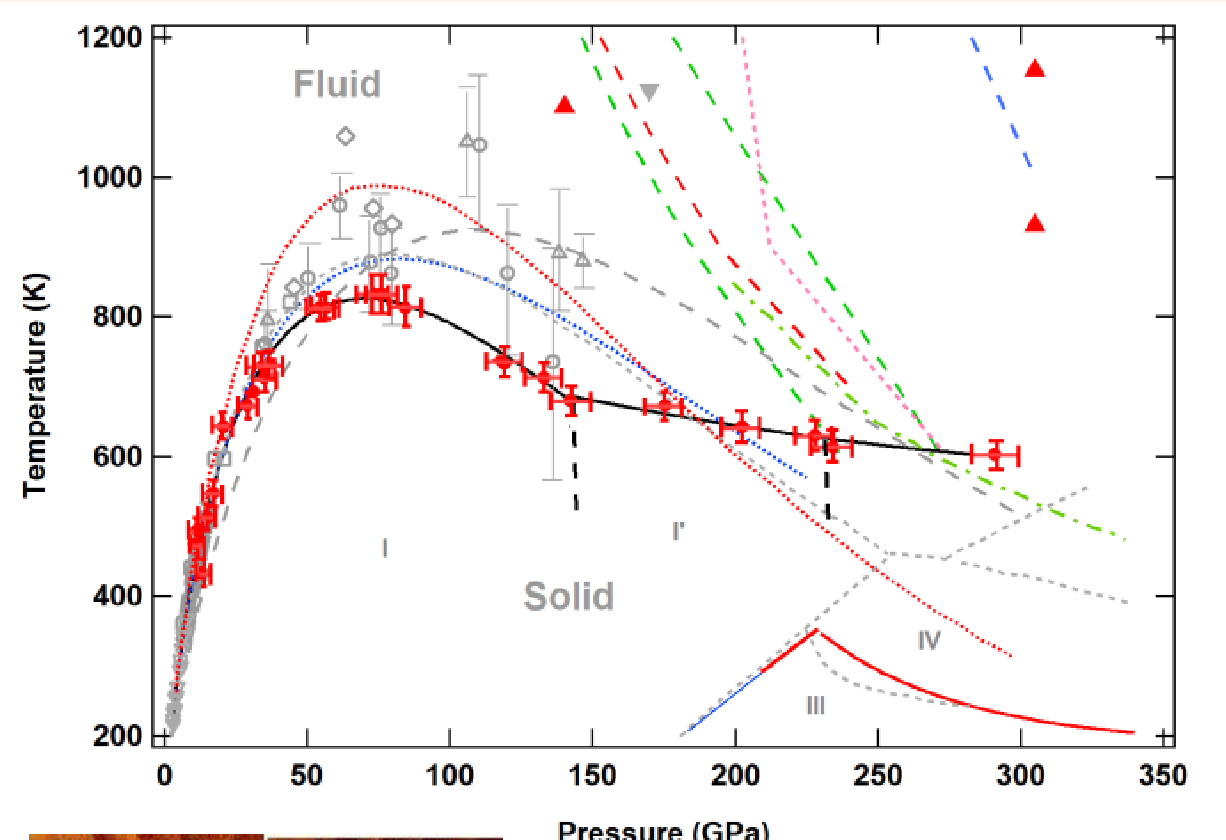
(a) Slab model for polar (0001) hP4-Na surface.
(b) The corresponding 2D band structure. Electrons (0.5 e/per 2D cell) move from one surface to the opposite surface to neutralize the "polarization catastrophe". As a result, a 2D electron gas appears similar to that of the renown SrTiO3/LaAlO3 interface.

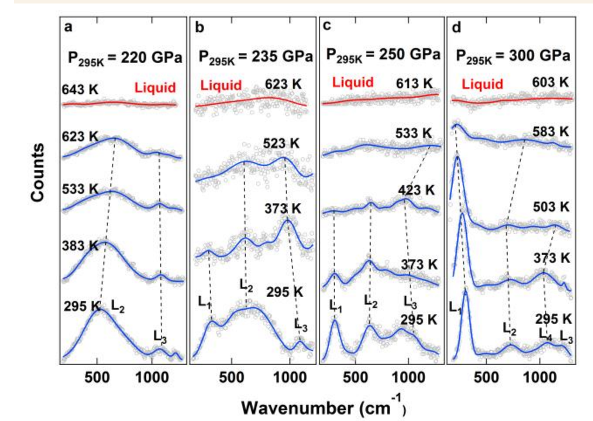
[I. I. Naumov and R. J. Hemley, *Phys. Rev. Lett*. (2016)]
[I. I. Naumov and R. J. Hemley, *submitted*]

CDAC

NNSA

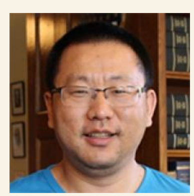
Topological surface states in dense hydrogen and other low-Z elements





Externally heated diamond anvil cell techniques in conjunction with *in situ* Raman measurements at each P-T point provide melting line data to 300 GPa when lattice mode disappeared. Vibrons changing with *P–T* indicate two transition points along the melting line. More details for high *P-T* phase diagram are in preparation.

C. S. Zha



Hanyu Liu

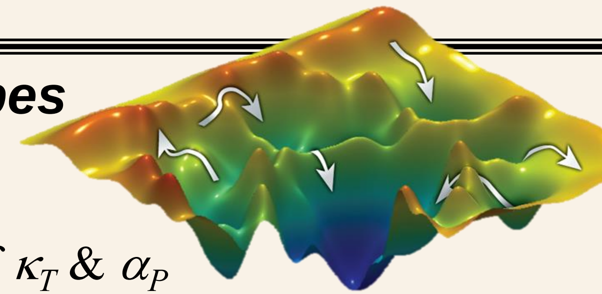
John Tse

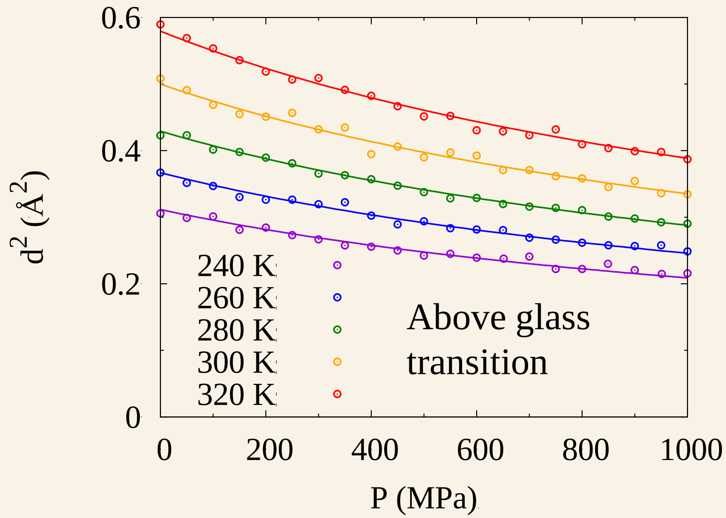
CDAC

NNSA

Pressure effects on energy landscapes of complex polymers

Quasiharmonic analysis of protein energy landscapes





- *P-T* fluctuations function of κ_T & α_P
- Above T_g:

$$d^2(P,T) = d_0^2 \frac{T}{T_0}\left[\exp(-\alpha_{P,0}\Delta T)(1+m\kappa_{T,0}\Delta P)^{1/m}\right]^{\left(-\frac{5}{3}+m\right)}$$

