ADVANCES AND OPPORTUNITIES FOR EFree AND DCO

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Carnegie Institution of Washington

CARNEGIE INSTITUTION FOR SCIENCE

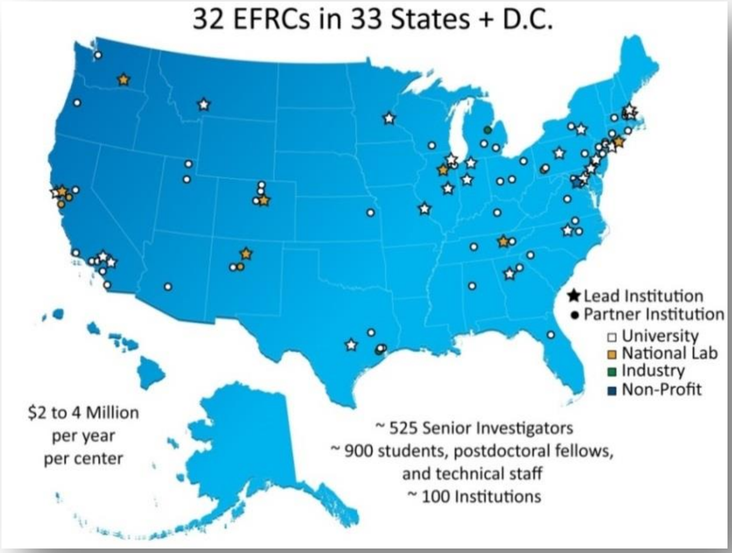
DCO Executive Committee Meeting

8-9 October 2015

Accademia Nazionale dei Lincei Rome, Italy

U.S. DEPARTMENT OF ENERGY | Office of Science

Energy Frontier Research Center



integrated, multi-investigator Centers involving partnerships among universities, national laboratories, nonprofit organizations.

generate, supply, transmit, store, and use energy

fundamental research focusing on one or more " energy grand challenges".

EFree Energy Frontier Research in Extreme Environments Center

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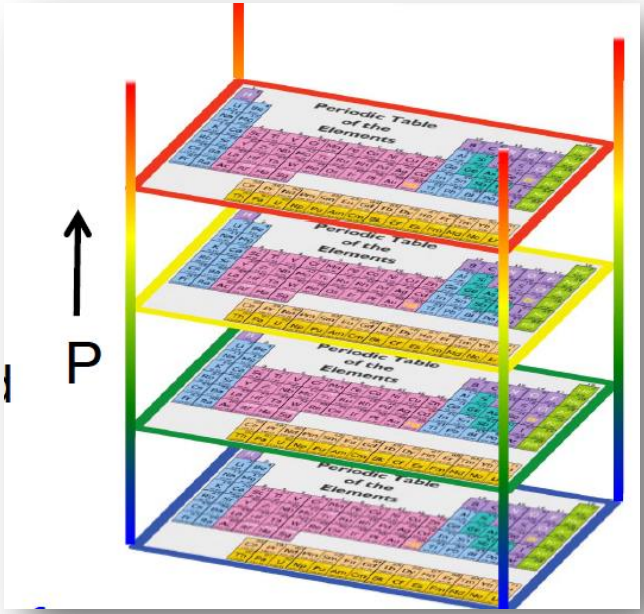
To accelerate the discovery and synthesis of new energy materials using extreme conditions

- High pressure is a unique variable to dramatically change the properties of materials. Novel phase and phenomena.

- Pressure provides a "**clean**" tool to decouple the interactions in a controlled manner. It is the ideal tool to deepen our understanding of material behavior.



