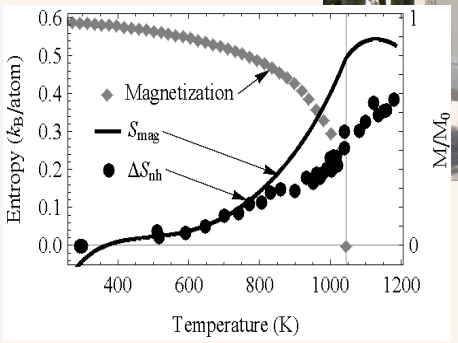
1



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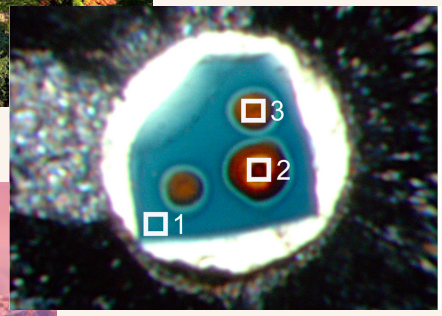


Carnegie-DOE Alliance Center: Student Science at HPCAT

Steve Gramsch
CDAC Coordinator

3

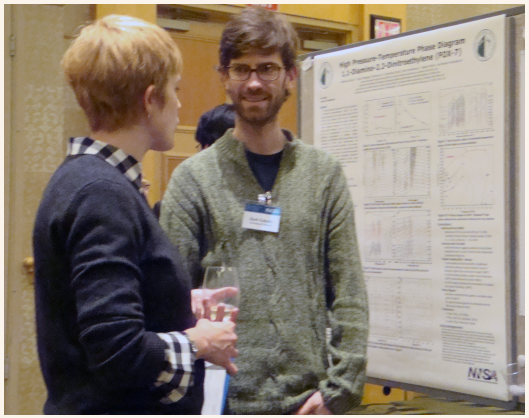
CDAC

CARNEGIE INSTITUTION FOR SCIENCE

CDAC is the SSAP Center for Materials at Extreme Conditions

- Founded in 2003 – 2 Renewals
- Currently 15 Academic Partners + Carnegie team
- 53 PhD degrees earned with CDAC support
- 228 student papers published with CDAC support
- ~ 50% of student papers describe work at HPCAT

John Lazarz, Tom Duffy



Emma Rainey, Zack Geballe

Wenk Group at HPCAT

A top priority of CDAC is graduate student education in high *P-T* materials science

- Academic Partners – leading high *P-T* research groups
  - A wide variety of disciplines represented
  - Reviewed annually by CDAC Steering Committee
    - Scientific Merit
    - Science aligned with NNSA mission
    - Applicability of skills toward NNSA Lab careers

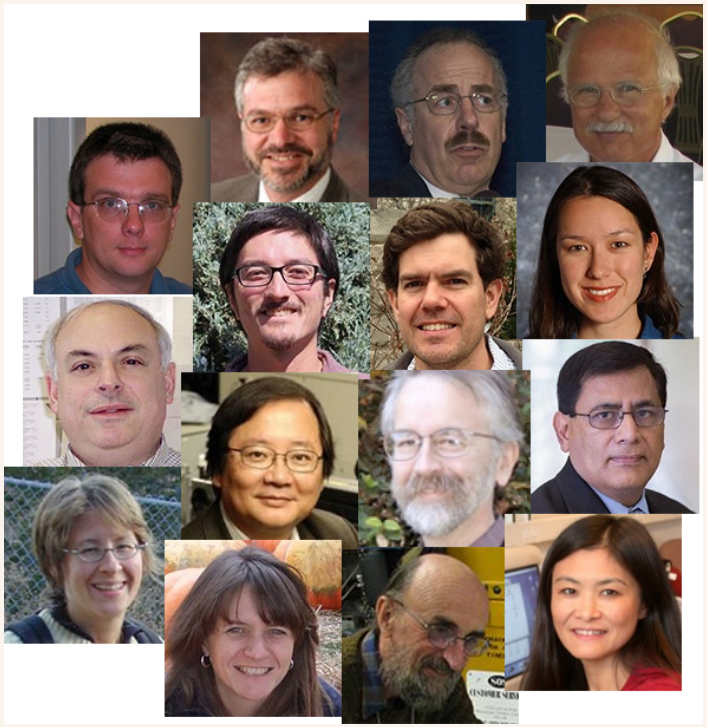
- 15 Current Partners – $1M from the core grant
  - Stipend
  - Tuition
  - Materials and Supplies Allowance
  - ~ 1 student per group
  - 17 FTE graduate students supported in Y13

- ~$40k/year in travel support to national user facilities (APS, NSLS, ALS) for experiments (+ workshops + SSAP events)