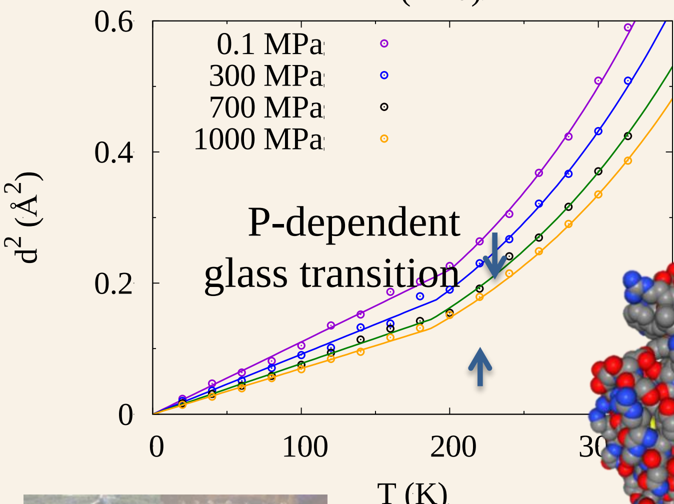
γ is Grüneisen and *m* & *n* are Mie potential parameter

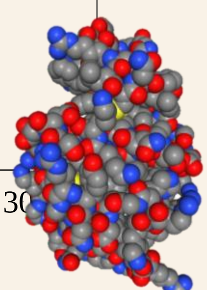
$$m = \frac{5}{3} - 2\gamma = (n+m+6)/3$$

- Below T_g:

$$d^2(P,T) = d_0^2 \frac{T}{T_0}\left[\exp(-\alpha_{P,0}(T_g(P)-T_0))(1+m\kappa_{T,0}\Delta P)^{1/m}\right]^{\left(-\frac{5}{3}+m\right)}$$

$$T_g(P) = T_{g,0} - \frac{1}{c\alpha_{P,0}}\log(1+c\kappa_{T,0}\Delta P)$$





Lysozyme

Pressure affects energy landscape by narrowing energy wells *and by lowering barriers between substates*

Toshiko Ichiye

Jocelyn Rodgers

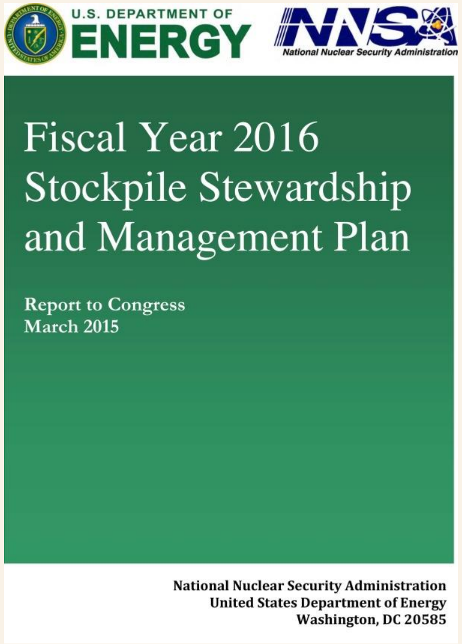
CDAC

Georgetown-Carnegie-GWU

NNSA

FUTURE OUTLOOK

- *How can we better understand and predict emergent complexity in highly compressed dense matter?*
- *What new physics may emerge in cold to warm dense matter at TPa pressures?*
- *Can we accurately determine fundamental thermodynamics at multimegabar P-T?*
- *How do defects, grain boundaries, and interfaces respond to high P-T-t conditions?*


U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

Fiscal Year 2016 Stockpile Stewardship and Management Plan

Report to Congress
March 2015

National Nuclear Security Administration
United States Department of Energy
Washington, DC 20585

- *How can we better measure time-dependent transformations, and bridge the gap between static and dynamic compression?*
- *Can we determine constitutive properties such as strength, plasticity, and rheology at ultrahigh (TPa) P-T conditions?*
- *Can we expand the synthetic chemistry frontier to very high P-T conditions to produce new optimized materials?*

CONCLUSIONS

1. Education and Training

- Diverse student program with a large group of university partners
- Continued placement of personnel in NNSA labs

2. Science Program

- Continued growth in number of high-profile publications
- Novel phenomena over a broad range of extreme conditions
- New opportunities for materials dynamics under extremes
- *Opportunities at APS for the NNSA labs*

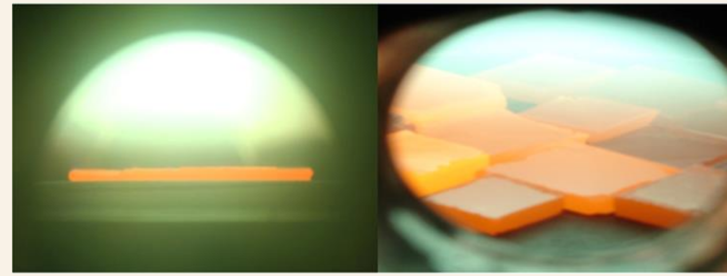
3. Technique Development

- Continued technique developments to support NNSA labs
- New x-ray techniques (imaging, time-resolved, static/dynamic)
- The APS upgrade provides new opportunities
- Opportunities for coordination across DOE facilities

BACKUP SLIDES

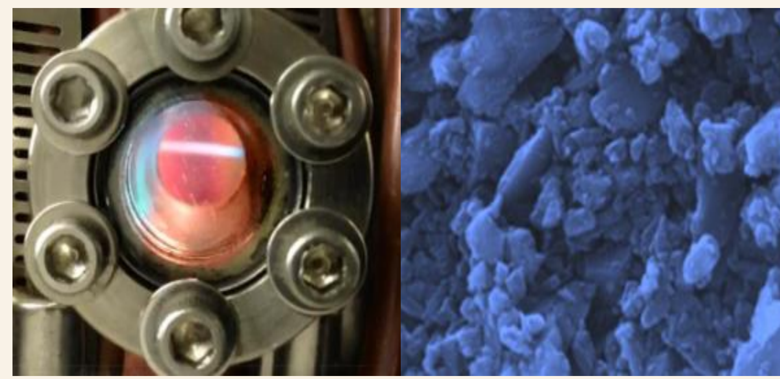
New developments in CVD diamond

1. **Growing diamond at atmospheric pressure**
   - *New micro-wave plasma CVD methods*
   - *Increasing pressure enhance diamond growth rates*
2. **Metastable growth of other materials**
   - *Other materials in kinetically stabilized states such as Si*
3. **N-V centers in nanodiamonds**



Single-crystal diamond grown at <200 torr

[K. Hemawan *et al*., *JVST A* (2015)]



Polycrystalline diamond produced by atmospheric pressure CVD

[K. Hemawan *et al*., *Appl. Phys. Lett*. (2015)]

Derek Keefer (Penn State)

Todd Zapata (TAMU)

