FORCE

ASU NSF

# 2nd Winter Workshop

## on Recent Advances in High Pressure Research

**January 3–4, 2024**

*Arizona State University, Tempe, AZ*

*Bateman Physical Sciences, F-Wing 101 & 186*



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# Wednesday January 3

## Morning Session – Chair: Tom Sharp (ASU)

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|---|---|---|
| 8:00 | Registration | PSF 186 |
| 8:30 | Workshop introduction<br>• 8:30: **Kurt Leinenweber** (ASU): Welcome and update on FORCE<br>• 8:55: **Dan Shim** (ASU): Workshop structure and breakout topics | PSF 101 |
| 9:00 | Invited speakers<br>• 9:00: **Carl Agee** (University of New Mexico): "High Pressure Experimental Petrology of the Solar System at FORCE"<br>• 9:15: **Andrew Campbell** (University of Chicago): "SEES: New Opportunities and Developments in Synchrotron Earth and Environmental Sciences" | PSF 101 |
| 9:30 | **Morning break** | PSF 186 |
| 9:45 | Invited speakers<br>• 9:45: **Tetsuo Irifune** (Ehime University) "Development of Kawai-type Multianvil High-pressure Technology"<br>• 10:40: **Megumi Kawasaki** (Oregon State University) "High-Pressure Torsion in Metal Processing: Characterization of Hetero-Nanostructure and Manufacturing Capabilities" | PSF 101 |
| 11:30 | Open discussion | PSF 101 |
| 12:00 | **Lunch** (personal arrangements) | |

## Afternoon Session – Chair: Kara Brugman (ASU)

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|---|---|---|
| 1:30 | **Emmanuel Soignard** (ASU): Overview of ASU supporting facilities | PSF 101 |
| 1:45 | Lab and analytical facilities tours | |
| | • **FORCE Press Hall** (PI: Kurt Leinenweber)<br>  ○ Ichiban: 6000 ton uniaxial multi-anvil<br>  ○ Twister: 500 ton high pressure torsion<br>  ○ Nebula: internally heated pressure vessel<br>  ○ Jasmine: 1500 ton cubic DIA-type multi-anvil | ISTB2 |
| | • **CXFEL** (PI: Robert Kaindl) | Biodesign C |
| | • **Nano Science Lab** (PI: Robert Nemanich) | Psych North |

- **Eyring Materials Center aberration-corrected microscopes** Schwada
    - FEI Titan 80/300 E-TEM
    - Nion Monochromated UltraSTEM 100
    - JEOL ARM 200F TEM/STEM

3:45 **Afternoon break** PSF 186
4:00 Poster flash talks PSF 101
4:15 Poster viewing PSF Lobby
5:45 Open discussion (optional) PSF 101
6:30 **Workshop dinner** at Uncle Maddio's 660 S College Ave Suite 221

# Thursday January 4

## Morning Session – Chair: Dave Smith (ASU)

9:00 Contribution from FORCE personnel PSF 101

- 9:00: **Damanveer Grewal** (ASU) "Origin of nitrogen and carbon in rocky bodies–an iron meteorite perspective"
- 9:15: **Kyusei Tsuno** (ASU) "Wetting property of Fe-Ni-N alloy melt in ringwoodite and application to nitrogen depletion in present-day bulk silicate Earth"
- 9:30: **Kara Brugman** (ASU) "Experimental determination of H solubility in primitive rocky planet melts"

9:45 Contributed talks PSF 101

- 9:45: **Zi-Kui Liu** (Penn State) "Zentropy theory for accurate prediction of thermodynamics of temperature-pressure diagrams"
- 10:00: **Yifeng Han** (ASU) "Thermodynamic Properties and Enhancement of Diamagnetism in Nitrogen Doped Lutetium Hydride Synthesized at High Pressure"
- 10:15: **Sibo Chen** (ASU) "Empowering FORCE Users: vibEELS – A Nondestructive Sub-Nanometer Probe for Hydrogen in High-Pressure Minerals"

