62nd European High Pressure Research Group Meeting

31 August–5 September 2025
The Lowry, Manchester, UK

IOP Institute of Physics

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Sunday 31 August

15:30	EHPRG Committee Meeting (Hexagon Room)
17:00	Registration and Refreshments (Pier Eight Foyer)
19:00	Welcome Reception (Quays Bar)
20:30	End

Monday 1 September

08:30	Registration with Refreshments (Quays Bar)
09:00	Opening Ceremony (Quays Theatre)
09:30	Plenary I: Multigrain crystallography and its applications for studying deep mantle water cycle **Li Zhang**, Center for High Pressure Science & Technology Advanced Research, HPSTAR
10:30	Coffee Break (Quays Bar)

	Session 1a: Nanomaterials **(Quays Theatre)**		**Session 1b: Metals, metalloids and alloys** **(Studio 1)**
11:00	(Invited) Novel forms of carbon synthesized from fullerene C_{60} at high pressure **Alexander Soldatov**, Yanshan University	11:00	(Invited) Pressure dependence of alloy solution phase diagrams: Experiments and thermodynamic modeling **Guy Makov**, Ben-Gurion University of the Negev
11:30	(Invited) Pressure-Driven Moiré Potential Enhancement and Tertiary Gap Opening in Graphene/h-BN Heterostructure **Yupeng Wang**, University of Science and Technology of China	11:30	The mechanism of the A7 to sc phase transition in arsenic **Matteo Ceppatelli**, ICCOM-CNR and LENS
12:00	A glimpse into the high-pressure behaviour of metal nanoclusters: the case of Au_{25} **Camino Martín-Sánchez**, University of Geneva	11:50	Electrical Resistivity of Liquid Fe-16wt%S-2wt%Si at High Pressures with Implications for Heat Flow in Sub-Earth Exoplanets **Erin Lenhart**, University of Western Ontario
12:20	Strain Dependent Optical Properties of Core/Shell Nanoplatelets **River Leversee**, University of Colorado, Boulder	12:10	Thermal equation of state of rhodium characterized by resistively and laser heated diamond anvil cell **Jose Luis Rodrigo Ramon**, Universitat De Valencia
12:40	Lunch (Quays Bar)	12:30	Lunch (Quays Bar)

	Parallel Session 2a: Superconductivity (Quays Theatre)		**Parallel Session 2b: Superhard and strongly bonded materials (Studio 1)**
13:30	Predicting new high T_c superconductors **Julia Contreras**, Sorbonne Université / CNRS	13:30	Design of boron based nano-structured super hard material (BP, $B_{12}P_2$) **Hicham Moutaabbid**, Sorbonne University
13:50	Probing high-pressure superconductivity with NV centers in diamond **Jean-Francois Roch**, ENS Paris-Saclay	13:50	Towards predicting tough multi-functional materials recoverable from high-pressure synthesis: Symmetry and vectorisation as an efficient tool for configuration space navigation **Florian Trybel**, Linköping University
14:10	Superconductivity near room temperature in LaH_{10} thin-films at megabar pressures **Sam Cross**, University of Bristol	14:10	High-pressure behavior of binary nitrogen-halogen systems **James Spender**, University of Edinburgh
14:30	Tea Break (Quays Bar)		
15:00	Mikhail Eremets Memorial Lecture (Quays Theatre)		
16:00	EHPRG General Assembly (Quays Theatre)		
18:00	End		

Tuesday 2 September

08:30	Registration with Refreshments (Quays Bar)		
09:00	(Quays Theatre) Plenary II: Diamond anvil cell research at the European XFEL **Rachel Husband**, DESY		
10:00	Coffee Break (Quays Bar)		
	Parallel Session 3a: Optical spectroscopy methods (Quays Theatre)		**Parallel Session 3b: Geoscience and planetary science (Studio 1)**
10:30	(Invited) How to Predict The Refractive Index of a Silicate Glass at High Pressure Based on The Chemical Composition? **Xiangdong Li**, Gfz Helmholtz Centre For Geosciences	10:30	(Invited) Insights into the fate of volatile species during the planetary life cycle from dynamic compression experiments **Alisha Clark**, University of Colorado Boulder
11:00	(Invited) Optical photothermal infrared spectroscopy of h-BN in diamond anvil cell **Francesco Capitani**, Synchrotron SOLEIL	11:00	Twin domain switching in neighborite (NaMgF$_3$) during oscillating deformation: potential implications for intrinsic seismic attenuation of the lower mantle **Simon Hunt**, University of Manchester
11:30	All-optical PVT EOS measurements in the diamond anvil cell **Reece O'Beirne**, University of Salford	11:20	Thermal conductivities of solid and molten silicates: Implications for dynamos in mercury-like proto-planets **Damien Freitas**, The University of Manchester at Harwell
11:50	High pressure reflectance characterization of YAB from mid infrared to the visible **Julio Pellicer-Porres**, University of Valencia	11:40	Structural changes in CaSiO$_3$ glass up to lower mantle pressures **Clemens Prescher**, Universität Freiburg, Geomaterialien und kristalline Werkstoffe
12:10	Measurement of the refractive index of samples in the diamond anvil cell using white light transmission microscopy only **John Proctor**, University of Salford	12:00	(Invited) High-pressure behavior Fe-O-H system in the deep Earth's interior **Elena Bykova**, Goethe-Universität Frankfurt

12:30 Lunch
(Quays Bar)

Women in High Pressure
(Quays Theatre)

	Parallel Session 4a: Inorganic Materials **(Quays Theatre)**		**Parallel Session 4b: Liquids** **(Studio 1)**
13:30	(Invited) Pyramidal inversion in $Ba(IO_3)_2 \cdot H_2O$ **Robin Turnbull**, University of Valencia	13:30	(Invited) X-ray Raman scattering spectroscopy elucidates the microscopic structure of water at high pressure **Simo Huotari**, Department of Physics, University of Helsinki
14:00	SiV centers of diamond as quantum sensors under pressure **Grégoire Le Caruyer**, Lumin, ENS Paris Saclay	14:00	Dynamic diamond anvil cell for time-resolved study: Application on Water **Florian Dembele**, CEA
14:20	Effect of uniaxial pressure on transport properties of MnTe **Karel Vyborny**, Fzu - Inst. Of Physics, Acad Sci Czech Rep	14:20	High-Pressure Structural Invariance in Liquid Bismuth Across the Melting Curve **Shir Ben Shalom**, Ben Gurion University of The Negev
14:40	Neutrons don’t lie: The case of ReO_3 under pressure **Stefan Klotz**, IMPMC, Sorbonne University	14:40	Is there a Liquid-Liquid transition in realgar (As_4S_4) under Extreme Conditions? A Comprehensive Synchrotron study **Rajaji Vincent**, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université
15:00	Full energy structure of the Cr3+ activator in $Cs_2(Ag,Na)InCl_6$ double halide perovskite hosts under pressure **Tadeusz Lesniewski**, University of Gdansk	15:00	The Frenkel line of nitrogen and an empirical equation for the coordination number of real fluids **Ciprian Pruteanu**, University of Edinburgh