Huiyang Gou

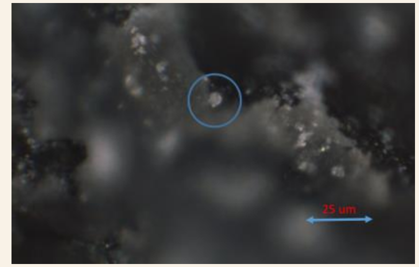
Kadek Hemawan

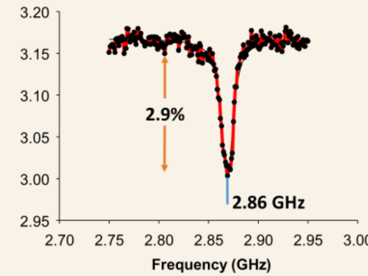
PSU-TAMU-Carnegie

New developments in CVD diamond

3. SCIENCE

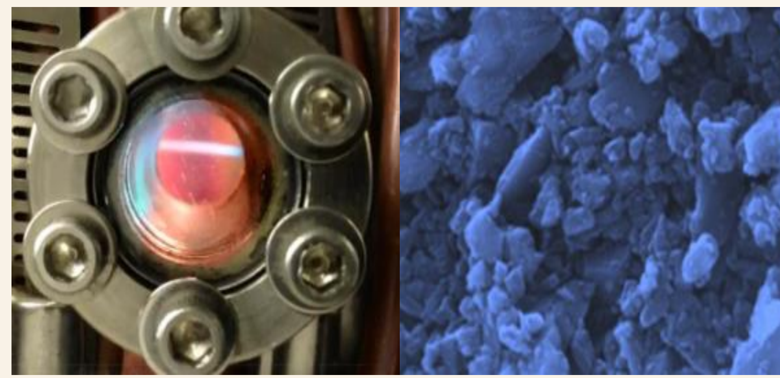
1. **Growing nanodiamond at HPHT conditions**
   - *New seeding technique*
   - *Allows direct placement of color-centers*
2. **Metastable growth of other materials**
   - *Other materials in kinetically stabilized states such as Si*
3. **N-V centers in nanodiamonds**





Organic nanodiamonds

[T. Zapata *et al*., arXiv:1702.06854]



Polycrystalline diamond produced by atmospheric pressure CVD

[K. Hemawan *et al*., *Appl. Phys. Lett*. (2015)]

Derek Keefer (Penn State)

Todd Zapata (TAMU)

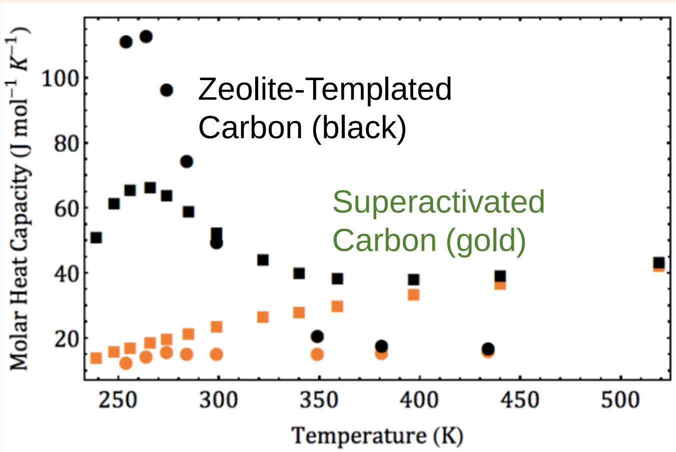
Huiyang Gou

Kadek Hemawan

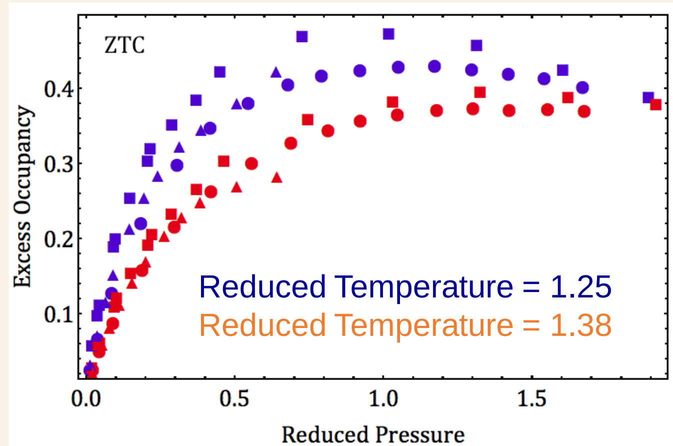
PSU-TAMU-Carnegie

A Generalized Law of Corresponding States for Nonideal Gas Physisorption

3. SCIENCE



Adsorbed-Phase Heat Capacity



Gas Uptake Normalized by Molecular Volume

Max Murialdo (Caltech)

Zeolite-Templated Carbon has anomalous thermodynamics due to cooperative interactions with methane, ethane and krypton

At corresponding conditions, adsorption data aligns for multiple gases at same reduced *T*, even with anomalous thermodynamics of adsorption.

[M. Murialdo, *et al.*, *J. Phys. Chem. C* (2016)]

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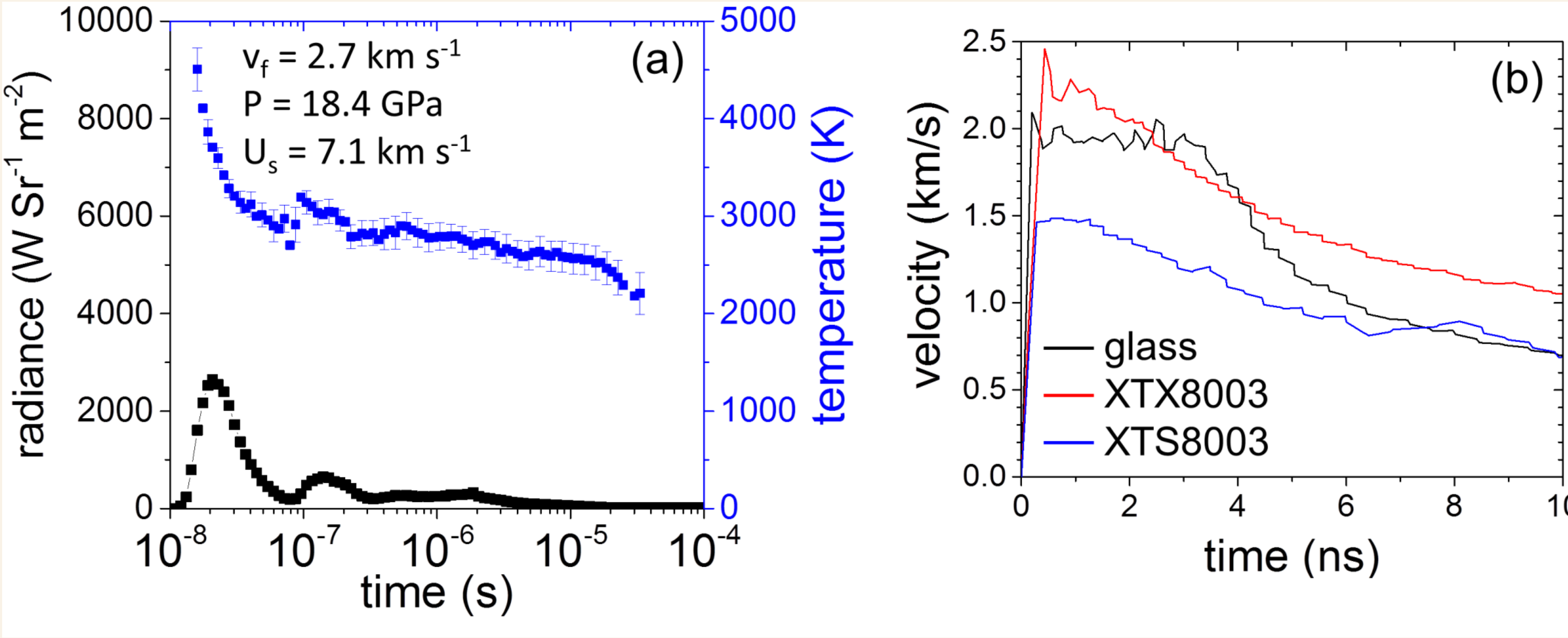
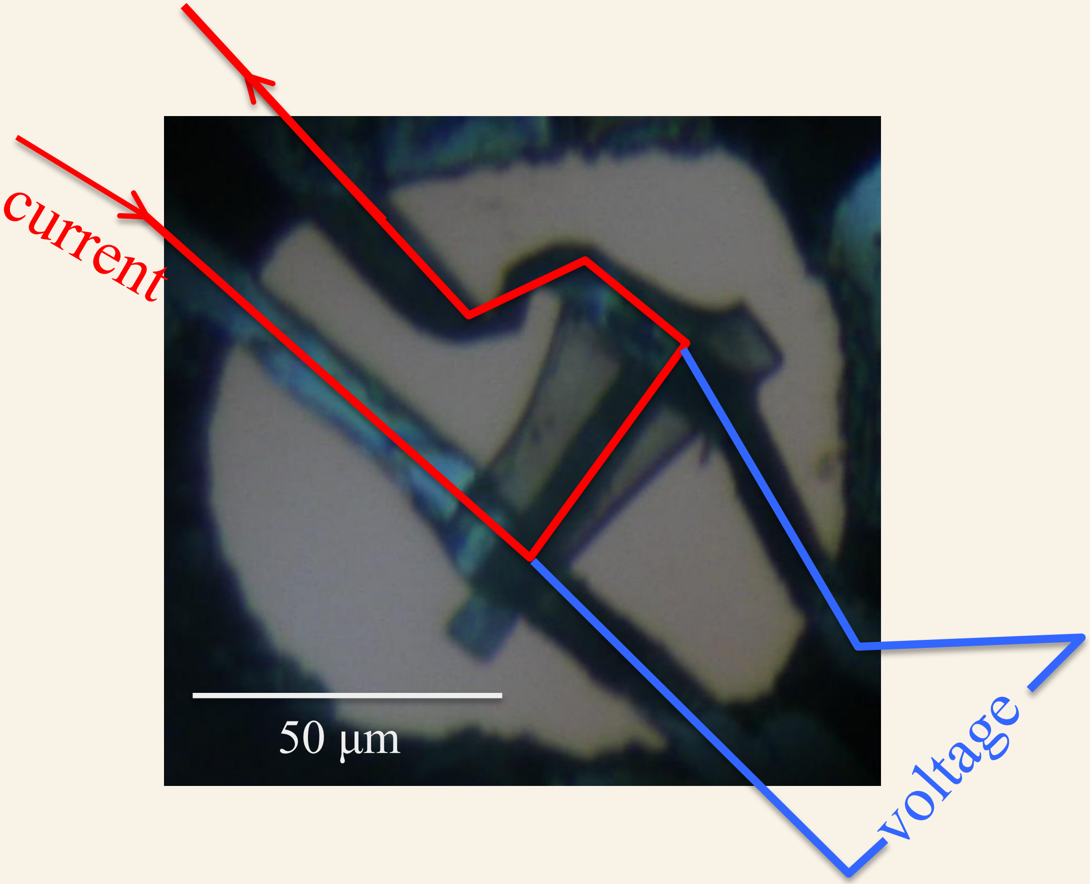
Probing detonation-strength shocks in the plastic-bonded explosive XTX8003