EFree Energy Frontier Research in Extreme Environments Center

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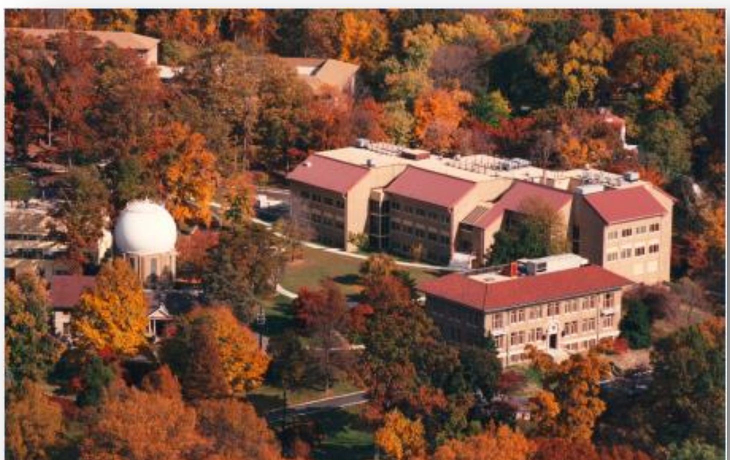
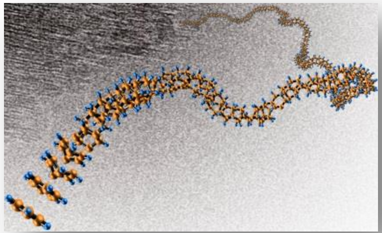
- Exploit extreme environments to manipulate matter for next-generation materials
- Understand fundamental factors that control performance
- Synthesis and/or stabilization at ambient pressure
- Broad university, national laboratory, industrial collaboration



EFree projects

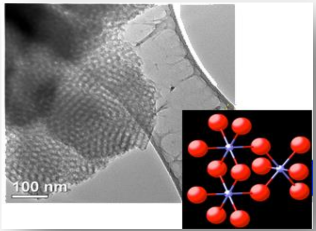


Carbon Nanothreads

1. New Nanophase Carbons

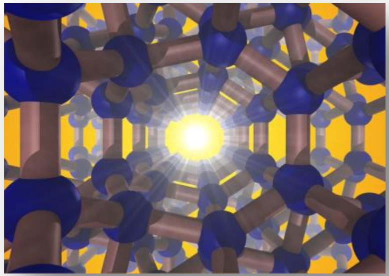
Goal: To stabilize and characterize new forms of carbon through tailored synthetic processes for the development of new structural materials *(Lead: Badding, Penn State)*.

Mesoporous Stishovite



2. Next Generation Mesoporous Materials

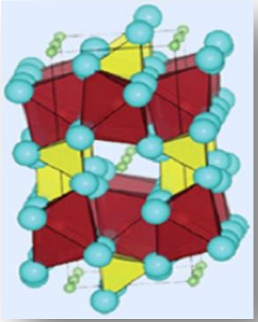
Goal: To obtain mesoporous and mesostructured crystalline materials through templated synthetic routes at high pressure for catalysis and related applications *(Lead: Landskron, Lehigh)*.



Open-Framework Si_{24}

3. New Solar Energy Materials

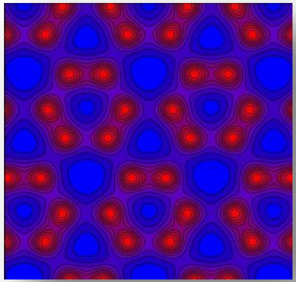
Goal: To synthesize new materials that will have a transformative impact on solar light absorption, conversion efficiencies and manufacturing costs *(Lead: Strobel, Carnegie)*.



Li_xFePO_4

4. Ion Transport Processes

Goal: To characterize the structural features that underlie ion transport in battery materials *(Lead: Fultz, Caltech)*.

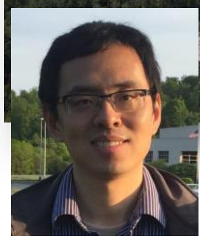


Graphenic Hydrogen

5. Novel Transport in Hydrogen-Rich Materials

Goal: To uncover novel electron transport in hydrogen-rich materials for enhanced electrical transport *(Lead: Hemley, Carnegie)*.