15:30 Poster Session 1 with Coffee
(Studio 2 and 3)

17:00 End

Wednesday 3 September

08:30 Registration with Refreshments
(Quays Bar)

09:00 (Compass Room)
EHPRG Award Lecture: When crystallography meets planetary science: insights into large icy moons of Jupiter and Saturn
Anna Pakhomova, European Synchrotron Radiation Facility

10:00 Coffee Break
(Quays Bar)

Parallel Session 5a: Molecular systems and mixtures
(Compass Room)

10:30 (Invited) Phase Stability and Stimulated Reactivity of Methane
Miriam Pena-Alvarez, University of Edinburgh

11:00 (Invited) The emptied hydrate: from the high pressure synthesis to the recovered functional material
Leonardo del Rosso, CNR - Institute of Applied Physics "Nello Carrara"

11:30 Large compositional variability in water-ammonia solid mixtures at high pressure and temperature
Sandra Ninet, Sorbonne Université - IMPMC

11:50 High Temperature properties of methane-hydrogen inclusion compounds
Leopoldine Parczanny, The University of Edinburgh

12:10 Quantum Diamond Magnetometry : High-Pressure Sensing for High-T$_c$ Superconductivity
Claire Roussy, Université Paris-Saclay

Parallel Session 5b: Hydrides and magnetic materials
(Studio 1)

10:30 High-Pressure Synthesis and Characterization of the Novel Potassium Superhydride KH$_9$
Tomas Marqueño Villanueva, University of Edinburgh

10:50 Ternary Sulfur Hydride Compounds
Israel Osmond, Centre For Science at Extreme Conditions, University of Edinburgh

11:10 Formation of Molybdenum Deuteride at High Pressure: A Neutron Diffraction Study
Zhongsheng Wei, STFC - ISIS Neutron and Muon Source

11:30 High Pressure Synthesis of Cesium Superhydrides
Mikhail Kuzovnikov, University of Edinburgh

11:50 Imaging magnetic fields using NV centers as quantum sensors - study of the magnetic transition of UH$_3$ under high pressure
Valentin Schmidt, CEA, DAM, DIF

		12:10	High-pressure modulation of breathing kagome lattice: Lifshitz transitions and evolution of the electronic structure **Marcos Vinicius Goncalves Faria**, Helmholtz-Zentrum Dresden-Rossendorf
12:30	Lunch (Quays Bar)		
	Parallel Session 6a: Central Facilities **(Compass Room)**		**Pressure Scale Workshop** **(Studio 1)**
13:30	(Invited) Developing the High Pressure Science Programme at the ISIS Neutron and Muon Source **Craig Bull**, ISIS Neutron and Muon Source		
14:00	(Invited) Dynamic compression experiments at the HED-HiBEF scientific instrument at European XFEL **Karen Appel**, European XFEL GmbH		**Parallel Session 6b: Geoscience and planetary science** **(Studio 1)**
14:30	Developing Neutron Techniques at Extreme Conditions: the High Pressure Neutron Diffractometer at China Spallation Neutron Source (CSNS) **Jinlong Zhu**, Department of Physics, Southern University of Science And Technology	14:30	(Invited) High-pressure data quality in today's data-centric world **Kamil Dziubek**, University of Vienna
14:50	High-pressure research at the HPCAT beamlines following the APS Upgrade **Maddury Somayazulu**, Argonne National Laboratory	15:00	Synthesis of chemically simple carbonates at moderate pressures and temperatures **Dominik Spahr**, Goethe University Frankfurt
15:10	Structural investigations of iron by X-ray heating and Diamond Anvil Cells at European Free Electron Laser **Zuzana Konopkova**, European XFEL GmbH	15:20	
15:30	Poster Session 2 with Coffee (Studio 2 and 3)		
17:00	End		
19:00	Conference Dinner (The Midland Hotel)		

Thursday 4 September

08:30 Registration with Refreshments
(Quays Bar)

09:00 (Compass Room)
Plenary III: The iron phase diagram at multiple timescales
Sébastien Merkel, Univ Lille, France

10:00 Coffee Break
(Quays Bar)

	Parallel Session 7a: Instrumentation and experimental methods **(Compass Room)**		**Parallel Session 7b: General Interest Talks** **(Studio 1)**
10:30	(Invited) A New X-ray Transparent Internally Heated Pressure Vessel for High-Pressure and High-Temperature in-situ view experiments **Barbara Bonechi**, The University of Manchester	10:30	(Invited) From between diamonds to the centres of planets – large scale impacts from tiny samples **Helen Maynard-Casely**, Australian Centre For Neutron Scattering
11:00	Pressure gradients inside the hydrostatic cavity of DACs loaded with silicone oil and methanol-ethanol 4:1 as pressure transmitting media **Ignacio Hernandez**, Universidad De Cantabria	11:00	(Invited) Crystallising phase relations of Earth’s outer core **Tetsuya Komabayashi**, School of GeoSciences, University of Edinburgh
11:20	Imaging in (Laser-Heated) Diamond Anvil Cells: From Phase Diagrams to Material Properties **Bernhard Massani**, University of Edinburgh	11:30	Engaging Students in High-Pressure Physics Through Sapphire Anvil Cell Experiments **Ilia Sholin**, Independent Researcher
11:40	Optimized Sample Geometry for X-ray Diffraction Experiments under Laser Heating in Diamond Anvil Cells.S **Gunnar Weck**, CEA	11:50	(Invited) How plastic water is? **Livia Eleonora Bove**, CNRS Paris & Università La Sapienza Roma
12:00	(Invited) Study of high pressure properties of geomaterials using time-resolved diagnostics **Guillaume Morard**, IMPMC-CNRS		

12:30 Lunch
(Quays Bar)

Parallel Session 8a: Melting curves and phenomena
(Compass Room)

13:30 Can we compute high-pressure melting curves without knowledge of the crystalline structure?
Stanimir Bonev, Lawrence Livermore National Laboratory