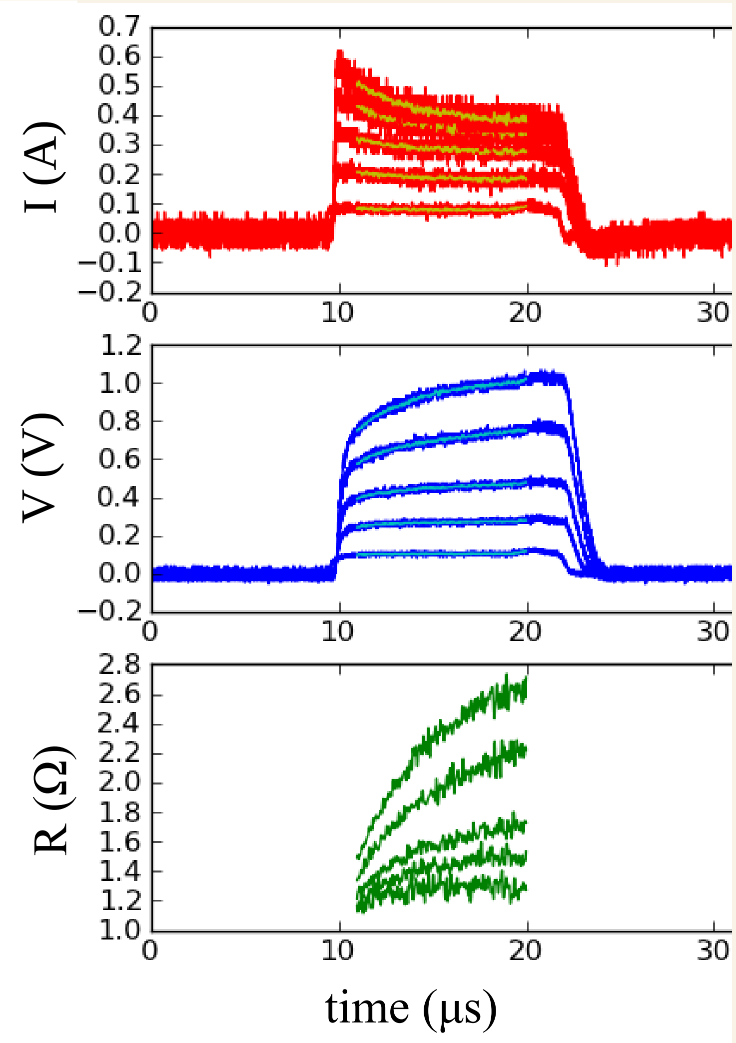


2017 GSCCM Early Career Award Winner

Will Bassett (Illinois)

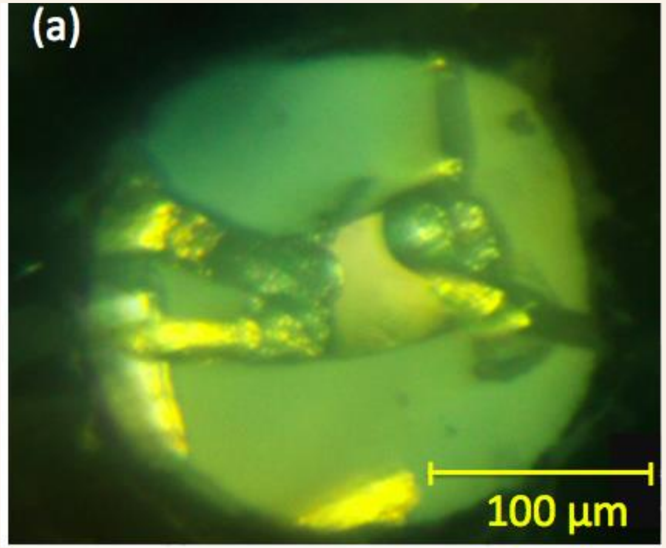
Pulsed electrical heating in diamond cells: application to synthesis of PdH_x