EFree resources

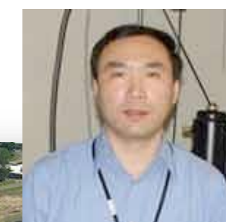


Spallation Neutron Source
(ORNL) - *NEUTRON SCATTERING*

Chen Li
Neutron Scattering Coordinator

Advanced Photon Source
(ANL) – *X-RAY*

Zhenxian Liu
Carnegie IR Lead



Maria Baldini
X-ray Coordinator

Synchrotron IR facility at NSLS II

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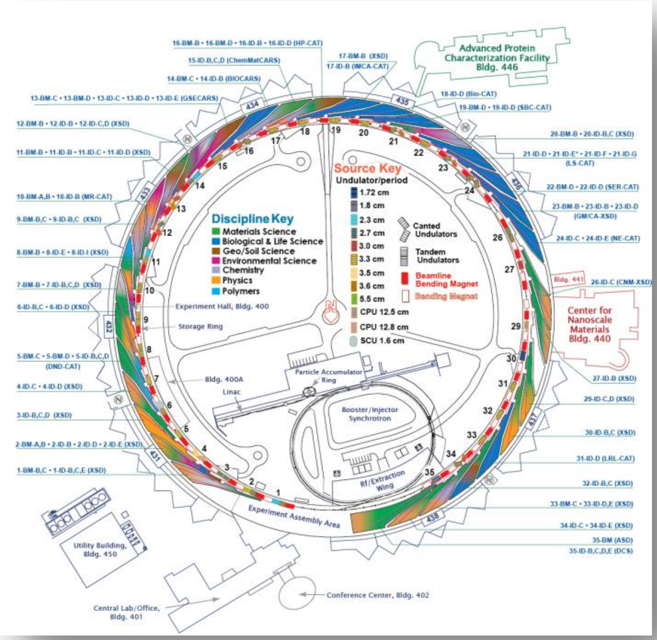
EFree resources



Spectroscopy, scattering and imaging

In-situ characterization

Micro, nano, amorphous

Magnetic and electronic properties

Structure and dynamics

Chemical bonding

Phonon density/oxidation state

- **X-ray diffraction, PDF, EXAFS= Structural characterization**
- **X-ray absorption, X-rayRaman spectroscopy= chemical bonding (sp2/sp3 bonding in C-related compounds)**
- **Transmission X-ray Microscopy (TXM), imaging= strain analysis, volume determination**
- **Small angle scattering= shape and distribution of porous**

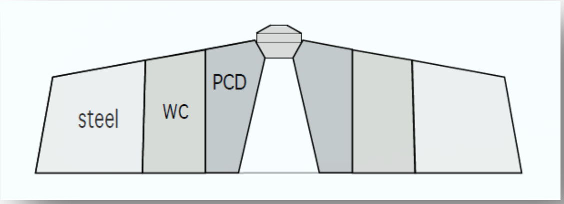
EFree resources

Reini Boehler

High P-T Technique Coordinator

- 90 GPa
- 82 degrees apertures

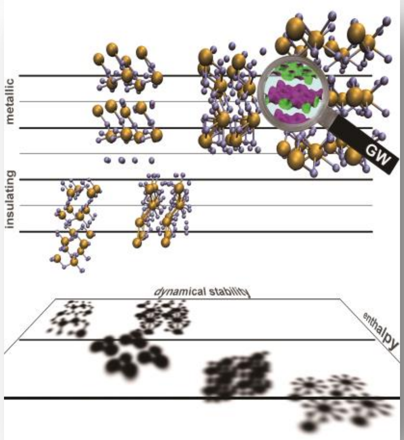
Cells for neutron diffraction and spectroscopy