CDAC students represent leading high *P-T* research groups from throughout the US

CDAC Academic Partners in Year 13

- **David Cahill** (Illinois)
- **Przemek Dera** (Hawai'i)
- **Dana Dlott** (Illinois)
- **Brent Fultz** (Caltech)
- **Toshiko Ichiye** (Georgetown)
- **Steven Jacobsen** (Northwestern)
- **Raymond Jeanloz** (Berkeley)
- **Abby Kavner** (UCLA)
- **Kanani Lee** (Yale)
- **Lowell Miyagi** (Utah)
- **James Schilling** (Washington - St. Louis)
- **Yogesh Vohra** (Alabama – Birmingham)
- **Hans-Rudolf Wenk** (Berkeley)
- **Choong-shik Yoo** (Washington State)
- **Eva Zurek** (Buffalo)



CDAC makes discretionary beam time at HPCAT available to graduate students and NNSA Lab partners

30% of beam time on each beamline goes to CDAC for discretionary use

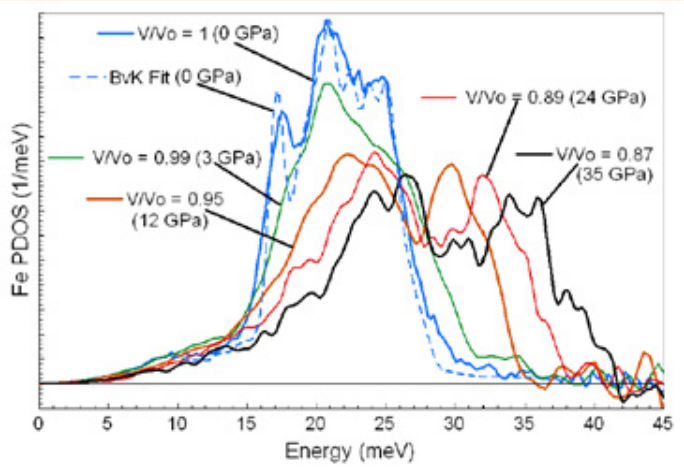
- General User Proposals (GUP)
- CDAC graduate students ~60%
- Carnegie CDAC staff ~15%
- Laboratory partners ~15%
  Programmatic research
  Development
  Personal research
- University collaborators / student work ~10%

Lisa Mauger, Caltech

CDAC is facilitating the preparation of students for leadership in the field

- 53 students have earned the PhD degree with CDAC support since 2004
- 37 students have accepted postdoctoral appointments
- 10 CDAC students have accepted postdoctoral positions in the NNSA Labs (6 since 2012)
- 4 CDAC students have taken permanent staff positions in the NNSA Labs
- 4 Carnegie / CDAC postdoctoral fellows have taken permanent staff positions at NNSA Labs
- 15 CDAC personnel have gone to NNSA Labs since 2005 (8 since 2012)
- 7 CDAC students to positions at other federal agencies / institutions
- 2 Carnegie / CDAC postdocs to positions at other federal agencies / institutions

The Caltech group uses nuclear resonant techniques to study vibrational thermodynamics



Stiffening of the phonon DOS from 12 to 24 GPa in Pd_3Fe is slower than at low pressure due to the Invar transition and a change in the magnetic moment at Fe.

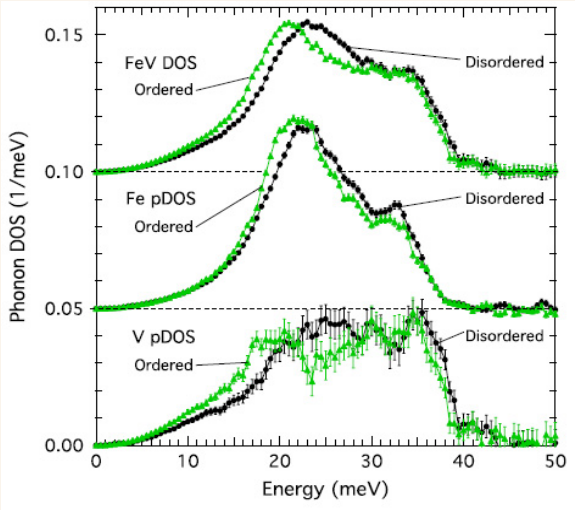
[*Phys. Rev. Lett.* **2009**, *102*, 237202]

Mike Winterrose, Caltech

The higher vibrational entropy of the ordered FeV alloy compared to the disordered material was determined using a combination of inelastic neutron scattering at ARCS/SNS and NRIXS at HPCAT.