10:30 **Morning break** PSF 186
10:45 Breakout 1: Future directions for high pressure research PSF 186, 226, 501, 543
11:45 Groups report back PSF 101
12:00 Group photo Outside PSF
12:15 **Lunch** (personal arrangements)

## Afternoon Session – Chair: Dan Shim (ASU)

| | | |
|---|---|---|
| 1:45 | Breakout 2: Challenges of running a user facility | PSF 186, 226, 501, 543 |
| 2:45 | Groups report back | PSF 101 |
| 3:15 | Open discussion | PSF 101 |
| 3:45 | Announcement of poster awards & photo of recipients | PSF 101 |
| 4:00 | Workshop adjourns | |

# Abstracts

## Invited Speaker Abstracts

**Carl Agee**[1]

**High Pressure Experimental Petrology of the Solar System at FORCE**

Facility for Open Research in a Compressed Environment (FORCE) offers the opportunity to explore an array of yet unsolved problems on the origin and differentiation of planets and small solar system bodies. The large sample volumes and high-pressure range of “Ichiban” and “Jasmine” can create near equilibrium conditions required for experiments on multi-component systems (“real rocks”) placing new constraints on differentiation of large terrestrial planets such as Earth, Venus, and Mars. For asteroids, the internally heated pressure vessel (IHPV) apparatus can reproduce the required modest pressure conditions present in these small bodies that are not achievable in a piston-cylinder device and or a 1-atm gas mixing furnace. This talk will highlight some unsolved problems than can be investigated at FORCE. These include 1) crystal fractionation in a deep terrestrial magma ocean, 2) constraints on the make-up of the Venusian interior, 3) silica-rich magmatism in small bodies of the early solar system.

*1University of New Mexico*

**Kara Brugman**[1], James Badro[2], George D. Cody[3], Jianhua Wang[3], Anat Shahar[3]

**Experimental determination of H solubility in primitive rocky planet melts**

To interpret and contextualize JWST exoplanet atmosphere data, scientists are modeling how solid planets and their atmospheres co-evolve. However, geochemical models that are applied to exoplanets are based on Earth’s chemistry and petrological relationships, many of which are still not well understood. For example, $H_2$ is the most abundant species in primary (nebula-derived) planetary atmospheres that may be in direct contact with primitive magma oceans for an extended time. The models needed to interpret exoplanet atmospheric data may depend on the solubility of H in molten rock, but studies of reduced volatiles in magma are not common. I will present the results of hydrogen solubility experiments performed at high and ambient pressures on two primitive compositions to help generalize the extension of experimental data to other rocky planet compositions.

*[1]Arizona State University, [2]Institut de Physique du Globe de Paris, [3]Carnegie Earth & Planets Laboratory*

**Andrew Campbell**[1]

**SEES: New Opportunities and Developments in Synchrotron Earth and Environmental Sciences**

SEES (Synchrotron Earth and Environmental Sciences) is a new organization to operate NSF-supported synchrotron beamlines that focus on geoscience user applications. SEES includes GSECARS and the former COMPRES-supported mineral physics beamlines, and will also facilitate new beamline access for applications in low-temperature geochemistry, environmental science, and in-situ studies of rock deformation at ALS, NSLS-II, APS, and SSRL. Coordinated management of these beamline facilities will improve service to the user community and enhance development across these existing X-ray and IR beamlines. The upcoming upgrades of the APS and ALS synchrotron sources will provide new possibilities for users in Earth and environmental science studies, and SEES will support beamline developments to exploit these and other opportunities in geoscience applications. Opportunities exist to couple the resources of FORCE and SEES to users' benefit.

