The DOE-NNSA (DE-NA 0003918) project on

Chemistry of Planetary Mixtures at Extreme Conditions

Graduate students: Alex Howard, Brittany Thiessen, Sohan Ahmed
PD Researchers: Jinhyuk Lim, Jialin Lei
Senior Scientist: Minseob Kim

Choong-Shik Yoo
Department of Chemistry, Institute for Shock Physics and Materials Science & Engineering, Washington State University, Pullman, Washington 99164
(509) 335 - 2712; csyoo@wsu.edu

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Overview: Chemistry of planetary mixtures under extreme conditions

- Investigate novel states, properties and chemistry of planetary mixtures under extreme conditions
- Develop enabling high PT technologies and real-time probes such as TR-XRD for d-DAC using the 3G (synchrotron) & 4G (XFEL) light sources
- Educate and train graduate students
- Collaborate with scientists at NNSA Labs at large scientific user facilities:
  - Z. Jenei, E. O’bannon, W. Evans at LLNL: dynamic-DAC at LLNL, HPCAT, PETRA, Eu-XFEL
  - A. Krygier, A. Jenei, J. Eggert, D. Swift at LLNL: NIF-DS shots on NaCl and CMAP shots at \(\Omega_{ER}\)
  - S. Duwal, C. Seagal at SNL: DAC and Z
  - B. Sturtevant, D. Dattelbaum at LANL: Eu-XFEL, LCLS
- Publication: six in 2021-2022

HPCAT is critical for the success of our research projects as well as student training
Progress: Properties of dense planetary solids under high pressures

Phase diagram and EOS

Chemical reaction and novel materials

EOS of ice X in $\text{H}_2$/He

Quantum effects

Crystallization of quantum solids

Lim & Yoo, PRL (2018); Lim & Yoo, PRB (2020); Ryu et al. JPCC (2017 & 2020); Yoo, MRE (2020), Duwal et al., JPPC (2020 & 2018); Lei et al., JPC Lett. (2021) & PRB (2021)
Emergence of PV compression curves between isoelectronic pairs of AX and RGS

Evidence for:
- New hcp phase in Ne and Ar
- B1-B2 transition in NaF


Similar PV curves of AX and RGS may signify reduced bond anisotropy, thus, packing over bonding at high P
Technology development: Dynamic-DAC and time-resolved (TR) probes

Dynamic-DAC to probe the dynamics of phase transitions under fast compression

TR Raman of \( \text{N}_2 \)

TR X-ray Diffraction of \( \text{N}_2 \)

Powder XRD patterns of \( \text{N}_2 \) were obtained in a ms resolution at the APS & PETRA
Compression behaviors of N$_2$ phases in static vs dynamic loading

No apparent difference observed in the onset of transition pressure (liq/$\beta$- or $\beta$/$\delta$-N$_2$), but $\beta$-N$_2$ (not $\delta$-N$_2$) shows distinctive compression behavior under dynamic compression.
Data obtained at a compression rate of $23.5\ \text{TPa/s}$ at the HED of Eu-XFEL (Oct. 2021), in collaboration with DESY (Liermann, Husband, Stronm), LLNL (Jenei, O'Bannon, Evans), LANL (Sturtevant, Dattelbaum), and WSU.

This dynamic-DAC achieves a strain rate of $\sim 10^3/\text{s}$, complementing static and shock experiments.
The PV curve of $\beta$-$N_2$ in dynamic condition is substantially stiffer than that in static, indicating a rapid increase of dynamic yield strength of $\beta$-$N_2$. 
Recent development of HP technologies at DOE-National Labs and HED facilities enables us to access the PT regime of cold-warm dense matters; 1 TPa and 1 eV (in T).

Collaboration: Novel states and new “core-electron” chemistry at TPa

Exotic Conducting States Theoretically Predicted:
- Metallic H$_2$ Suoerfluid at 0.5 TPa
- Metallic carbon at 10 TPa
- Metallic H$_2$O, N$_2$ at 2-4 TPa
- Metallic salt NaCl at 0.5-1.0 TPa
- Metallic He at 40 TPa
- Electrides at 10-100 TPa
- etc. etc
NIF-DS: to exploit novel metallic phases with predominantly ionic structures predicted for NaCl at NIF-accessible pressure (~1 TPa)

Four NIF-DS shots on NaCl have been scheduled in FY2021-22

WSU: Choong-Shik Yoo (PI) and Minseob Kim
LLNL: Andy Krygier (RI), Jon Eggert, Amy Jenei, Damian Swift

Academic collaborators: Chris Pickard at Cambridge; Evan Reed at Stanford; Eva Zurek at U. Buffalo, Michelle Marshall at U. Rochester

Chen & Ma, EPL 100, 26005 (2012).
Shot N210210: Ramp compression of NaCl to ~600 GPa

The diffraction analysis is currently in progress, while more shots are planned.

1. Ti blanks at t=0 (why?)
2. Initial shock reaches Be/NaCl
3. Shock breakout into LiF
4. Peak pressure of ramp
Scientific Progresses:

- Determined various properties of dense planetary mixtures (H2-He): phase diagram, EOS, chemical reactions, crystallization, and quantum effects.
- Investigated the crystal structure and EOS of ice X in He and H2, suggesting evidence for ice X to be a covalent solid with 2e-3c bonding: $B_0^X = 225$ GPa, $B_0^\text{VII} = 5$ GPa.
- Found the evidence of new hcp phase in Ne and Ar and the emergence of PV compression curves between isoelectronic pairs of AX and RGS.
- Investigated the structure evolution of CO2, N2 and CH4 under rapid laser heating, utilizing advanced 3G (synchrotron) and 4G (XFEL) light sources.

Collaboration and Technology Development:

- Time-resolved X-ray diffraction using dynamic-DAC and Eu-XFEL and PETRA-IV in collaboration with the LLNL and DESY groups.
- NIF-DS shots on Chemistry under extreme conditions (XCHEM) on NaCl to 1 TPa.

We continue to emphasize enabling collaboration with DOE-SC and NNSA laboratories.