[*Phys. Rev. Lett.* **2011**, *107*, 115501]

Jorge Muñoz, Caltech



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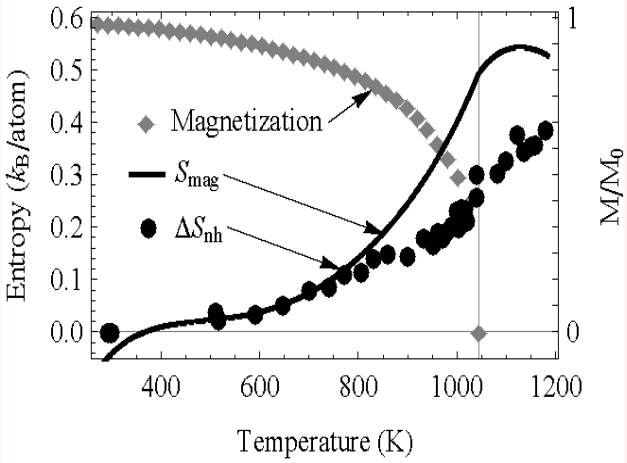
Carnegie Institution for Science

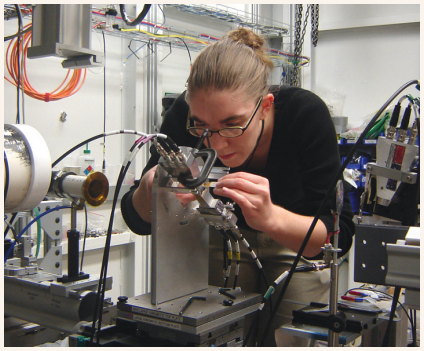
NNSA

Work on 16-ID-D is opening up new frontiers in the dynamics of iron and iron-containing materials

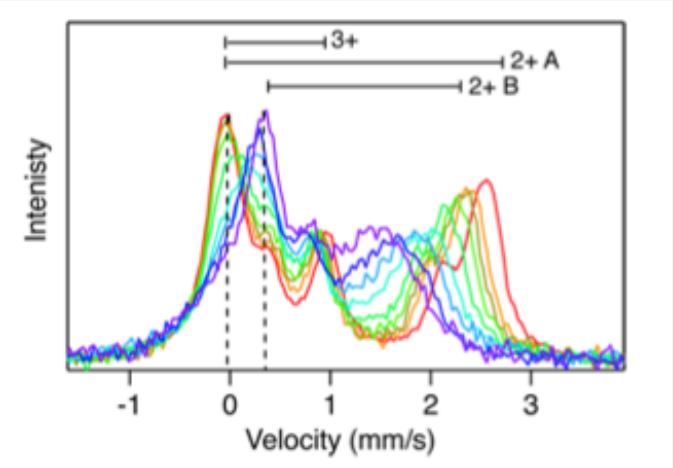
NRIXS measurements are used to separate the effects of magnons and phonons as they interact to enhance the stability of *bcc*-Fe at high temperatures. The results increase the fundamental understanding of the bcc-fcc phase transition.

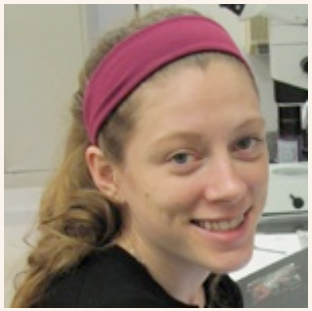
[*Phys. Rev.* **2014**, *B90*, 064303]





Lisa Mauger, Caltech





Sally Tracy, Caltech

A combination of x-ray diffraction and NFS spectroscopy shows that the onset of fast electron dynamics is correlated with the loss of local order on the sodium sublattice in the battery material Na_xFePO_4 (triphylite).

[*Chem. Mater.* **2016**, *28*, 3051-3059]