[1]*University of Chicago*

**Damanveer Grewal**[1]

**Origin of nitrogen and carbon in rocky bodies–an iron meteorite perspective**

Long-term habitability of rocky planet surfaces relies heavily on the exchange of life-essential volatiles like nitrogen and carbon between the atmosphere and silicate reservoirs. However, when and how did Earth-like rocky planets acquire their volatile inventories is poorly understood. The rocky planet forming region in the inner Solar System is believed to have been too hot for volatiles to condense, resulting in almost volatile-free rocky protoplanets. A small cargo of outer Solar System materials is, therefore, assumed to exclusively supply the volatile inventory to the inner Solar System – resulting in volatile-poor rocky planets. In this talk, I will present some of my new observations based on meteorites and laboratory experiments that challenge this paradigm.

[1]*Arizona State University*

**Tetsuo Irifune**[1]

**Development of Kawai-type Multianvil High-pressure Technology**

Since the large-volume press with a double-stage multi-anvil system was invented by late Professor Naoto Kawai, this apparatus (Kawai-type multi-anvil apparatus or KMA) has been developed for higher pressure generation, in situ X-ray and neutron observations, deformation experiments, measurements of physical properties, synthesis of high-pressure phases, etc., utilizing its large sample volume and ability in stable and homogeneous high temperature generation relative to those of competitive diamond anvil cell. Such developments in KMA technology have been made mainly by Japanese scientists and engineers, which provided a number of new experimental data on phase transitions, melting relations, and physical properties of minerals and rocks, leading to important constraints on the structures, chemical compositions, and dynamics of the deep Earth. KMA technology has also been used for synthesis of novel functional materials such as nano-polycrystalline diamond and transparent nano-ceramics, opening a new research field of ultrahigh-pressure materials science.

[1]*Ehime University*

**Megumi Kawasaki**[1]

**High-Pressure Torsion in Metal Processing: Characterization of Hetero-Nanostructure and Manufacturing Capabilities**

Metal processing through the application of high-pressure torsion (HPT) enables the production of bulk nanostructured metals and materials. One unique aspect of HPT is its ability to process general engineering metals and alloys at ambient temperatures for a short duration, introducing true nanometer-sized grains without microstructural recovery through hydrostatic compressive pressure. HPT-processed nanocrystalline metals often exhibit superior mechanical properties and functionality. This presentation provides principles for the processing of bulk nanostructured metals through the application of HPT, along with recent studies on characterizing undiscovered hetero-nanostructures in the HPT-processed metals. Special emphasis is placed on exploring the manufacturing capability of HPT for the rapid fabrication of metal matrix nanocomposites and metastable alloys, as well as the scaling up of severely deformed metals using the HPT facility with additional HPT accessories.

[1]*Oregon State University*

**Kyusei Tsuno**[1]

**Wetting property of Fe-Ni-N alloy melt in ringwoodite and application to nitrogen depletion in present-day bulk silicate Earth**

The abundance of nitrogen (N) in present-day bulk silicate Earth (BSE) is distinctively lower than carbon and hydrogen because N can be effectively partitioned into core-forming alloy melt than silicate magma ocean. I hypothesize that disequilibrium reaction between them may have resulted in higher N content in the magma ocean than in BSE, and after the early Earth differentiation, the N content in the deep mantle reached its present-day level. To assess whether N removal from the deep mantle occurred by percolation of alloy melt produced by disproportionation of ferrous iron in silicate minerals after the early Earth differentiation, we experimentally measured the dihedral angles of Fe-Ni-N melt in ringwoodite. The measured dihedral angle is much larger than wetting boundary, therefore, this scenario does not hold so far. Jasmine, an Osugi-type press to be installed at ASU, will be a powerful device to obtain the dihedral angle at higher pressures.

[1]*Arizona State University*

## Contributed Abstracts

**Godwin Agbanga**[1], Alexandra Navrotsky[1], Manuel Scharrer[1]

**Structure and thermodynamic stability of rare earth carbonates (RECs)**

Rare earth elements (REEs) are an essential key to modern technology and a highly valued critical commodity. High prices and potentially politically unstable supply chains have increased the demand for new sources of REEs. One of these is the promising extraction of REEs from REE-bearing waste sludges from aluminum production (red mud) using supercritical CO2. To model the fractionation and mobility between the REEs as well as optimize the extraction processes, it is therefore essential to fully constrain the REE-CO2-H2O system. This is done by hydrothermal synthesis of end members, structural characterization by XRD and FTIR, thermal analysis by DSC, and enthalpic analysis by high-temperature oxide melt drop solution calorimetry. The inability to synthesize heavy REE bastnaesites at <250°C requires the future use of higher-pressure synthesis methods such as the piston-cylinder method.