13:50 Melting at Extreme Conditions: X-ray diffraction Meets Phase-Contrast Imaging
Emma Ehrenreich-Petersen, Deutsches Elektronen-Synchrotron (DESY)

14:10 Grain-size, grain-growth and melting under extreme conditions: A novel approach to melt identification
Tara R McElhinney, University of Manchester

Parallel Session 8b: General Interest Talks
(Studio 1)

13:30 (Invited) Life under extreme conditions
Judith Peters, Univ. Grenoble Alpes

14:00 (Invited) From Snails to Fitting High-Pressure Raman Data
David Dunstan, Queen Mary University of London

14:30 Excursions / Free Time

Friday 5 September

08:30 Registration with Refreshments
(Quays Bar)

09:00 (Compass Room)
Plenary IV: Will hydrogen-based superconductors come out of the DAC?
Ion Errea, University of The Basque Country

10:00 Coffee Break
(Quays Bar)

	Parallel Session 9a: Chemical Bonding **(Compass Room)**		**Session 9b: Theoretical and computational methods** **(Studio 1)**
10:30	Molecular orbital theory for bonding in high-pressure boron and hydrogen clusters **Harry Morgan**, University of Manchester	10:30	(Invited) Elastic constants with anharmonic corrections using quasiparticle theory **Ernesto J Blancas**, University of Oviedo
10:50	(Invited) Pressure-Induced Multicenter Bonding in $CsIO_3$: A New Perspective on Main-group Perovskite Formation Mechanism **Francisco Javier Manjón**, Universitat Politecnica De Valencia	11:00	Formation of new hydro-carbonitrides under pressure: kinetics versus thermodynamics **Andreas Hermann**, The University of Edinburgh
11:20	Machine learned interatomic potential study of NH_3-H_2O-CH_4 mixture under extreme pressures and temperatures **Gracie Chaney**, Sorbonne University	11:20	AIASSE - Ab Initio Augmented Structure Solving Engine: A Hybrid Approach to Atomic and Electronic Structure Characterization of Disordered Materials **Ayobami Daramola**, University of Edinburgh
		11:40	Powder-Diffraction-Based Structural Comparison for Crystal Structure Prediction Under Pressure **Alberto Otero De La Roza**, University Of Oviedo

12:00 Closing Ceremony
(Compass Room)

12:30 Lunch and Depart
(Quays Bar)

Poster Session 1

(Studio 2 and 3)

P1	Dispersion of the KCl refractive index at high pressure **Reece O'Beirne**, University of Salford
P3	High-Pressure Phase Evolution of Bi–Ga Alloys Driven by Polymorphism, Anomalous Melting, and Liquid Miscibility Gap **Shir Ben Shalom**, Ben Gurion University of The Negev
P5	Melting curve of Phosphorus: Evidence for a solid-liquid-liquid triple point **Frédéric Datchi**, IMPMC, Sorbonne Université, CNRS & MNHN
P7	Heat capacity and other thermodynamic properties of hcp-CrH **Mikhail Kuzovnikov**, University of Edinburgh
P9	Investigating the Stability of High Entropy Sulphides at High Pressures: Delineation of Solid-State Phase Transformations **Josh Littleton**, University of Manchester
P11	The pressure response of the K2[Ru(bipy)(CN)4]·3H2O coordination polymer studied by Raman and photoluminescence spectroscopy **Olga Karabinaki**, Faculty of Engineering, Aristotle University of Thessaloniki
P13	Structural- and valence-state changes in EuT$_2$X$_2$ **Jiří Prchal**, Charles University, Faculty of Mathematics and Physics
P15	Clathrate-like CeB$_{12}$ with Superior Hardness **Bole Chen**, Chongqing University of Posts and Telecommunications
P17	Comparing DFT calculated P-V equation of states of high-pressure hydrides to experimental XRD results **Milo Dixon**, University of Edinburgh
P19	Novel Chromium Silicides MoSi$_2$-type CrSi$_2$ and PdGa$_5$-type CrSi$_5$ Synthesized under High-Pressure **Takuya Sasaki**, Department of Materials Physics, Nagoya University
P21	Phase transitions in ferroelectric van der Waals crystals under pressure **Nada Alghofaili**, School of Physics & Astronomy, University of Nottingham
P23	Electrical Resistivity of Liquid Fe-16wt%S-2wt%Si at High Pressures with Implications for Heat Flow in Sub-Earth Exoplanets **Erin Lenhart**, University of Western Ontario

Poster Session 2

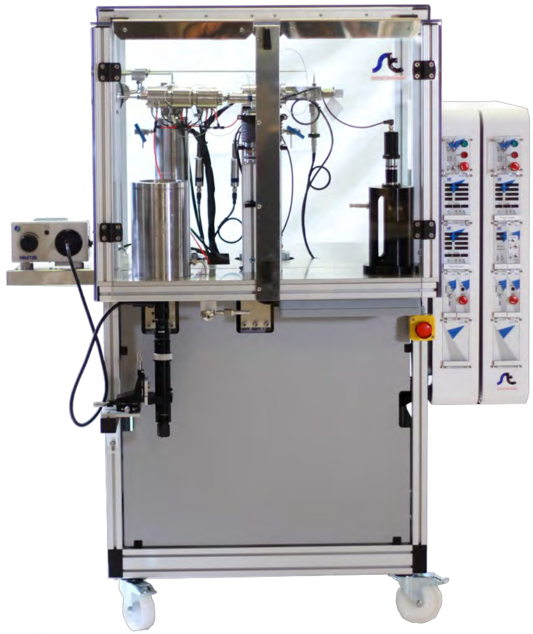
(Studio 2 and 3)