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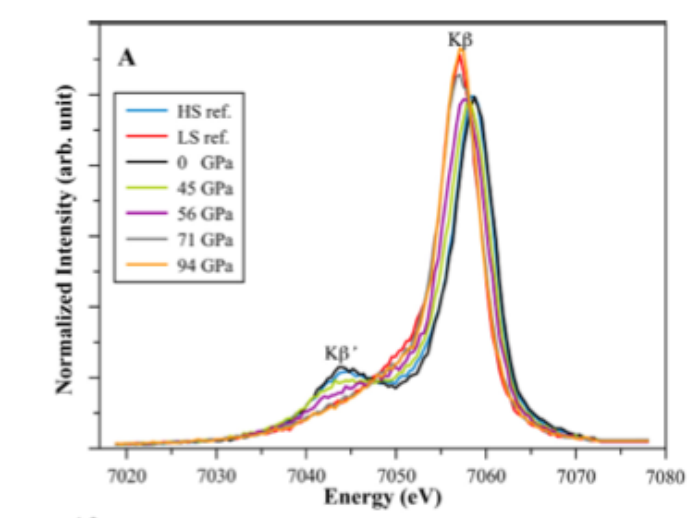
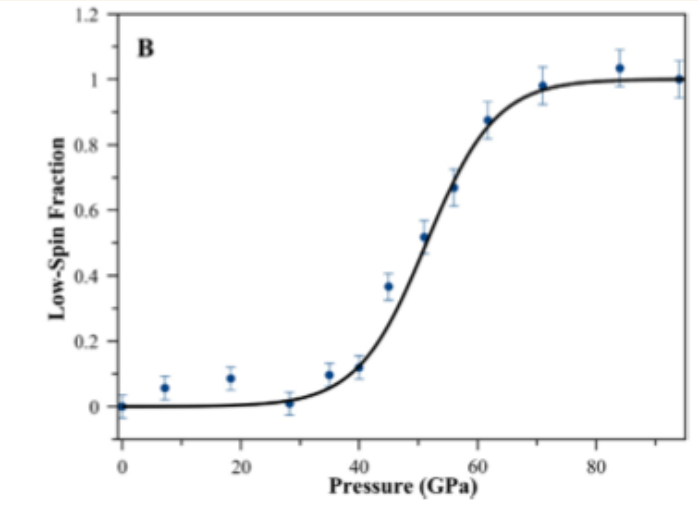
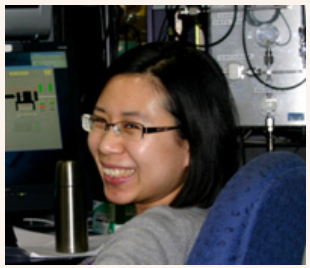
X-ray emission provides detailed information on the electronic structures of complex materials



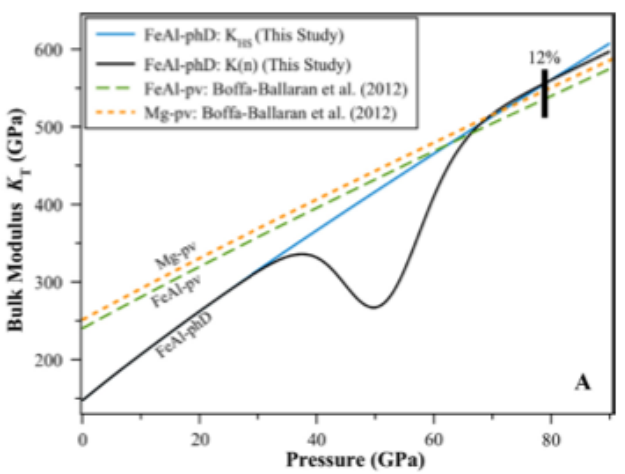
The high- to low-spin transition at Fe^{3+} in Phase D -- $MgSi_2O_4(OH)_2$ is captured with high precision and allows a comparison with diffraction data on the pressure of a discontinuity in the *P-V* curve. The data support the association of water-rich material with subducted oceanic crust into the lower mantle, and an alternative to silicate perovskite for the origin of small-scale seismic scatterers in Earth's mid-lower mantle.

[*Earth Planet. Sci. Lett.* **2013**, *382*,1-9]





Yun-yuan Chang, Northwestern



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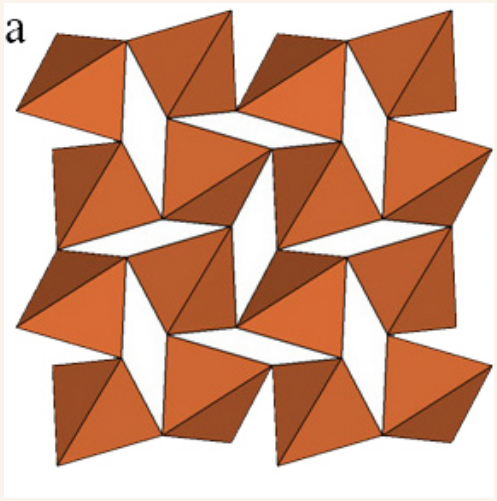
The photon flux at ID-B allows refinement of structures with light elements, including hydrogen