The hydrothermal synthesis of REE carbonates from room temperature to 250°C shows that the formation of different REE carbonates (amorphous, lanthanite, tengerite, kozoite, and bastnasite) is not only limited by thermodynamic factors but also largely depends on kinetics (time and size of the experimental setup). The lanthanite structure is constrained to low temperatures with light REEs, which is a result of thermodynamic destabilization relative to tengerite for intermediate REEs and probably also to the amorphous phase for heavy REEs.

[1]*Arizona State University*

**Benjamin Brugman**[1], Yifeng Han[1], Logan J. Leinbach[1], Kurt Leinenweber[1], Axel van de Walle[2], Sergey V. Ushakov[1], Qi-Jun Hong[1], Alexandra Navrotsky[1]

**YO: computationally led high pressure synthesis and experimental thermodynamics of rocksalt yttrium monoxide**

Yttrium monoxide (YO) is among a group of several yttrium oxides recently predicted to stabilize at high pressure. YO was predicted to exhibit superconductivity with a critical temperature that increases as pressure decreases. Despite this, there are no reported syntheses of bulk YO. We used density functional theory and molecular dynamics to predict the stability of YO above 8.6 GPa and at high temperature and successfully synthesized YO in a multi-anvil press. The optimal synthesis conditions were 15 GPa and 1600 °C. The fcc structure was confirmed by powder X-ray diffraction. YO decomposes rapidly when heated, so we used a combination of experiments and theory to obtain its formation enthalpy and calculate the P-T slope for the reaction Y + Y2O3 = 3YO. The enthalpy of the reaction is 35.7 kJ/mol, which compares favorably with the predicted value of 32.7 kJ/mol. The slope of the P-T boundary is slightly positive, decreasing to 8.68 GPa at 0 K. This agrees with the 8.6 GPa DFT prediction and indicates YO is metastable at ambient pressure for all temperatures. Our results illustrate the importance of using pressure as a chemical synthesis parameter and the valuable role theoretical calculations can play in guiding experiments.

[1]*Arizona State University* [2]*Brown University*

**Miguel Bustamante**[1]

**Enthalpies of Mixing for Alloys Liquid Below Room Temperature Determined by Oxidative Solution Calorimetry**

Fusible alloys, and gallium-based liquid metal alloys (Ga-LMA) in particular, have applications in soft robotics, microelectronics, self-healing battery components, and 2D materials synthesis, making the study of their thermodynamic properties critical to improvement and development of hybrid materials. To determine the enthalpies of formation/mixing of the binary Ga-In, the ternary Ga-In-Sn, and the quaternary Ga-In-Sn-Zn eutectics, a novel experimental calorimetric technique based on oxidative solution calorimetry was developed. The experimental results for the discreet binary and ternary alloy composition are consistent with previous data obtained by direct reaction and solution calorimetry, demonstrating the viability and precision of the experimental technique, making applicable to a large variety of multi component systems that are complex in composition and liquid at or below room temperature. The heats of mixing of the quaternary system represent the first reported experimental value. Both the standard geometrical models and FactSage were used to define enthalpy analogs for these systems which agreed with the experimental data, providing a foundation to analyze the thermodynamics of other unknown Ga-based alloys liquid alloy systems.