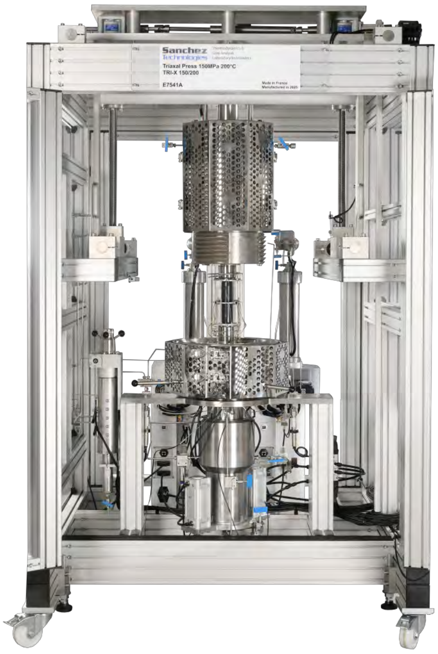
P2	New instrumentation at P02.2, PETRA III, DESY employing Soller slits for structural measurements of non-crystalline materials at extreme conditions **Christoph Otzen**, University of Freiburg, Institute of Earth and Environmental Sciences
P4	Softening of fcc and hcp metals at high homologous temperatures contribute to effective elastic softening in the inner-core **Tara R McElhinney**, University of Manchester
P6	Bonding changes in solid nitrogen under high pressure and temperature **Gordon Scholz**, TU Dortmund / Experimentelle Physik Ia
P8	Phase Transitions of Solid and Liquid Fe-Si Alloys with Applications to Planetary Core Composition and Dynamo Processes **Ben Kalman**, University of Western Ontario
P10	Pressure-Induced Occupancy Changes in Methane Hydrate II: Implications for Planetary Ices **Cerian Robertson**, The University of Edinburgh
P12	Styrkja: a pressure intensifier for miniature HP-HT devices for 4D synchrotron X-ray microtomography **Damien Freitas**, The University of Manchester at Harwell
P14	Li-Battery Cathode Materials: Investigating the High Pressure-Temperature Phase Stability Field of Olivine-Structured $\mathrm{Li(Fe,Ni,Mn)PO_4}$ **Josh Littleton**, University of Manchester
P16	Effect of high-pressure processed apple on human gut microbiota, phenolic metabolites and short chain fatty acids by using a dynamic in vitro colonic fermentation system **Begoña De Ancos**, ICTAN-CSIC
P18	Metadynamics study of kinetic pathways of coesite densification **David Vrba**, Comenius University
P20	High Energy Scattering Capabilities at Beamline I15 **Dominik Daisenberger**, Diamond Light Source
P22	Digital temperature controller for the externally heated diamond anvil cell **Ivan Badger Holmes**, University of Salford
P24	High Pressure Hydrogen capabilities at ISIS Neutron and Muon Facility **Ian Hickman**, ISIS Neutron and Muon Source

P25

Strain Dependent Optical Properties of Core/Shell Nanoplatelets

River Leversee, University of Colorado, Boulder



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HIGH PRESSURE RESEARCH

Plenary Talk I

Multigrain crystallography and its applications for studying deep mantle water cycle

Li Zhang[1]
[1] Center for High Pressure Science & Technology Advanced Research, HPSTAR, Japan

High water contents were observed in basalts of ocean islands and large igneous provinces, suggesting the presence of H2O-rich sources in the lower mantle or even above the core-mantle boundary. Whether water in subducted slabs can be transported to the core-mantle boundary depends on H2O storage capacity in the assemblage of minerals under the pressure-temperature conditions along the subduction path. The H2O effect on the lower mantle mineralogy can further place constraints on the geochemical and geophysical models of the deep lower mantle.

To investigate deep H2O cycle in the lower mantle, we used multigrain diffraction methods to sort out individual grains in a complex multiphase system at megabar pressures [1, 2]. Combining with ex situ chemical analysis, we are able to obtain detailed crystal structure and chemical composition of submicron-sized grains under the lower mantle conditions.

Our new results indicate that H2O-bearing NiAs-type alumina-rich silica (Nt) phase is stable in subducted oceanic crust along normal geotherm conditions to the core-mantle boundary, supporting the existence of H2O-rich reservoirs at the base of the mantle. Although Bridgmanite is nearly dry in coexistence with a hydrous phase [3], the presence of H2O greatly alters the chemistry of bridgmanite. We also found that the presence of H2O stabilizes ferrous iron in bridgmanite at depths greater than 2300 km in the lower mantle [4]. H2O-induced phase transition and phase chemistry change, dehydration melting and the existence of water reservoirs above the core-mantle boundary could play a key role in generation of plumes rooted at the base of the Earth's mantle [5].

[1] L. Zhang, Y. Meng, P. Dera, W. Yang, W.L. Mao, H.-k. Mao, Single-crystal structure determination of (Mg,Fe)SiO3 postperovskite, Proceedings of the National Academy of Sciences, 110 (2013) 6292-6295.
[2] L. Zhang, H. Yuan, Y. Meng, H.-K. Mao, Development of High-Pressure Multigrain X-Ray Diffraction for Exploring the Earth's Interior, Engineering, 5 (2019) 441-447.
[3] T. Ishii, E. Ohtani, A. Shatskiy, Aluminum and hydrogen partitioning between bridgmanite and high-pressure hydrous phases: Implications for water storage in the lower mantle, Earth and Planetary Science Letters, 583 (2022) 117441.
[4] L. Zhang, Y. Chen, Z. Yang, L. Liu, Y. Yang, P. Dalladay-Simpson, J. Wang, H.-k. Mao, Pressure stabilizes ferrous iron in bridgmanite under hydrous deep lower mantle conditions, Nature Communications, 15 (2024) 4333.
[5] S.W. French, B. Romanowicz, Broad plumes rooted at the base of the Earth's mantle beneath major hotspots, Nature, 525 (2015) 95-99.

(Invited) Novel forms of carbon synthesized from fullerene C60 at high pressure

Alexander Soldatov[1]
[1]Yanshan University, Qinhuangdao, China

Since the discovery of fullerene C60 followed by synthesis of other molecular forms of carbon – e.g., nanotubes and graphene - these intrinsically nanostructured systems have been in focus of attention of the scientific community due to rich assortment of outstanding chemical, optical, electrical and mechanical properties these materials exhibit [1]. Intermolecular interaction in these systems is governed by weak van der Waals forces that makes high pressure a suitable tool for tuning their physical properties and creating novel carbon-based nanostructured materials.