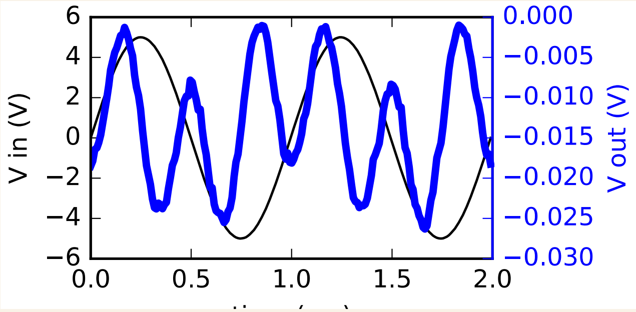


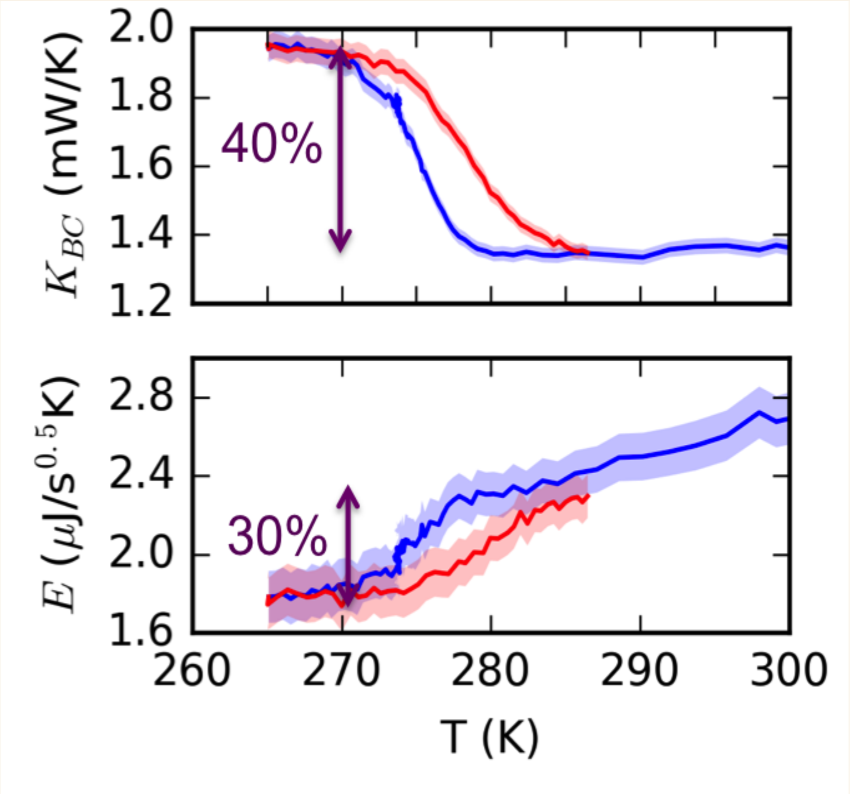


- Synthesis of PdH_x
- Potential applications to high-pressure melting, equations of state, chemical reactions

Modulation calorimetry in diamond cells: application to H_2O





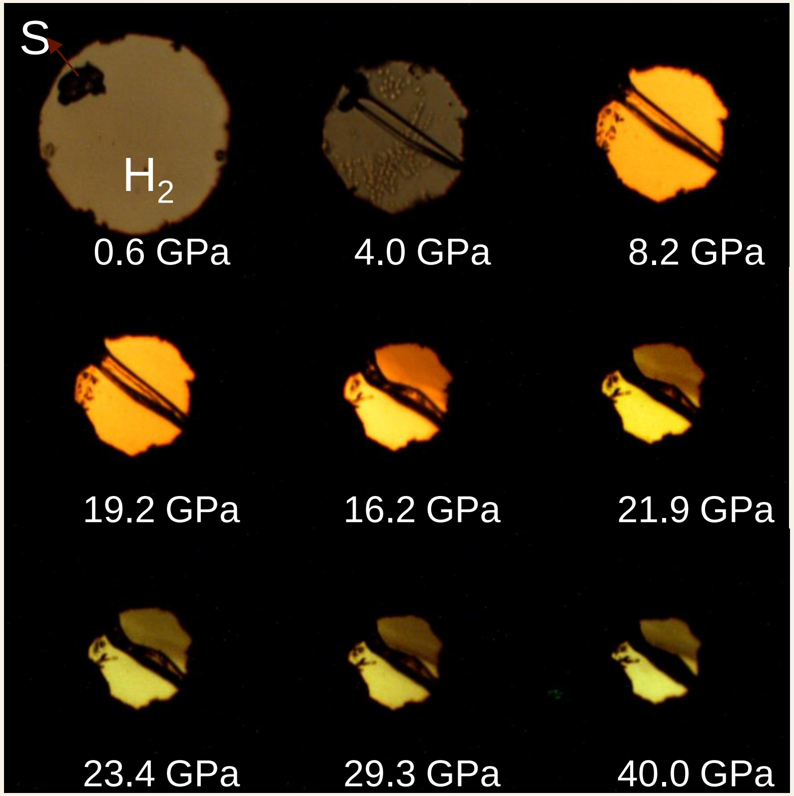


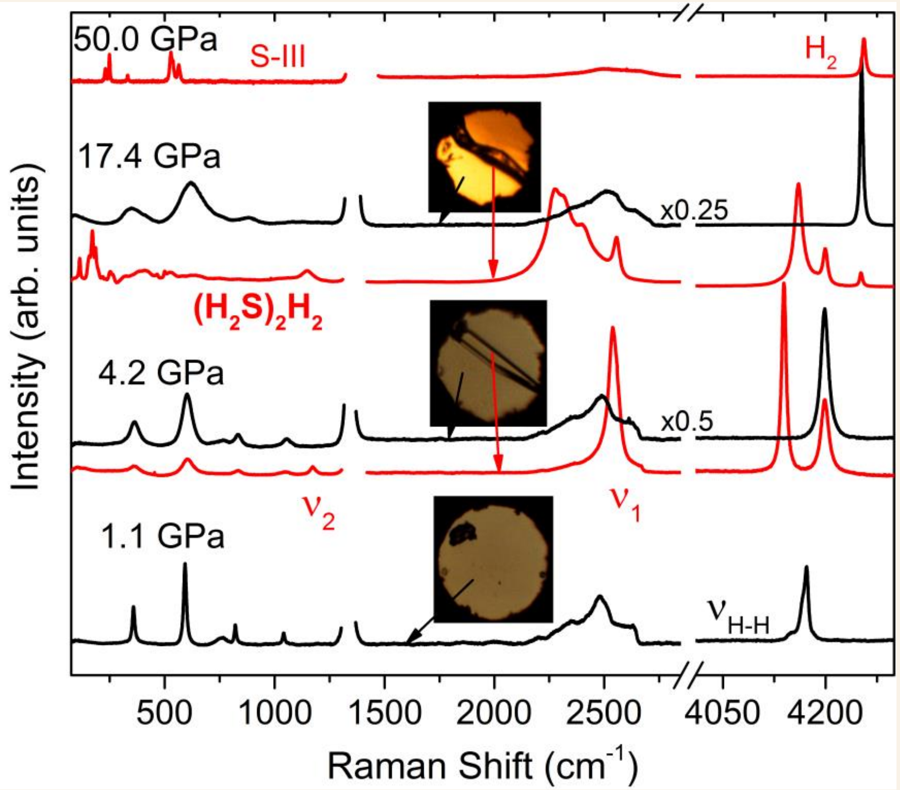
[Z. M. Geballe & V. V. Struzhkin, *J. Appl. Phys*, submitted]

- **Calorimetry with thin-film heaters surrounded by insulating sample → high signal:noise**
- **Thermal property changes across ice VII-VIII, VI-water boundaries up to 9 GPa**