[1]*Arizona State University*

**Luisa Chavarria**[1], Hannah Bausch[2], Allison Pease[1], Vitali Prakapenka[3], Maddury Somayazulu[4], Susannah M. Dorfman[1]

**Role Of Iron Concentration In The Incorporation Of Sodium Into Ferropericlase In The Earth's Lower Mantle**

The storage and mobility of sodium in the mantle can be related to processes such as mantle mixing of subducted crust and cycling of volatiles. The main host phase for sodium in the mantle may be ferropericlase, the second most abundant mineral in a pyrolitic lower mantle. However, the quantity, conditions, and mechanisms of sodium incorporation in ferropericlase in the lower mantle are not well understood. Accurate thermodynamic modeling of the stable mantle phase assemblage depends on including constraints on sodium chemistry. In this study, we reacted synthetic (Mg0.75-0.50, Fe0.25-0.50)O ferropericlase with NaCl in the laser-heated diamond anvil cell at lower mantle conditions of 40-90 GPa and 1900-2300 K. After recovery from high pressures and temperatures, ex situ Energy Dispersive X-Ray spectroscopy (EDX) analysis detected sodium in less iron-rich (Mg0.75, Fe0.25)O under certain time and pressure conditions, compared with more iron-rich (Mg0.50, Fe0.50)O at 72 GPa and 2100 K conditions. These results suggest that the solubility of sodium is strongly enhanced in Fe-rich (Fe, Mg)O. In addition, solubility is pressure-dependent, and higher concentrations of sodium are observed in samples recovered from pressures above ~70 GPa. Sodium solubility in ferropericlase in the lower mantle may be enhanced in iron-rich mantle heterogeneities.

*[1]Michigan State University [2]Northwestern University [3]University of Chicago [4]Argonne National Laboratory*

**Sibo Chen**[1], Shize Yang[2], Taehyun Kim[1], Xuehui Wei[1], Sang-Heon Shim[1]

**Empowering FORCE Users: vibEELS – A Nondestructive Sub-Nanometer Probe for Hydrogen in High-Pressure Minerals**

Understanding hydrogen transportation and storage is important for planetary habitability. In Earth's mantle, hydrogen can be stored in lattice defects, affecting mineral properties. While infrared spectroscopy examines hydrogen in high-pressure minerals, its large beam size limits detection in sub-micron phases common in high-pressure samples. Recent Ultra High Energy Resolution Scanning Transmission Electron Microscope (UHER-STEM) advances introduce vibrational electron energy loss spectroscopy (vibEELS). With <1 nm spatial resolution and aloof spectroscopy capabilities, vibEELS avoids damaging sensitive high-pressure minerals.

Using a NION UltraSTEM at Arizona State University, we applied vibEELS to nanoscale hydrous minerals, nominally anhydrous minerals, and hydrogen-bearing amorphous phases. The resulting spectra revealed hydrogen peaks at 0.3-0.5 eV, aligning with IR-active modes, and robust lattice mode observations at 0.03-0.2 eV for nanometer-scale phase identification. This technique holds promise for quantifying H partitioning in multi-phase rocky mantle systems. Future FORCE users can conveniently utilize the large volume press and UHER-STEM at Arizona State University for both experimentation and analysis, streamlining research processes.

*[1]Arizona State University [2]Yale University*

**Shanece Esdaille**[1], Vadym Drozd[2], Jiuhua Chen[3]

**Is the Earth's Core Rusting?: A Synchrotron discovery**

One of Earth's lower mantle enigmas is the origin of seismic heterogeneity near the core-mantle boundary (CMB). Among these are Ultra-low velocity zones (ULVZ) that exhibit much slower seismic velocities in comparison to the surrounding mantle. A proposed candidate for this origin is high-pressure polymorphs of iron oxyhydroxides (FeOOH) which is a primary component of rust that is produced when iron meets moisture. Water carried down by subduction slabs may react with the iron-rich core, producing patches of high-pressure solid phase FeOOH with a pyrite structure (py-FeOOH).

To address the knowledge gap surrounding whether py-FeOOH remains stable when surrounded by molten iron -representative of the outer core- we conducted simultaneous high pressure-high temperature in-situ synchrotron X-ray Diffraction measurements on py-FeOOH with iron using a Laser-heated Diamond Anvil Cell. We observed transformation reactions and reaction limits up to CMB conditions (~136 GPa and ~3500K) to better determine the equilibrium conditions of py-FeOOH. Moreover, since the true composition of the DLM is unknown, we examined the synthesis of py-FeOOH using an Fe-Ni alloy and water at DLM conditions. This project aims to determine the thermal and compositional stability boundaries of high-pressure core rust in equilibrium with molten iron at CMB conditions.