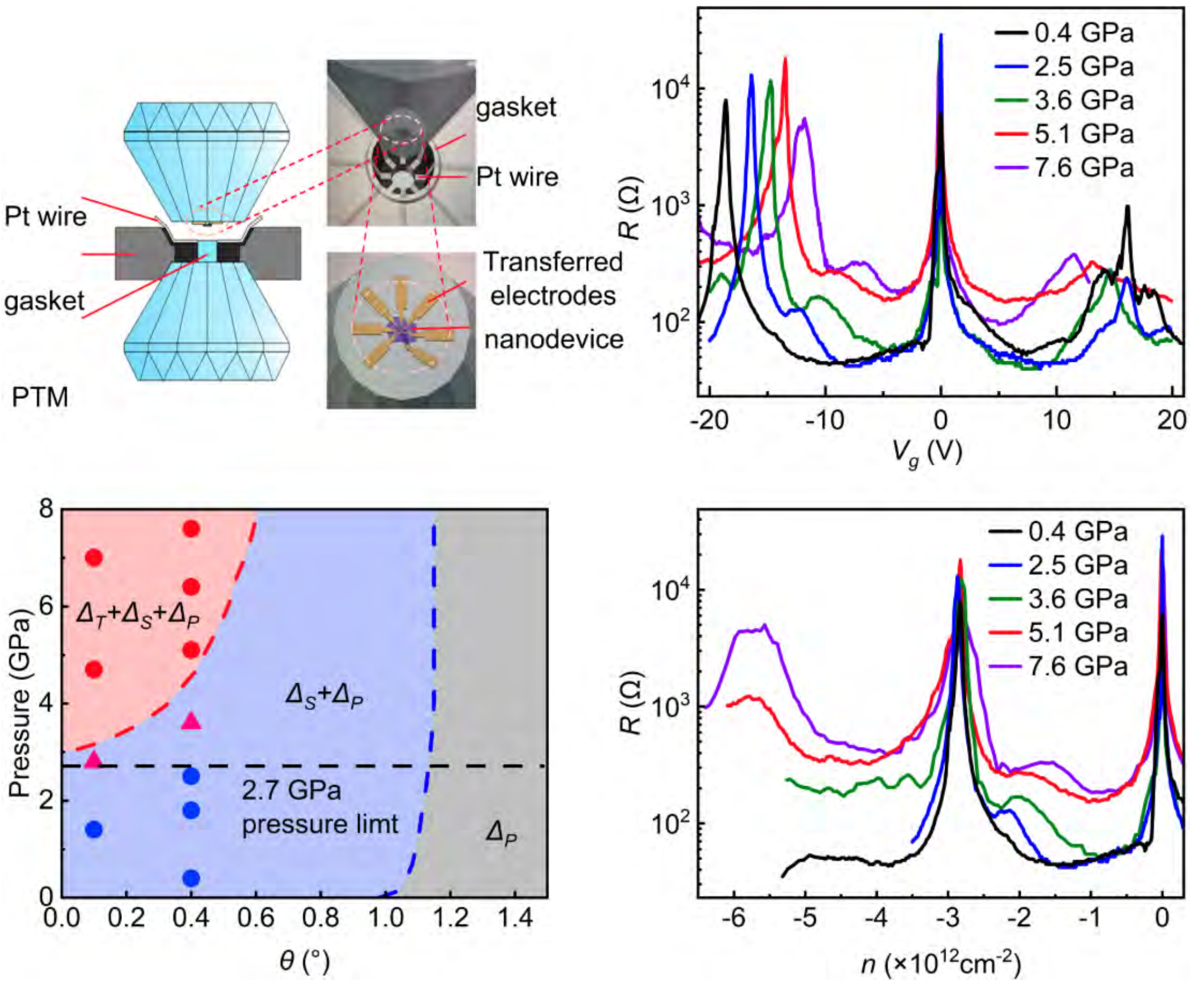
We review our recent results on high pressure synthesis of new forms of nanostructured carbon from C60 fullerene. The materials exhibit a remarkable combination of mechanical and electronic properties (ultra-hardness, superior wear resistance and semiconducting behaviour) [2]. They were characterized by multi-excitation Raman spectroscopy, SEM, High-resolution scanning TEM/EELS. Prospective uses of these novel materials are discussed.

[1] S. Srinivasan, et al. Nature Communications. (2022) 13:3251.
[2] C. Liu, et al. Unpublished.

(Invited) Pressure-Driven Moiré Potential Enhancement and Tertiary Gap Opening in Graphene/h-BN Heterostructure

Yupeng Wang[1], and Zengming Zhang[1]
[1]University of Science and Technology of China, China

Moiré superlattices enable engineering of correlated quantum states through tunable periodic potentials, where twist angle controls periodicity but dynamic potential strength modulation remains challenging. Here, we develop a high-pressure quantum transport technique for van der Waals heterostructures, achieving the ultimate pressure limit (~9 GPa) in encapsulated moiré devices. In aligned graphene/h-BN, we demonstrate that pressure induces a substantial enhancement of the moiré potential strength, evidenced by the suppression of the first valence bandwidth and the near-doubling of the primary bandgap. Moreover, we report the first observation of a tertiary gap emerging above 6.4 GPa, verifying theoretical predictions. Our results establish hydrostatic pressure as a universal parameter to reshape moiré band structures. By enabling quantum transport studies at previously inaccessible pressure regimes, this work expands the accessible parameter space for exploring correlated phases in moiré systems.



A glimpse into the high-pressure behaviour of metal nanoclusters: the case of Au_{25}

Camino Martín-Sánchez[1], Arnulf Rosspeintner[1], Khadijetou Ahmed Ethmane[1], Abolfazl Ziarati[1], Daniele Rosa-Gastaldo[1], Michal Swierczewski[1], and Thomas Bürgi[1]
[1]University of Geneva, Switzerland

Atomically precise monolayer-protected metal nanoclusters (MPCs) are emerging nanomaterials that are currently the focus of interest due to their interesting size-dependent-tunable properties, which give rise to a rich variety of applications in different fields, such as catalysis, bioimaging and optoelectronics. Pressure represents a powerful yet largely overlooked tool to tune and enhance the properties of MPCs, offering new opportunities for their functional exploitation. Former works indicate that high pressure induces important changes in the optical properties of MPCs, both in the absorption and the emission spectra, increasing, for example, MPCs photoluminescence up to two orders of magnitude [1-3]. Although these works open up new ways of research to understand the behavior of these complex systems through high pressure, there is a systematic lack of correlation between the optical properties and the structural changes that MPCs undergo upon compression.

In this work, we present a systematic spectroscopic and structural study on the influence of pressure on the absorption spectrum of $Au_{25}(SR)_{18}$ (SR = thiolate ligand), in correlation with Raman spectroscopy and X-ray diffraction as structural probes. Our results reveal that, within the 0–10 GPa range, $Au_{25}(SR)_{18}$ clusters undergo two pressure-induced structural transitions that primarily affect the ligand shell, while the metallic core remains largely intact. These phase transitions are intrinsic to the cluster structure and occur independently of the ligand type, charge state, or pressurization conditions.

[1] M. Zhang et al. J. Phys. Chem. C, 2013, 117, 639-647.
[2] Q. Li et al. ACS Nano, 2020, 14, 11888-11896.
[3] Q. Li et al. ACS Nano, 2021, 15, 16095-16105.