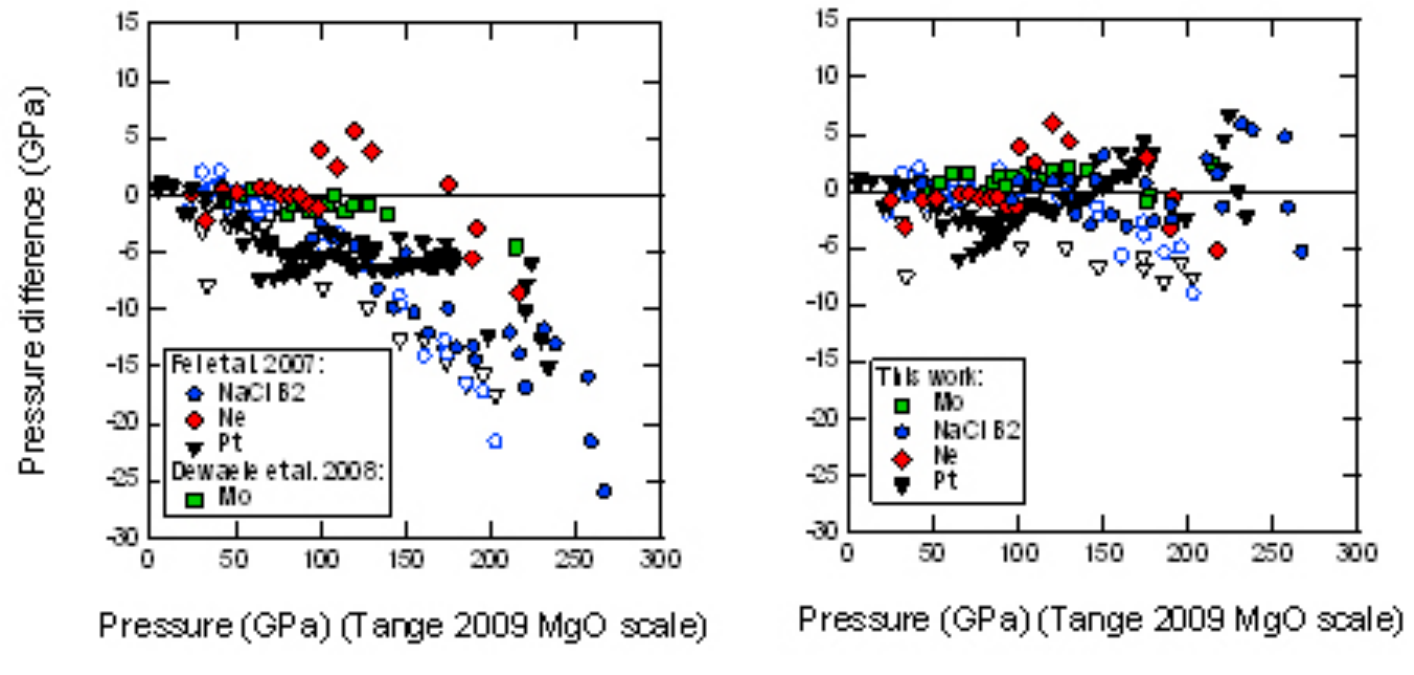
Powder diffraction measurements complimented single crystal diffraction experiments on the structure of $Be(OH)_2$ and allowed an understanding of the role of hydrogen bonding during pressure-induced phase transformations. Phase transformations in $Be(OH)_2$ are closely related to, but distinct from, transformations in $Zn(OH)_2$ and SiO_2.

[*Phys. Chem. Minerals* **2016**, *43*, in press]

Madison. Barkley, Arizona

Hannah Shelton, Hawai'i

Microbeam capabilities allow analysis of several samples simultaneously in the diamond anvil cell