*[1]Florida International University [2]Argonne National Laboratory [3]Lawrence Berkeley National Laboratory*

**Minkyung Han**[1], Cheng Peng[2], Ruyi Song[2]; Feng Ke[2], Youssef S. G. Nashed[2], Wendy L. Mao[1,2], Chunjing Jia[3],and Yu Lin[2]

**Machine Learning-Empowered Study of Metastable γ-CsPbI3 under Pressure and Strain**

Metastable γ-CsPbI3 is a promising solar cell material due to its suitable band gap and chemical stability. While this metastable perovskite structure can be achieved via introducing external pressure or strain, experimenting with this material is still challenging due to its phase instability. In this work, we present the first instance of exploiting various machine learning (ML) models to efficiently predict the band gap and enthalpy of metastable γ-CsPbI3 under pressure or strain while identifying key structural features that determine these properties. ML models trained on experimentally benchmarked, first-principles calculation datasets exhibit excellent performance in predicting the behavior of tuned systems, comparable to predictions made for ambient material databases. In particular, graph neural networks (GNNs) that explicitly include a graph encoding the bond angle information outperform other ML models in most scenarios. The pressure-tuned system demonstrates a strong linear relationship between structural features and properties, effectively captured by global structural features using linear regression models. In contrast, the strain-tuned system shows a non-linear relationship, exhibiting superior prediction performance using GNNs trained on local environments. This study opens up opportunities to apply and develop ML models for understanding and designing materials at extreme conditions.

*[1]Stanford University [2]SLAC National Accelerator Laboratory [3]University of Florida*

**Yifeng Han**[1], Yunbo Oub[1], Hualei Sun[2], Jan Kopaczek[1,3], Gerson Leonel[1], Xin Guo[1], Benjamin Brugman[1], Kurt D. Leinenweber[1], Hongwu Xu[1], Meng Wang[2], Sefaattin Tongay[1], Alexandra Navrotsky[1]

**Thermodynamic Properties and Enhancement of Diamagnetism in Nitrogen Doped Lutetium Hydride Synthesized at High Pressure**

Nitrogen doped lutetium hydride has drawn global attention in the pursuit of room temperature superconductivity near ambient pressure and temperature. However, variable synthesis techniques and uncertainty surrounding nitrogen concentration have contributed to extensive debate within the scientific community about this material and its properties. We used a solid state approach to synthesize nitrogen doped lutetium hydride in multi-anvil (5GPa, 1273 K) and analyzed the residual starting materials to determine its nitrogen content. High temperature oxide melt solution calorimetry determined the formation enthalpy of LuH1.96N0.02 (LHN) from LuH2 and LuN to be -28.4 ± 11.4 kJ/mol. Magnetic measurements indicated diamagnetism which increased with nitrogen content. Ambient pressure conductivity measurements observed metallic behavior from 5 to 350 K, and the constant and parabolic magnetoresistance changed with increasing temperature. High pressure conductivity measurements revealed that LHN does not exhibit superconductivity up to 26.6 GPa. We compressed LHN in a diamond anvil cell to 13.7 GPa and measured the Raman signal at each step, with no evidence of any phase transition. Despite the absence of superconductivity, a color change from blue to purple to red was observed on increasing pressure. Thus, our findings confirm the thermodynamic stability of LHN, do not support superconductivity, and provide insights into the origins of its diamagnetism.