Strain Dependent Optical Properties of Core/Shell Nanoplatelets

River Leversee[1], Zifei Chen[2], Arun Ashokan[2], Paul Mulvaney[2], and J. Mathias Weber[3]
[1]JILA and the Department of Physics, University of Colorado, USA [2]ARC Centre of Excellence in Exciton Science, School of Chemistry, University of Melbourne, Australia [3]JILA and the Department of Chemistry, University of Colorado, Boulder, USA

Colloidal nanoplatelets are promising materials with tunable narrow emission bands and large photoluminescence quantum yields. In this work we utilize high hydrostatic pressure to investigate the effects of lattice strain on the optical properties of CdSe/CdZnS core/shell nanoplatelets. This work incorporates experimental photoluminescence spectra measured in a diamond anvil cell with hydrostatic pressures up to ~6 GPa, as well as comparison with theoretical models and density functional theory to investigate strain dependent bandgap shifts in colloidal nanoplatelets. This modeling allows for insight into how band structure, confinement, electrostatic effects alter the measured photoluminescence spectra.

(Invited) Pressure dependence of alloy solution phase diagrams: Experiments and thermodynamic modeling

Shir Ben Shalom[1], Moran Emuna[3], Yaron Greenberg[3], Joonho Lee[2], Eyal Yahel[3], and **Guy Makov**[1]
[1]Ben-Gurion University of the Negev, Israel, [2]Korea University, Korea, [3]NRCN, Israel

The experimental determination of phase diagrams necessitates not only structural analyses but also precise and well-equilibrated thermophysical measurements to establish equilibrium thermodynamic conditions. Hence, it took many decades to map the phase space of thousands of binary systems at ambient conditions. Pressure affects phase diagrams both by altering the interactions, which control the nature of the diagram and through stabilizing new elemental and alloy phases. Determining structures under pressure is well-developed. However, measuring thermophysical properties and their transitions under pressure is technically challenging and consequently rarer. Therefore, it is useful to combine experimental measurements with thermodynamic modeling to explore the pressure evolution of alloy systems.

In the present contribution, we study the pressure evolution of several alloy systems through a combination of experimental techniques and thermodynamic modeling. Specifically, we studied several types of alloy systems, including isomorphous Bi-Sb, eutectic Ga-In, monotectic Bi-Ga with a liquid miscibility gap, and the ternary Bi-Sb-Pb system. Through a thermodynamic model, supported by physical measurements of sound velocity and density, we were able to construct phase diagrams up to several GPa of these alloys. To validate our predictions, we undertook high-pressure measurements, including x-ray diffraction in a diamond anvil cell (DAC) and resistivity measurements in a Paris-Edinburgh (PE) large-volume press. These studies validate the predictions of our thermodynamic model of the pressure dependence of the alloy systems, including changes in the nature of the diagram from isomorphous to eutectic, disappearance of the miscibility gap, shifts of eutectic points, and the evolution of interaction parameters with pressure.

The mechanism of the A7 to sc phase transition in arsenic

Matteo Ceppatelli[1,2], Marta Morana[3], Manuel Serrano-Ruiz[1], Kamil Dziubek[4], Enrico Berretti[1], Konstantin Glazyrin[5], Demetrio Scelta[1,2], Roberto Bini[2,6], and Maurizio Peruzzini[1]
[1]ICCOM-CNR - Institute of Chemistry of OrganoMetallic Compounds, National Research Council of Italy, Italy, [2]LENS - European Laboratory for Non-Linear Spectroscopy, Italy, [3]Dipartimento di Scienze della Terra, Università degli Studi di Firenze, Italy, [4]Institut für Mineralogie und Kristallographie, Universität Wien, Austria, [5]DESY - Deutsches Elektronen-Synchrotron, Germany, [6]Dipartimento di Chimica "Ugo Schiff", Università degli Studi di Firenze, Italy

The phase diagram of arsenic is known up to 250 GPa along the room T isotherm, from ambient pressure hexagonal As-I (A7), to simple cubic (sc) As-II, host-guest incommensurately modulated As-III, and bcc As-IV [1]. Nevertheless, the prototype phase transition from the layered A7 structure to the non-layered sc one, underlying inter-layer chemical bond formation and trigonal-pyramidal to octahedral change in As coordination, still remains debated and experimentally elusive.

Two powder X-ray diffraction studies have represented the experimental benchmarks so far, reporting contrasting transition pressures at 25 [2] and 32 GPa [3] with first-order character, while different theoretical studies have calculated transition pressures spreading across 18 GPa [4,5], suggesting higher order.

In this study we used room T single-crystal synchrotron X-ray diffraction to investigate the pressure-induced A7 to sc phase transition in As between 0.3 and 37.7 GPa, using a membrane diamond anvil cell for pressure generation and He as hydrostatic compression medium.

Single-crystal determination allowed the detailed monitoring of lattice parameters, atomic positions and nearest-neighbor distances in rhombohedral setting throughout the investigated pressure range with unprecedented pressure resolution and the identification of a two-step inter-layer bond formation mechanism analogous to that observed in phosphorus [6], finally providing experimental evidence to solve the long-standing debate about the nature of the A7 to sc phase transition in As. Implications concern bond theory, superconductivity in As and the synthesis of innovative As-based layered materials.

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Electrical Resistivity of Liquid Fe-16wt%S-2wt%Si at High Pressures with Implications for Heat Flow in Sub-Earth Exoplanets