Photochemical reaction of H_2+S forming $(H_2S)_2H_2$

H_2 + S mixture with increasing pressure

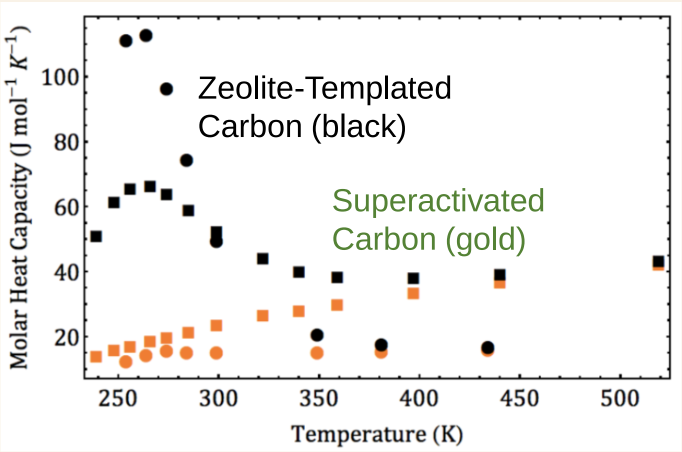




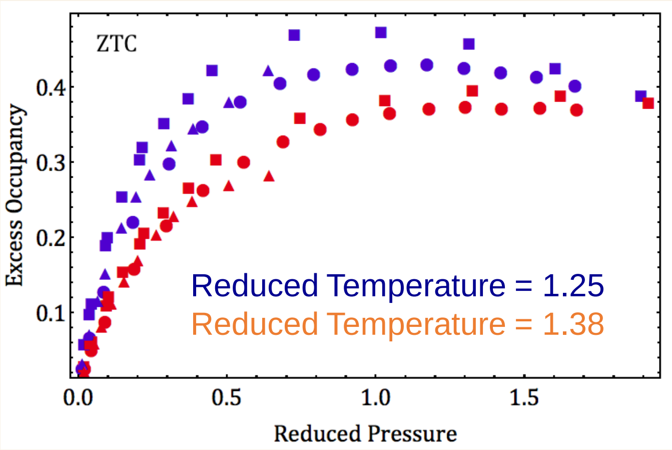
[S. Duwal and C. S. Yoo, *submitted*]

A Generalized Law of Corresponding States for Nonideal Gas Physisorption

3. SCIENCE



Adsorbed-Phase Heat Capacity



Gas Uptake Normalized
by Molecular Volume

Max Murialdo (Caltech)

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At corresponding conditions, adsorption data aligns for multiple gases at same reduced *T*, even with anomalous thermodynamics of adsorption.

[M. Murialdo, *et al.*, *J. Phys. Chem. C* (2016)]

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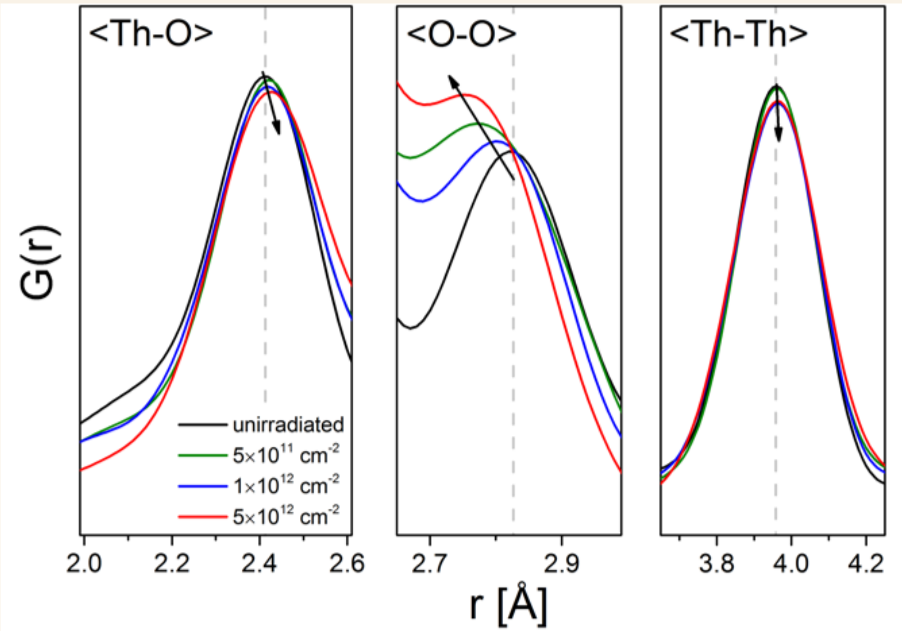
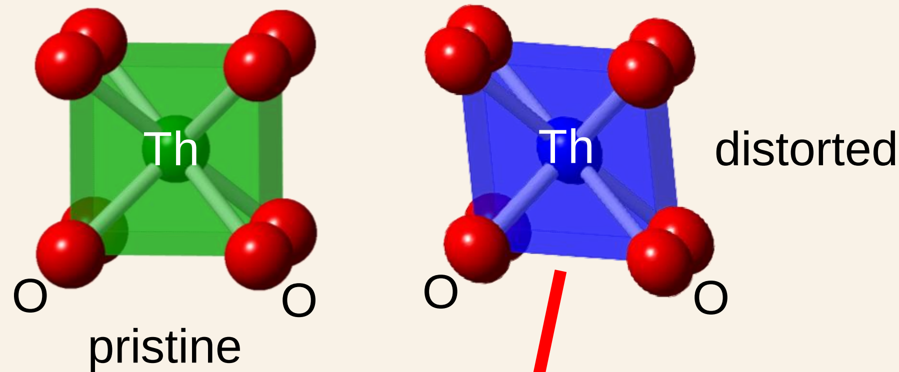
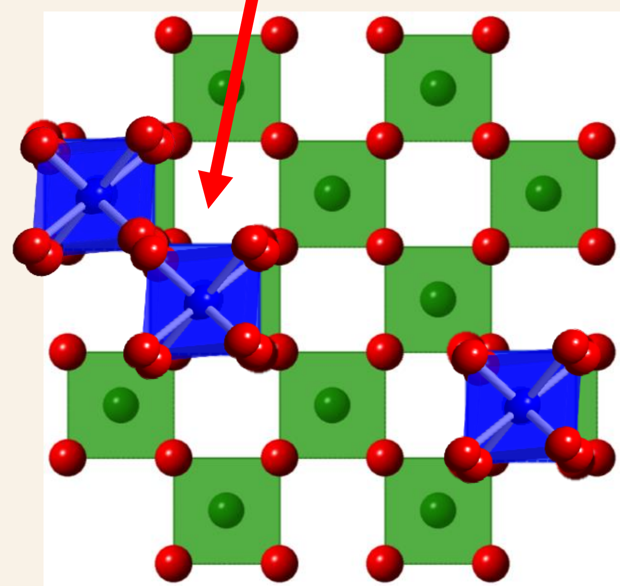
Actinide materials under extreme conditions