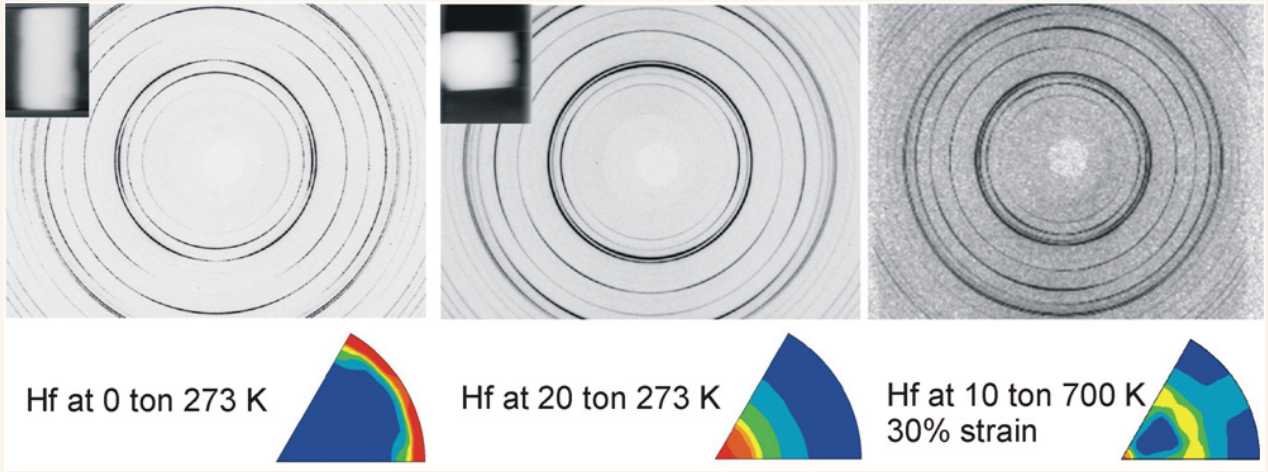


Susannah Dorfman, Princeton
EPF Laussane
Michigan State
New CDAC Partner in 2016

Diffraction of several standard samples in the DAC at the same time has resulted in an internally consistent pressure scale that reduces uncertainties from 10% to 3% at 250 GPa.

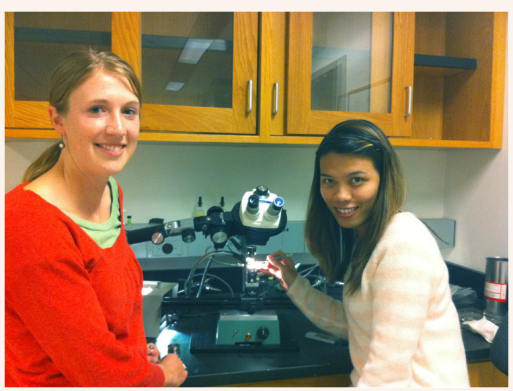
[*J. Geophys. Res.* **2012**, *117*, B08210]

CDAC students at Berkeley use radial diffraction methods for information on texture development at high pressure



Diffraction pattern

Pole figure



Pamela Kaercher, Jane Kanitpanyacharoen, Eloisa Zepeda
UC-Berkeley

Challenging radial diffraction experiments show that in most hexagonal metals, increasing temperature will decrease twinning activity, even at high plastic strain.

[*Acta Mater.* **2012**, *60*, 430-442;
Phys. Rev. Lett. **2013**,*111*, 195701]

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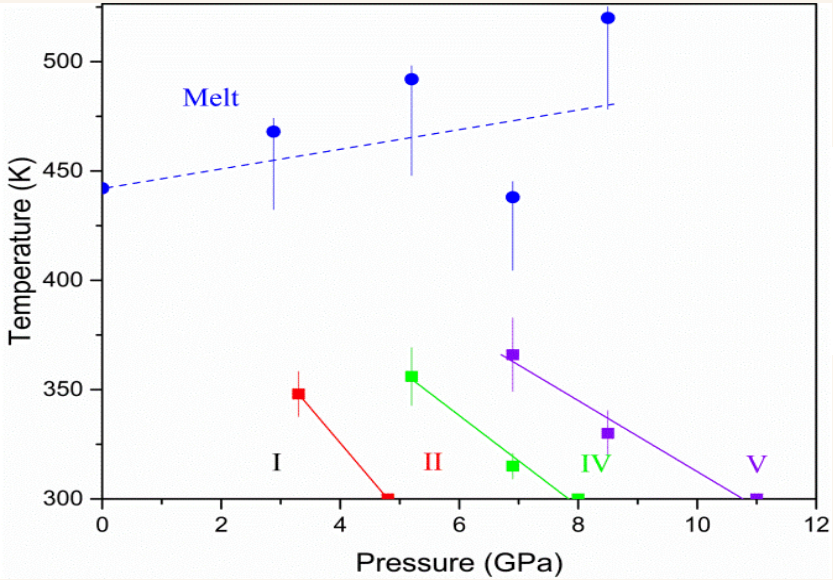
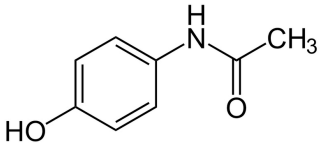
The membrane controller allows finely tuned increases in pressure for EOS and phase diagram measurements