- **anvil:** type 1 natural (4 mm diameter)
- **seat:** polycryst. diamond

DuckYoung Kim

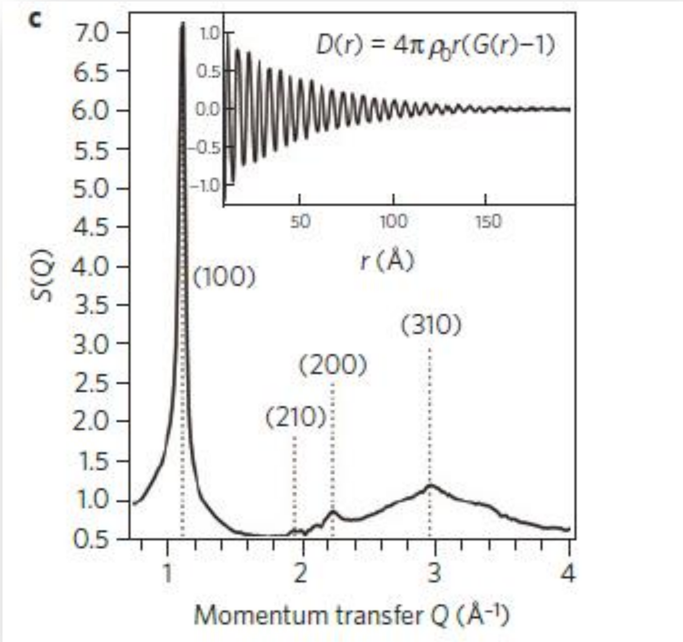
Computational Theory Coordinator



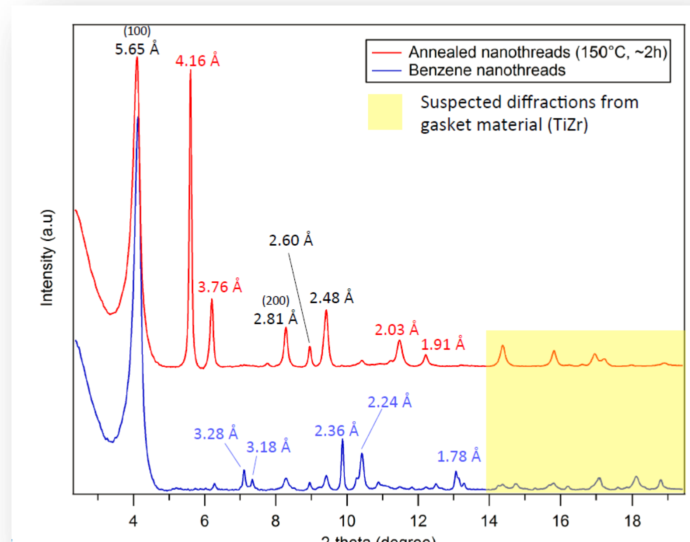
<u>**Crystal structure predictions**</u>

<u>**Electronic structure analysis**</u>

Benzene-derived carbon nanothreads



Synthesis of a new carbon nanomaterial from benzene under pressure that is the thinnest possible thread of the diamond structure

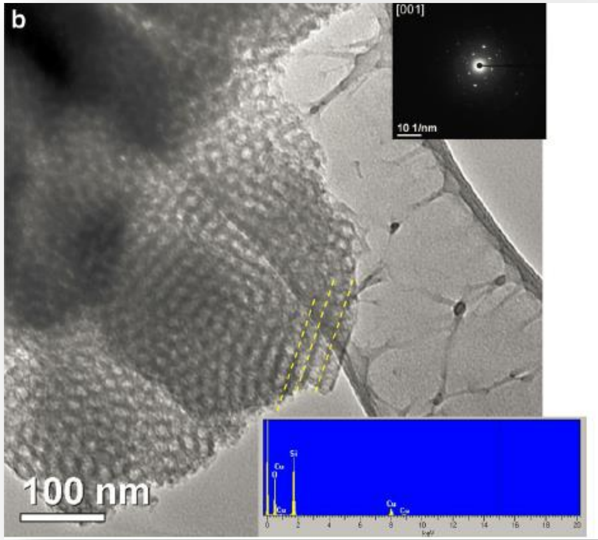


These sp3 nanothreads should have diverse applications owing to their unique properties, including strength, compared to conventional sp2 carbon nanotubes

Fitzgibbons, T.C.,et al.., *Nat Mater, (2014)*
Xu E.-S. et al., *Nano Letters*, (2015)

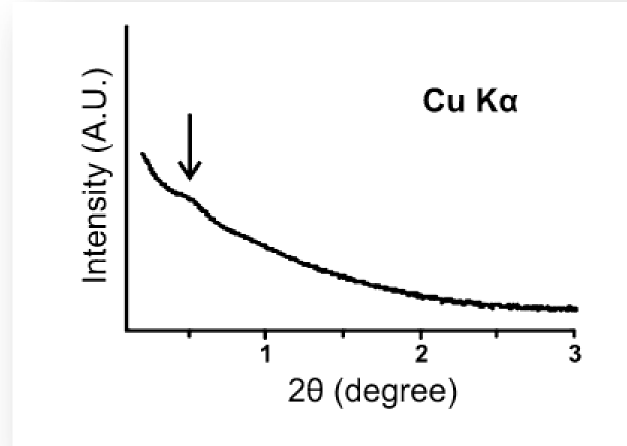
synchrotron x-ray diffraction, neutron diffraction, TEM, Raman spectroscopy, NMR, and first principles calculations.