*[1]Arizona State University [2]Sun Yat-Sen University [3]Wroclaw University of Science and Technology*

**Heidi Krauss**[1], Allen K. McNamara[1]

**Superpiles: A Low Density Explanation for LLSVPs**

One hypothesis for the formation of Large Low Shear Velocity Provinces (LLSVPs) is that they formed from an intrinsically more dense compositional reservoir in the lower mantle. The possibility of mantle plumes originating from this compositional reservoir could provide an explanation for the observed trace element geochemistry differences between mid ocean ridge basalts (MORBs) and ocean island basalts (OIBs). Our geodynamic models have shown compositional reservoirs tend to form either active superplume, or passive pile morphology. Tomography models indicate the LLSVPs have a morphology which resembles superplumes. The thermal initial condition of a geodynamic model greatly impacts the morphology of these compositional reservoirs. A hot thermal initial condition increases the upwards buoyancy or effective density of the surrounding mantle. This causes the compositional reservoir to form a new type of pile morphology at smaller than expected density differences, a superpile. Superpiles are tall features resembling superplumes, but they are passive features formed by mantle convection the same as a pile morphology. If LLSVPs have a superpile morphology they could have a density similar to the surrounding mantle while explaining the tall LLSVP morphology.

[1]*Michigan State University*

**Logan Leinbach**[1], Kara Brugman[1], Kurt Leineweber[1], Alexandra Navrotsky[1], Thomas Sharp[1], Sang-Heon Shim[1], David Smith[1], Kyusei Tsuno[1]

**FORCE (Facility for Open Research in a Compressed Environment) Progress and Future Advances**

The Facility for Open Research in a Compressed Environment (FORCE), will provide a research laboratory to enable the high-pressure science community to gain access to state-of-the-art, large-volume high-pressure equipment previously only accessible outside of the United States. The implementation of FORCE is being supported by NSF as a Mid-scale Research Infrastructure (RI-1) Project. Four major pieces of equipment will be installed in FORCE:

1. A 6000-ton uniaxial Kawai-type multi-anvil press (Ichiban) from Sumitomo Heavy Industries will be employed for the synthesis of single-crystal and polycrystalline large-volume samples up to 25 GPa.
2. A 1500-ton DIA cubic press (Jasmine) from Max Voggenreiter GmbH will generate ultra-high pressures (40–100 GPa) samples and will be useful for studying materials of the upper to the deep mantle.
3. A 500-ton high pressure torsion device (Twister) from Riken Corporation will be utilized for studies involving shear and torsional forces.
4. An internally heated pressure vessel (Nebula) from Wille Geotechnik will be important for planetary crust studies as well as synthesis of starting materials for use in the other apparatus.

The first two pieces of equipment, Ichiban and Twister, arrived in Summer 2023 and have completed their requisite commissioning.

[1]*Arizona State University*

**Zi-Kui Liu**[1]

**Zentropy theory for accurate prediction of thermodynamics of temperature-pressure diagrams**

Pressure is an important variable in many systems, particularly in Earth and Planetary Science. However, the prediction of its combined effects with temperature on phase stability remains elusive. The pressure and volume are conjugate variables in thermodynamics and related to each other by derivatives of free energy. Therefore, the fundamental challenge is to accurately predict the free energy of a system as a function of temperature and pressure. Based on statistical mechanics, a macroscopically homogeneous system is composed of all possible independent configurations that the system embraces. The macroscopical properties of the system are thus determined by the properties and statistical probabilities of those configurations with respect to external conditions. In this presentation, our multiscale entropy approach (recently termed as zentropy theory) will be discussed to demonstrate its capability to accurately predict free energy and temperature-pressure phase diagrams with only inputs from first-principles calculations based on density functional theory (DFT) combined with a revised statistical mechanical formula without additional models and fitting parameters. It is shown that the anharmonicity and non-linear emergent behaviors originate from the statistical probabilities of competing configurations, including singularity at a critical point.