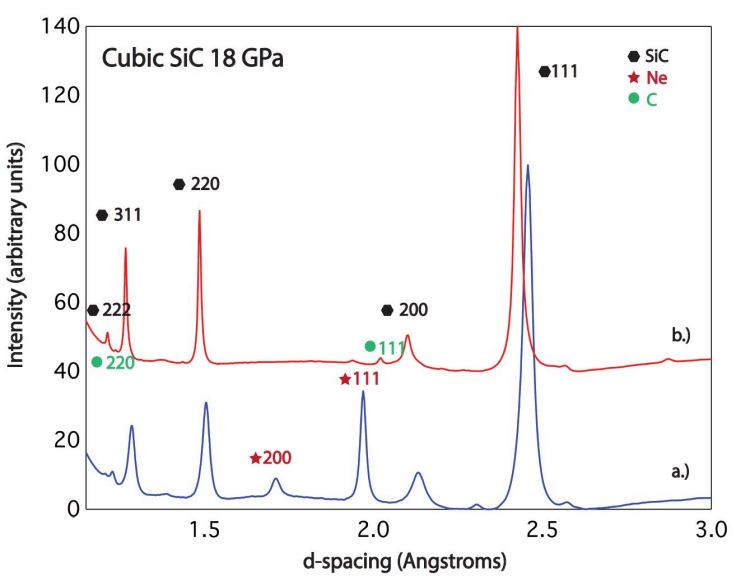


Spencer Smith, Alabama-Birmingham

Low-pressure phase transitions in paracetamol are relevant to its role as an analogue for energetic materials and to its role as an important pharmaceutical substance. Ongoing work at HPCAT is providing information on how organic crystals transform under pressure.

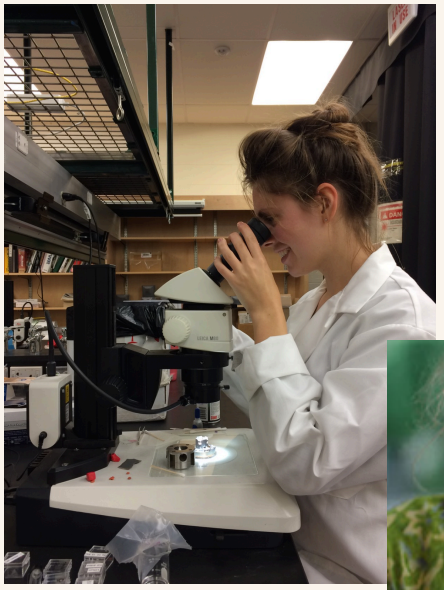
[*J. Phys. Chem. A* **2014**, *118*, 6068-6077;
J. Phys.:Condens. Matter **2016**,*28*, 035101]

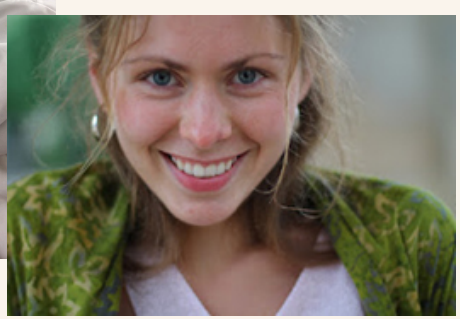
Modeling of planetary interiors is possible with the laser-heated diamond anvil cell



Quenched from 2500 K

298 K





Kierstin Daviau, Yale

High P-T x-ray diffraction at 16-ID-B is helping to resolve whether SiC melts congruently at high pressure, or decomposes into Si and C. Diffraction data support results from Raman spectroscopy that dissociation into the elements is the preferred pathway. This work is helping to provide clues as to the nature of planetary interiors containing carbon.

[*EOS Trans AGU: Fall Mtg. Suppl.* **2015**,DI43A-2602]

CDAC

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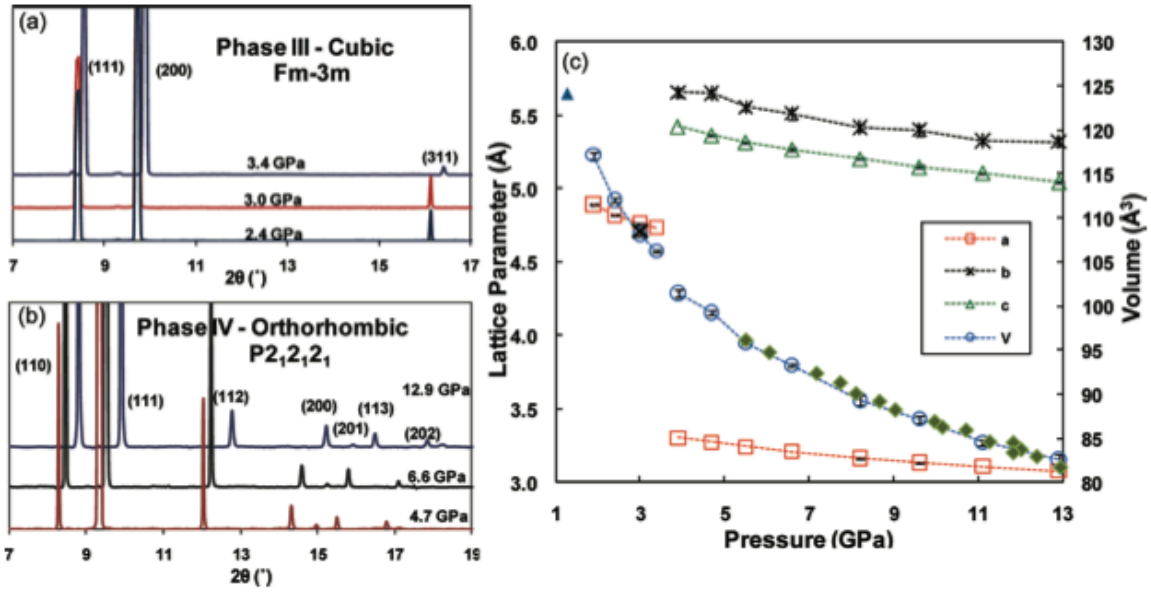
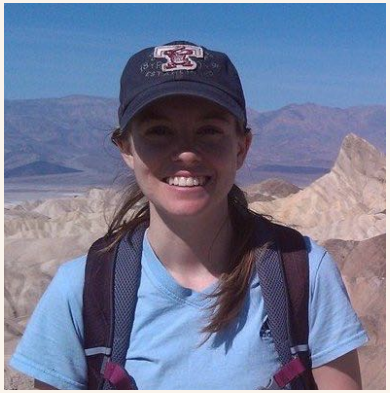
NNSA