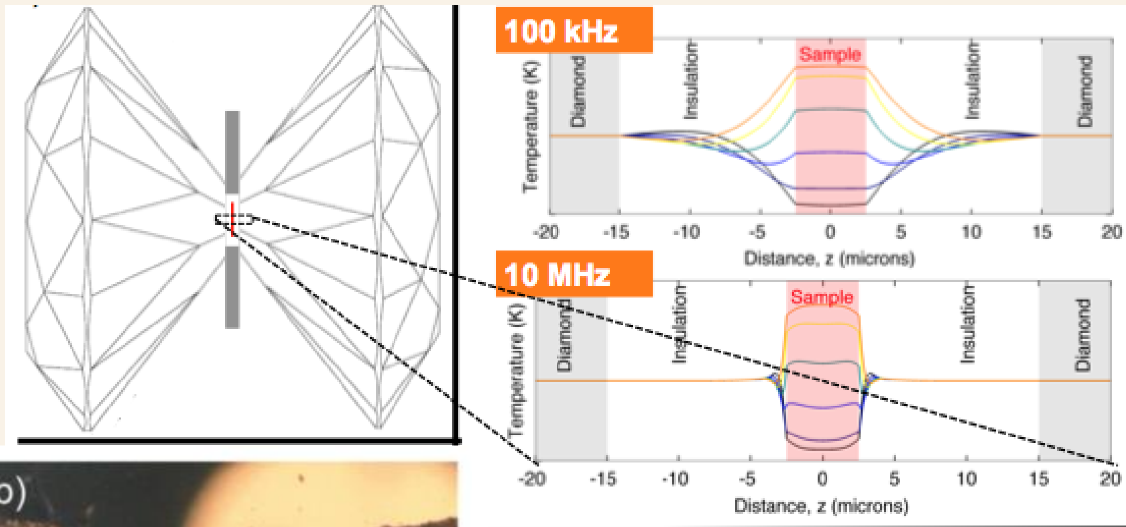
Raul Palomeras (Tennessee)

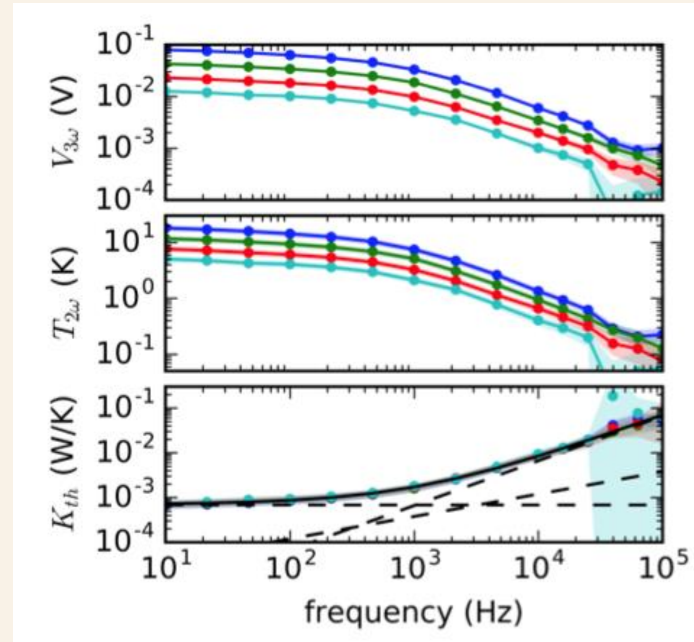
- Monitoring CeO_2 and ThO_2 bond lengths as a function of ion fluence (ions/cm^2)
- Electronic structure and redox behavior influence resultant defect structure
- CeO_2: Ce^{3+} and peroxide formation
- ThO_2: distortion of local polyhedra

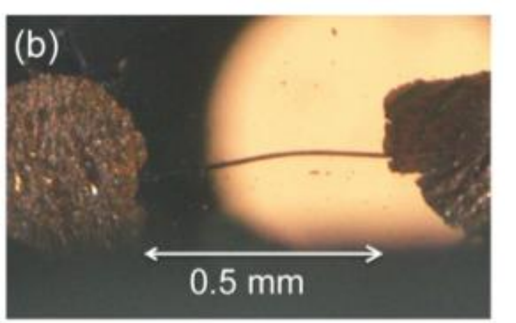
[R. I. Palomares, *et al.*, *J. Mater. Chem. A, submitted*]

Modulation calorimetry in diamond cells: designs and prototypes

3. SCIENCE





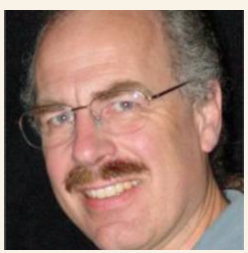


[Z. M. Geballe, et al., *J. Appl. Phys.* 121, 145902 (2017);
Z. M. Geballe, et al., *J. Appl. Phys.* 121, 145903 (2017)]

- Motivated by C_p, L measurements in laser-shock
- Numerical simulations of heat flow in diamond cell
- Design of Joule-heating experiment
- Testing of Fe, Pt, Ni, Pt-coated glass prototypes


Zachary Geballe


G. W. Collins

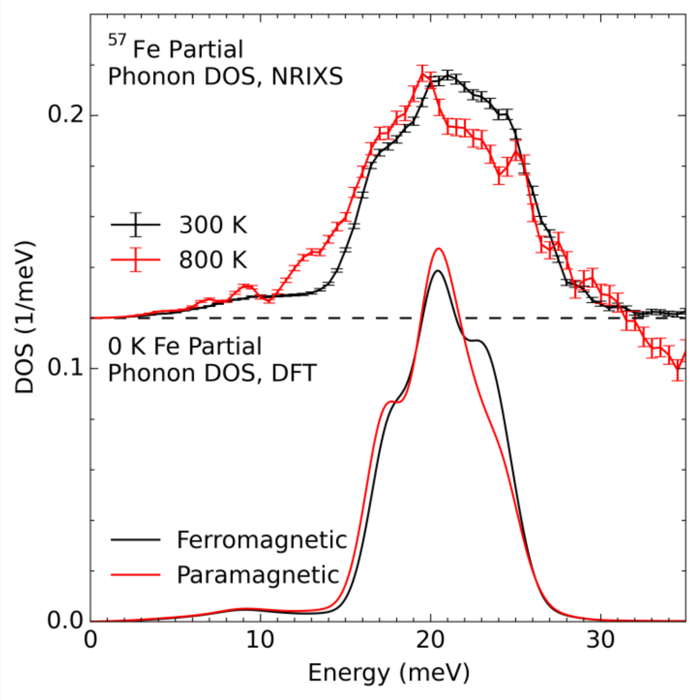

Raymond Jeanloz

CDAC

Berkeley-Carnegie-LLNL

NNSA

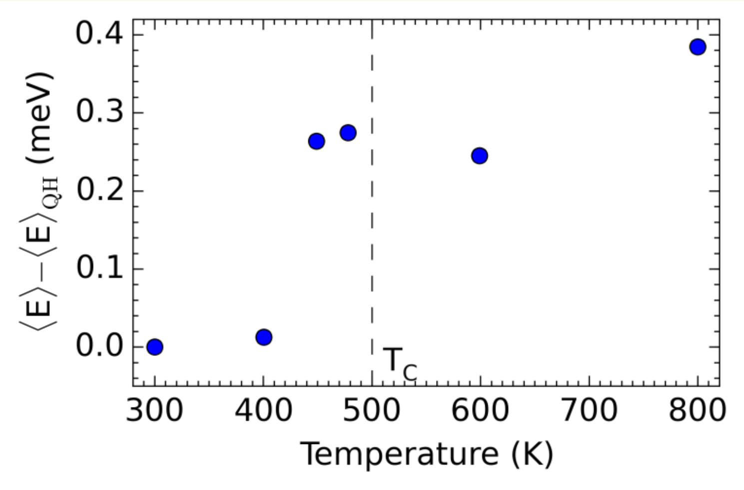
Magnon-Phonon Interaction in Pd_3Fe



- Investigate lattice dynamics across magnetic transition under *T, P*
- Nuclear resonant spectroscopy at HPCAT: NRIXS, NFS
- Shift in phonon energy near Curie temperature – indicates magnon-phonon interaction