Next generation measoporous materials



- 9 GPa and 500 °C in a multianvil apparatus

- Mesopores with a wide pore size distribution, ~ 45 m^2/g, and pore volume~ 0.15 cm^3/g



Stagno, V., et al. *Phys. Chem. Minerals* (2015).

The synthesis of mesoporous silica polymorphs offers the opportunity to investigate thermochemical properties for the interaction between stishovite and various guests, such as water H2, CH4, CO2, CO to model fluid sequestration, mineral dissolution and growth under geologic conditions.

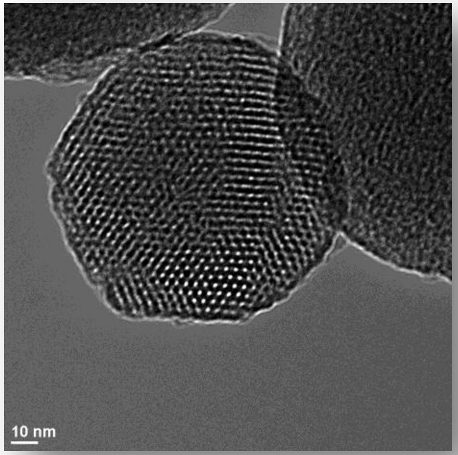
TEM, electron microscopy, gas adsorption, SAXS.

Next generation measoporous materials

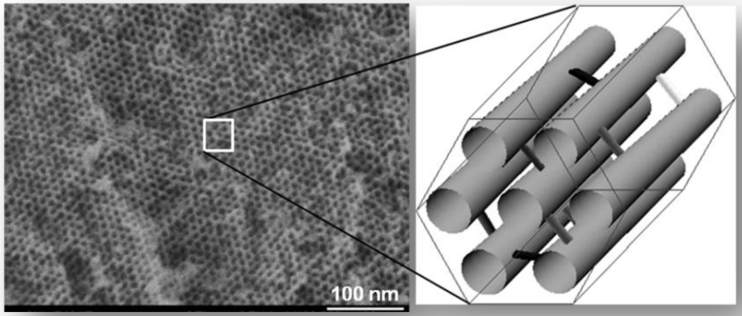
Synthesize a periodic diamond-like mesostructures in mesoporous silicas at high pressure.

Benzene

SBA-16: cubic structure
spherical meso-pores



SBA-15: hexagonal structure
1D meso-channel

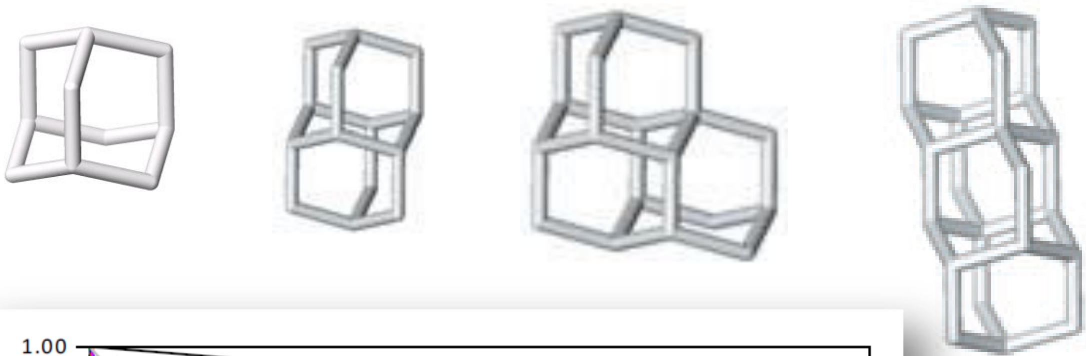


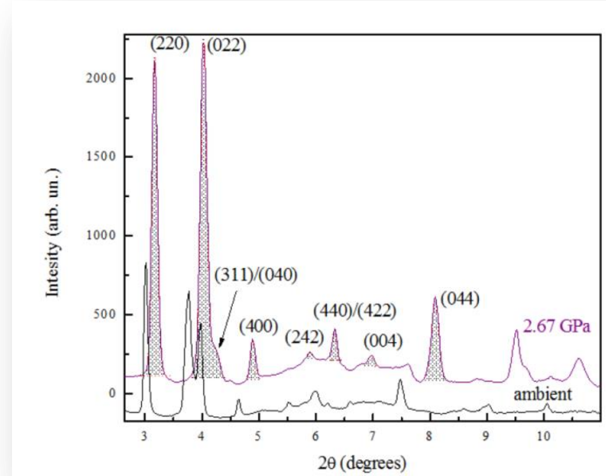
If polymerization into a three-dimensional polymer occurs