The behavior of light element-containing small molecules at high pressure is accessible on 16-ID-B



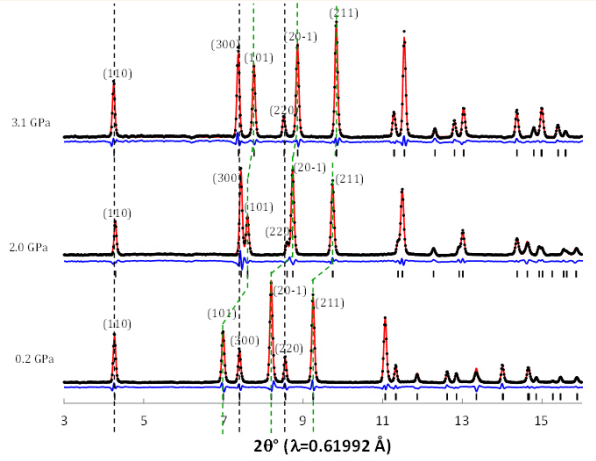


Bethany Chidester, University of Toledo
University of Chicago

X-ray diffraction data indicate that the compressional behavior of solid NH_3 in the NH_3-H_2 system is identical to that observed for pure NH_3, and confirm the observation of phase separation at high pressure.

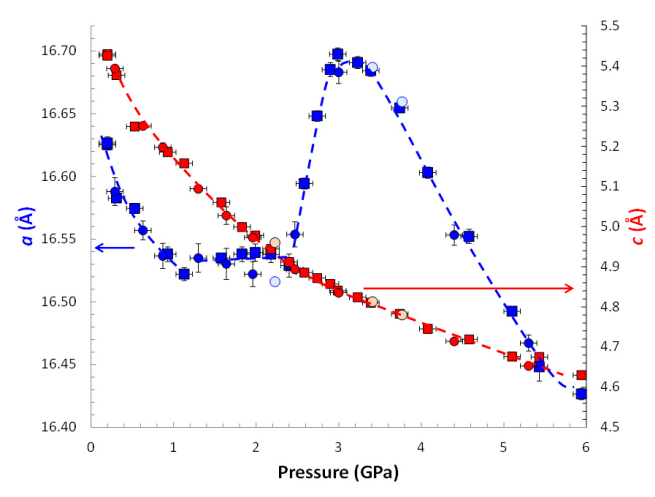
[*J. Phys. Chem. A* **2011**, *115*, 10437]

Small compositional changes in H_2-containing solids are resolved with data from 16-ID-B



Powder diffraction data show that an anomalous increase in the *a* lattice parameter of the β-hydroquinone-H_2 clathrate is the result of an increase in H_2 occupancy from 1 to 3 under pressure.

[*J. Phys. Chem. Lett.* **2014**, *5*, 1880-1884]



Victor Rosza, Hillsdale College
University of Chicago

HPCAT has been crucial to the success of the CDAC mission in student education and training

Summary

- CDAC graduate students are completing cutting-edge research for their PhD degrees with data obtained at HPCAT
- CDAC students are publishing their work in high-impact journals, based on experimental techniques that are unique and highly developed
- The beamline staff has devoted a significant amount of time and resources to students who come to HPCAT and are a major reason for the success of the CDAC program

8

9

Quiz Answers

1

2

3

4

5

1. Caltech
2. Northwestern
3. Utah
4. Alabama-Birmingham
5. Berkeley
6. Washington-St. Louis
7. Buffalo
8. Washington State
9. UCLA (Jackie Robinson Field)

6

7

8

9