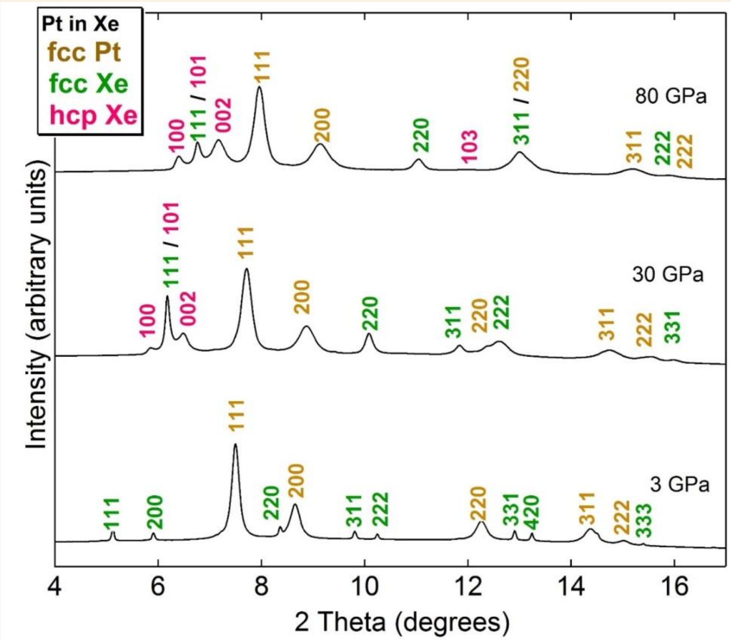
Fred Yang (Caltech)

Discrepancy between quasiharmonic approximation and experimental result with temperature



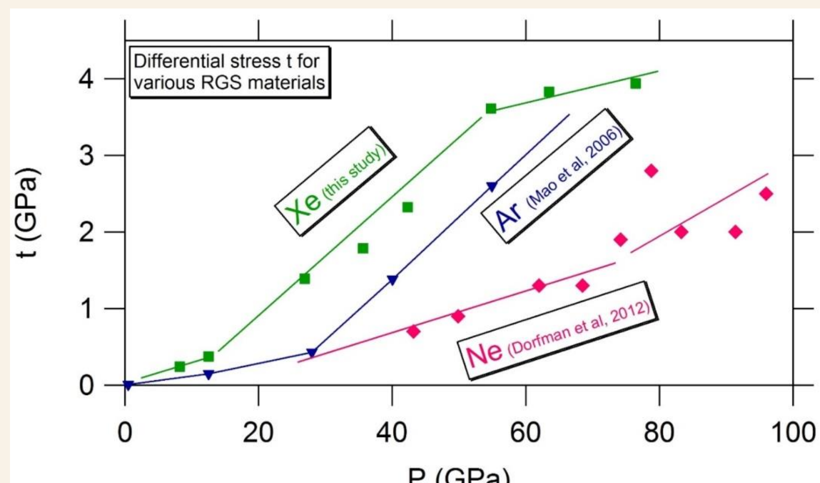
[F. C. Yang, *et al*. *Phys. Rev. Lett.* (2016)]

Rare gas solids at high pressure



- Xenon compressed in diamond anvil cell with Pt standard to 80 GPa
- Uniaxial differential stress determined by lattice strain analysis in both Xe and Pt
- Strength increases with Z for rare gas solids

Ben Brugman
Michigan State



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[B. Brugman. *et* al. *in preparation*]

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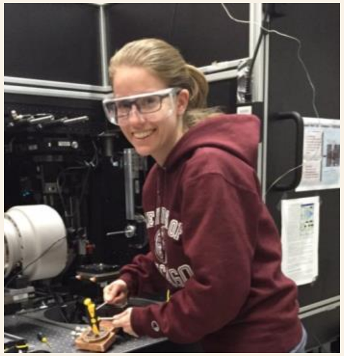
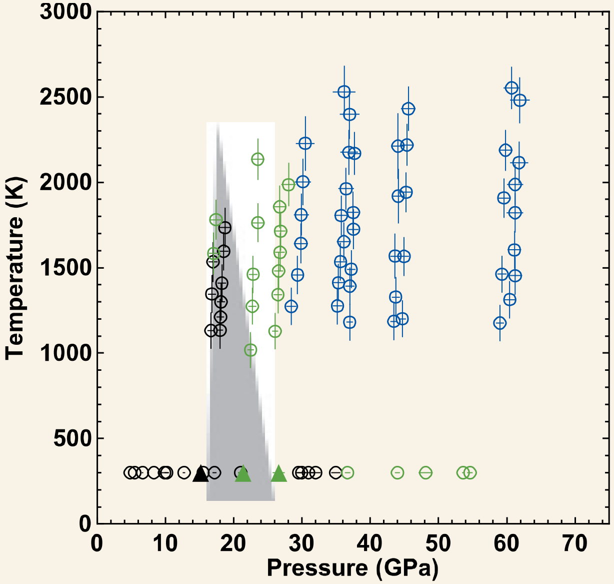
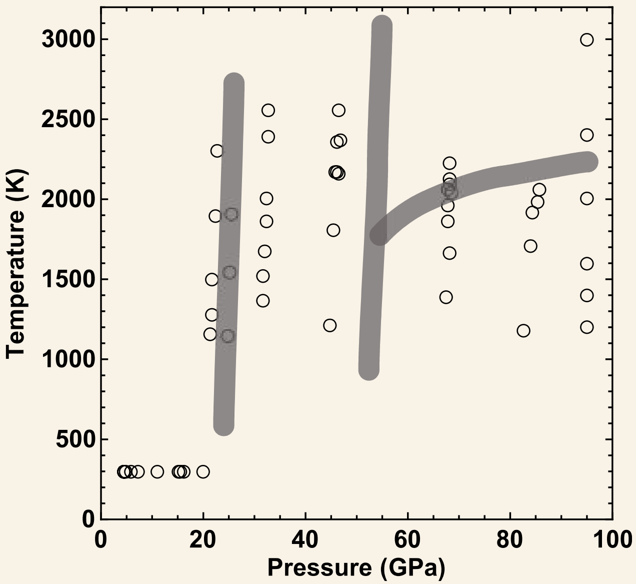
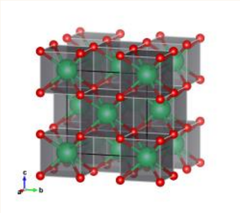
Actinide oxides at high *P-T*



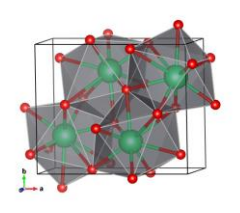
Bethany Chidester (Chicago)





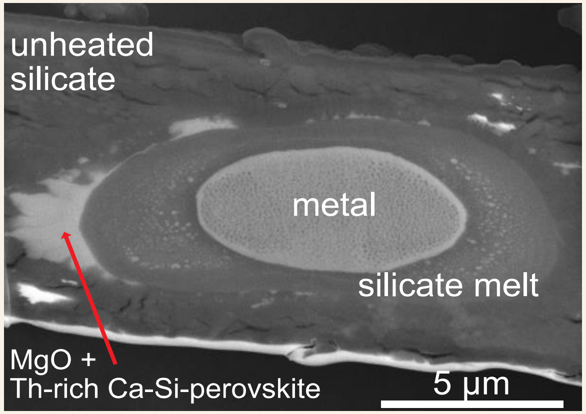


Flourite-type



Cotunnite-type

- Fluorite-type to cotunnite-type transitions in both ThO_2 and UO_2 at moderate pressures
- Tetragonal and monoclinic Structures observed in UO_2 at Higher *P* and *T*
- Interest in ThO_2 and UO_2 phases arises from possible appearance in metal-silicate partitioning experiments



[B. Chidester *et al., in preparation* (2016)]

CDAC

NNSA