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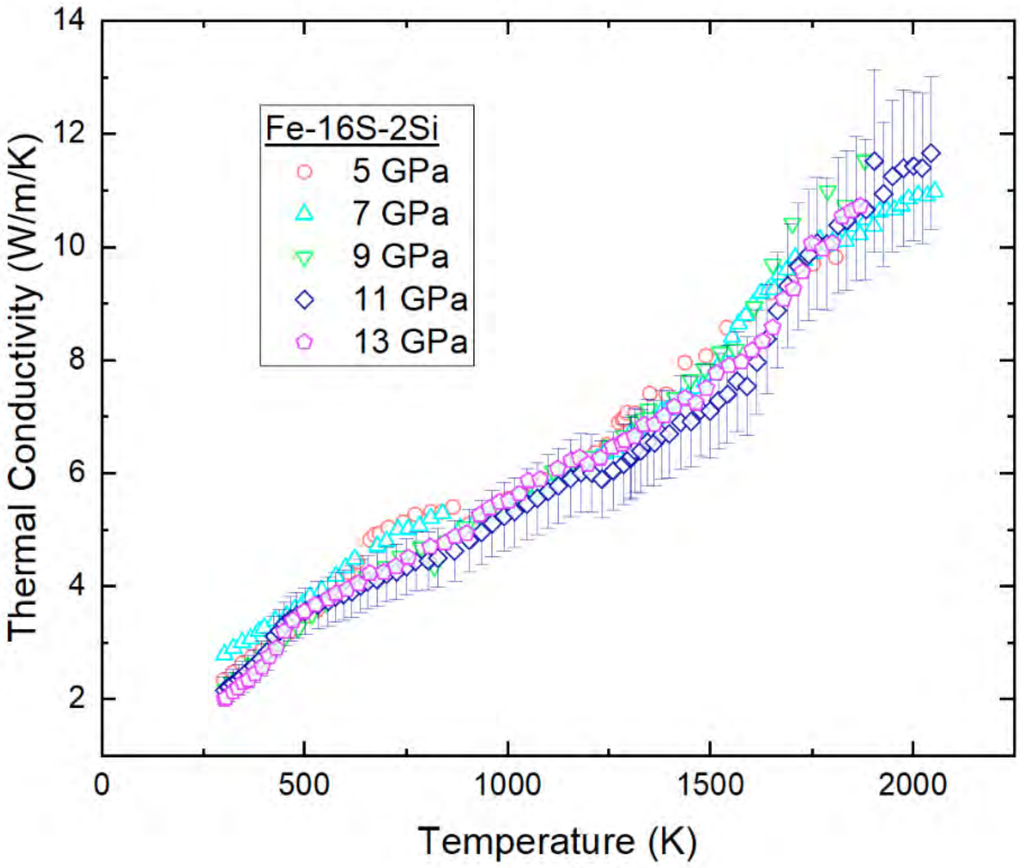
The heat flow contributing to magnetic field generation at the pressures of terrestrial planetary cores may be constrained using high-pressure experiments. To find thermal convective force in the core, thermal evolution models may be combined with adiabatic heat flow estimates, which require thermal conductivity values, which may in turn be obtained from electrical resistivity measurements. Previous electrical resistivity measurements have been performed at pressures up to 5 GPa on liquid Fe-S alloys at the eutectic composition or higher. This study provides novel measurements up to 13 GPa in the moderate 10-20wt% S compositional range of Fe alloys corresponding to the estimated core compositions of Vesta and Mars along with the maximum miscible amount of Si alloyed into the liquid. This allows for characterization of the adiabatic heat flow in the core of sub-Earth exoplanet TRAPPIST-1h, which likely formed near the frost line of its host star.

Experiments were performed in a 3000 ton multi-anvil press on Fe-16wt%S-2wt%Si powder samples. One thermocouple on each end of the sample completed a 4-wire circuit in situ, allowing voltage drop across the sample as a function of temperature to be measured into the melt at 5-13 GPa. Post-experimental recovered samples were polished to a cross-section for geometry measurement and electron microprobe analysis. Electrical resistivity was then calculated, from which thermal conductivity was estimated according to the Wiedemann-Franz Law.

For pressures of 5-13 GPa, electrical resistivity of 400-500 μΩ·cm was found in the complete melt with no discernible dependence on pressure within the error of measurement. Thermal conductivity values of 5-8 W/m/K were calculated for the region of partial melt prior to complete melting at ~1650 K. Thermal conductivity then increases to 11±0.5 W/m/K at the maximum experimental temperature of 2000K. For TRAPPIST-1h, an adiabatic heat flow at the top of the core is estimated.



Thermal equation of state of rhodium characterized by resistively and laser heated diamond anvil cell

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Transition metals, characterized by their partially filled d-band, have attracted significant interest due to pressure-induced phenomena such as topological transitions of the Fermi surface1-2, which can strongly influence their structural, thermal, and transport properties. Rhodium, a 4d transition metal from the platinum group, essential to a wide range of industrial and consumer applications[3] has therefore become the focus of considerable research under extreme pressure-temperature conditions.

Valued for its high melting point, hardness, and corrosion resistance, Rh is widely used in electrical contacts, Pt and Pd alloys, and as a catalyst3-4. Its exceptional robustness also makes it suitable for components in nuclear reactors and high-power laser systems operating under intense thermal loads5. Given its importance understanding of the extreme conditions stability of Rh is crucial.

In this study, we combined synchrotron X-ray diffraction measurements using resistively heated diamond anvil cells and laser-heated diamond anvil cells with DFT calculations to investigate Rh's structural, mechanical, and dynamical stability at high P-T.

Isothermal compression data were fitted using the Rydberg–Vinet equation of state (EoS): V_0 = 55.046(16) Å^3, K_0 = 251(3) GPa, and K'_0 = 5.7(2)6. The thermal EoS was described using the Holland and Powell model, with a thermal expansion coefficient $\alpha_0 = 3.08(5) \times 10^{-5}$ K^{-1}.

The measured equation of state and structural parameters have been compared to the results of simulations. The agreement between ab initio simulations and experiments is generally quite good.

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Keywords: Transition Metals; Extreme Conditions; RH-DAC;LH-DAC

Predicting new high Tc superconductors

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We present a novel high-throughput workflow for the prediction of high-pressure superconductors, combining variable-composition crystal structure prediction with TcESTIME, a newly developed tool for fast estimation of critical temperatures. This approach enables rapid screening of large compositional spaces by evaluating four key electronic structure features: hydrogen content, hydrogen-projected density of states at the Fermi level, electron delocalization (networking value), and molecular character; the latter two being derived from derived from the Electron Localization Function.

Using this method, we performed crystal structure prediction searches on ternary Z-Sr-H systems (Z = Si, S, B, Al, P, Ge, Se, Te, Pb) at 200 and 300 GPa, identifying several promising high-Tc candidates as potential examples of the approach. Notably, we will show some predictions in the range 130–220 K, which have been further validated via Migdal-Eliashberg calculations. Our workflow dramatically reduces computational cost—from thousands of CPU hours to seconds per compound—making it a practical route to explore wide chemical spaces and discover new superconductors. The entire pipeline is now accessible to the community via a dedicated web server.

Probing high-pressure superconductivity with NV centers in diamond

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Pressure is a key parameter for tuning or revealing superconductivity in materials and compounds. Many measurements of superconducting phase transition temperatures have been performed using diamond anvil cells (DACs), which provide a wide pressure range while allowing microscopic structural characterization of the sample. However, the inherently small sample volumes in DACs complicate the unambiguous detection of the Meissner effect, the hallmark of superconductivity. Recently, the Meissner effect in superconductors inside a DAC has been successfully demonstrated using diamond nitrogen-vacancy (N-V) magnetometry, a non-invasive optical technique.