[1]*Pennsylvania State University*

**Jiaqi Lu**[1], Jie Li[1]

**High-pressure melting behaviors of potassium carbonate: Carbon transportation in the mantle and deep carbon cycle**

Carbon is the chemical backbone of life on Earth and one of the major volatile elements in the mantle. The carbon cycle occurring near the Earth's surface is widely recognized as a crucial control on the environment and climate that supports life on our carbon-based planet. As potential carriers of carbon back to deep Earth through subducted slab, carbonates are highlighted due to its significance for the deep carbon cycle. Previous high-pressure melting studies of K2CO3 have yielded inconsistent results especially at above 3 GPa and large discrepancies of more than 180 °C at above 3 GPa remained mysterious. This research conducted high-pressure ionic-conductivity experiments in a 1000-ton multi-anvil press to resolve these discrepancies of the melting curve. Oil pressure was calibrated to provide more reliable pressure value, using the established high-pressure melting curve of NaCl. Melting point of K2CO3 at 3 GPa is reported as 1380 °C and the discrepancies at high-pressure are potentially caused by the water sealed in the closed system in previous studies. This ongoing research will also measure the melting temperature of K2CO3 using platinum marker experiments for comparisons and cross-validation on the influence of water.

[1]*University of Michigan*

**Ivan G. Matyushov**[1], Blaine G. Aberra[1], Ben L. Brugman[1], Logan J. Leinbach[1], Kurt D. Leinenweber[1], Sergey V. Ushakov[1], Alexandra Navrotsky[1]

**Thermal Analysis in the Multi-Anvil (TAiM)**

The multi-anvil press is widely used in experiments to generate high pressure conditions. New phases recovered from high P and T inform research from Earth and planetary science to materials chemistry. However, not all high P-T phases are recoverable to ambient pressure, and outside of synchrotron facilities, there are few diagnostics available for in situ property measurements in the press. The purpose of TAiM is to determine if the thermocouple and voltage controller setup used to monitor and control temperature in multi-anvil experiment can also be used for in situ thermal analysis. Heat effects from melting or solid-solid phase transitions may be detectable in power-temperature data recorded during heating. In this preliminary work, we drive phase changes in rare earth sesquioxides and melting in neodymium metal at high P-T (up to 1400 °C and 4 GPa) to test the sensitivity of the thermocouple to changes in heat flow. A large volume of sample is used to maximize the detectible heat effect. Power-temperature profiles will be used to construct a baseline and observe changes in the detected heat flow. Further thermodynamic experiments may be conducted on recovered high P phases. Additional details and preliminary results will be presented on the poster.

*[1]Arizona State University*

**Allison Pease**[1], Mario Cueva Calderon[1], Stella Chariton[2], Vitali Prakapenka[2], Susannah Dorfman[1]

**Thermal Equation of State of Transition-Metal-Bearing Davemaoite and Implications for Large Low Shear Velocity Provinces (LLSVPs)**

Davemaoite is proposed to be a major mineral phase in Earth's lower mantle, and Fe-bearing davemaoite may represent the physical properties of subducted basalt in the lower mantle. However, the thermoelastic behavior of transition metal enriched davemaoite has not been measured. In this study, we synthesized homogeneous (Ca, Fe, Mn)SiO3 starting materials from oxide powders in a vacuum-sealed glass ampule. Samples were loaded into a diamond anvil cell and transformed to the perovskite structure above 35 GPa and 1500 K. To constrain the thermal equation of state and tetragonal-cubic phase transition of transition metal enriched davemaoite, in situ X-ray diffraction data were obtained at GSECARS. High-temperature volume data were fit to a Mie-Gruneisen equation of state. The 300 K equation of state was determined based on a third-order Birch-Murnaghan equation of state. We observe that Ca0.82Mn0.18SiO3 and Ca0.69Mn0.16Fe0.15SiO3 have 1-3% lower unit cell volumes than CaSiO3. When K' is fixed to 4, the bulk modulus increases by 5-10% compared to CaSiO3 and up to 5% compared to the MnSiO3 end member. For natural Fe, Mn-bearing davemaoite, the incompressibility is higher relative to pure CaSiO3. Variation of the thermal equation of state with increasing transition metal content provides insight into the thermal gradient and heat storage within the lower mantle's large low shear velocity provinces (LLSVPs).

*[1]Michigan State University [2]University of Chicago*