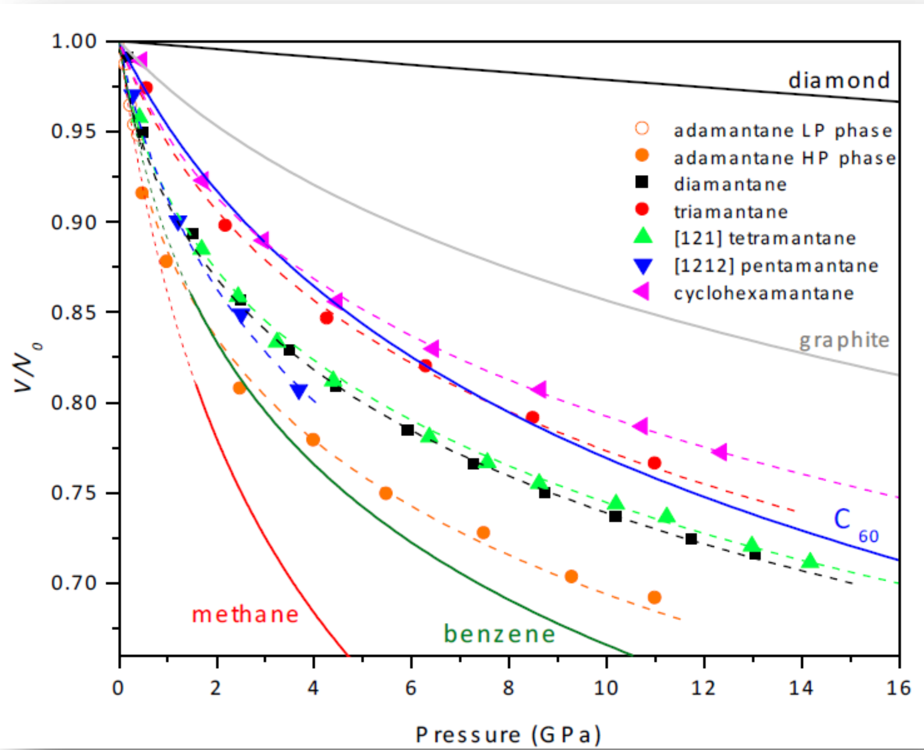
adsorption, separation, and catalysis applications.

Diamondoids

Carbon cage molecules terminated with C-H bonds





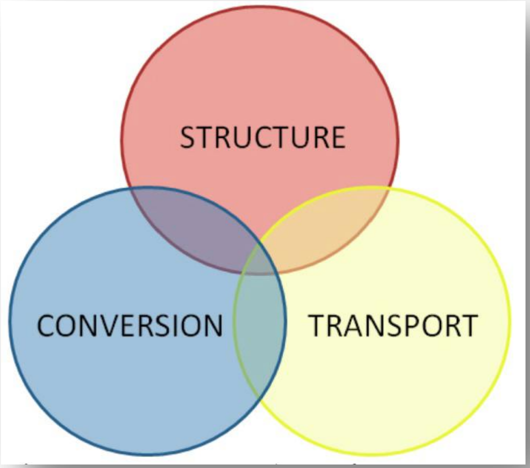


High compressibility, easily triggered pressure-induced phase transitions. Large structural rigidity and molecular geometry dependent bulk modulus.

Y. Fang et al. J. Phys. Chem. C, **2014**, 118, 7683-7689

Conclusions

- **Design, Synthesis and Kinetic Stabilization of Revolutionary Materials for Energy Conversion, Storage and Transport**
  - *Recovery from high P-T*
  - *Scale up*



- **Center for extreme conditions science**
  - *Interactions with national lab facilities*
  - *Technique development*

- **Synergy between theory and experiment**