We will describe that under hydrostatic conditions, the sensing efficiency of the NV center remains robust up to megabar pressures [1]. Under this condition, the symmetry of the NV center within the diamond lattice, which determines the quantum eigenstates, is preserved, leading to a response to an applied magnetic field as under ambient pressure.

We will also show that N-V magnetometry can map superconductivity with micrometer resolution. The technique is applied to a microcrystal of the mercury-based cuprate superconductor Hg-1223 under a pressure of 4 GPa [2]. We then detect the magnetic field expulsion and heterogeneities in the sample, visible in a set of characteristic parameters as the local critical temperature Tc. Flux pinning zones are identified by flux trapping maps. This approach could enable detailed studies of the superconductivity of a wide range of materials.

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Superconductivity near room temperature in LaH10 thin-films at megabar pressures

Sam Cross[1], Lawrence Nobbs[1], Will Thomas[1], Xiaojiao Liu[2], Annette Kleppe[2], Oliver Lord[3], Sven Friedemann[1], and Jonathan Buhot[1]
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The discovery of the hydride superconductor H_3S in 2015 with a Tc record of 203 K at 155 GPa ignited the search for high-Tc superconductivity in compressed hydride compounds [1]. Since, several other hydride compounds have been synthesised such as LaH_{10} [2, 3], YH_6 [4, 5] and YH_9 [5], exhibiting superconductivity close to room temperature under megabar pressures. Nevertheless, electrical characterisation of hydrides remains a challenge owing to the extreme pressures required. Our group has developed a novel approach to synthesise hydrides from an elemental thin film evaporated directly onto the diamond anvil, with ammonia borane (NH_3BH_3) as a hydrogen donor [6, 7]. This approach ensures a high hydrogen to metal ratio during synthesis, which is critical to produce superhydrides such as LaH_{10}. Thin film deposition techniques are also used to fabricate strong electrodes, with low electrical resistance, capable to withstand pressures up to 250 GPa. As an illustration, we will demonstrate our recent synthesis of superconducting LaH_{10} thin films at pressures in the range 170-180 GPa with Tc ~ 250 K. The cubic Fm-3m lanthanum sublattice is resolved in synchrotron powder XRD measurements, and superconductivity evidenced in resistance measurements, including the characteristic suppression of Tc in magnetic fields up to 14 T. We demonstrate that thin-film LaH_{10} has structural and electrical properties consistent with those reported for bulk LaH_{10} in previous studies [2,3].

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Session 2b: Superhard and strongly bonded materials

Design of boron based nano-structured super hard material (BP, $B_{12}P_2$)

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Hot sintering combined with the high pressure (HP-SPS) is a technique for sintering powder under moderate uniaxial pressure (max. 10 GPa) and high temperature HT (up to 2500 °C) in PE press. It has been widely used over the last few years as it can achieve full densification of ceramic or metal powders with lower sintering temperature and shorter processing time compared to conventional processes, opening up new possibilities for nanomaterials densification and preservation of the nanoscale grain size to produce bulk nanostructured ceramics, for which grain growth control is one of the main issues.

The yield strength σ varies with grain size according to Hall–Petch equation
σy = σy,0 + k/dx k is a constant, d is the average grain diameter, and σy,0 is the original yield stress.

Here, we present recent results on boron based nano-structured hard material (BP and $B_{12}P_2$). From HP-HT design below 5 GPa (1700°C) to physical properties, we obtained sintered and dense compact polycrystalline sample. High Vickers hardness (up to 48 GPa) and semiconducting (2 eV band gap) optical properties open possible use to replace WC tungsten carbide materials in industries. However, new frontiers of opportunities are now emerging by coupling SPS with large volume (i.e., at least for samples greater than several cubic millimeters, DIA module) high-pressure technology (up to ~10 GPa), allowing the full densification of hard-to-sinter materials.

Funding: This project has received financial support from the CNRS through the ANR Capbap Contract n° 20-ASTR-0020-02 and the MITI interdisciplinary programs through its exploratory research program.

Towards predicting tough multi-functional materials recoverable from high-pressure synthesis: Symmetry and vectorisation as an efficient tool for configuration space navigation

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One of the prime challenges for today’s scientific community is the discovery of sustainable materials with advanced, technologically relevant properties, allowing the optimization of energy production, transport, and usage. A broad range of materials with the desired functionalities can be synthesized under high-pressure high-temperature conditions, but their exceptional properties or even phase stability often vanish under decompression to ambient conditions. These materials show new chemistry,[1,2] superconducting behavior,[2,5] high hardness,[2,3,4] high energy densities,[2,3,4] wide (direct) band gaps,[2,4] piezo-electricity,[3] and even combined multi-functionalities.[2,3,4]

Strongly bonded materials, however, can remarkably be trapped in meta-stable states and recovered to ambient conditions.[2,3,4] Recently recovered materials feature furthermore ultra-incompressible CN4 tetrahedra,[4,5] ideal building blocks for the search for hard or even tough materials with additional functionalities.

Unfortunately, the synthesized compounds are often surprisingly complex. Unexpected chemistry with large numbers of atoms per unit cell, strongly non-cubic lattice vectors and strong meta-stability at ambient conditions, make these compounds often complex to predict using standard structure search computations.[1,2,3,4]

I will present our novel fully vectorised computational approach for the precise and comprehensive exploration of the high-dimensional structure-composition-space of materials containing incompressible covalent building blocks, e.g., CN4 tetrahedra, with the goal of discovering tough, recoverable materials that exhibit multiple advanced properties.

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High-pressure behavior of binary nitrogen-halogen systems

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High-pressure chemistry of binary nitrogen compounds has been extensively investigated over the past decade. Initial studies focused on the combination of nitrogen with elements of significantly lower electronegativity, including alkalis, alkaline earths, and transition metals, resulting in the formation of anionic polynitrogen species. More recently, the focus has shifted to elements closer in electronegativity to nitrogen, such as those in the first few columns of groups XIII, XIV, XV, and XVI of the periodic table. These elements are more likely to form heteroatomic covalent bonds with nitrogen, giving rise to compounds with markedly different crystal chemistry.

As it stands, one group of elements has been left untouched in the high-pressure investigation of binary nitrogen solids: halogens. This group of elements can be split into two with iodine and bromine having electronegativities similar to that of nitrogen, while chlorine and fluorine are more electronegative. The former are thus expected to form covalent bonds with nitrogen, while the latter are anticipated to result in the formation of cationic polynitrogen species.

This talk will show our experimental study of the binary nitrogen-halogen systems (Cl-N, Br-N, and I-N) at pressures up to 120 GPa using a laser-heated diamond anvil cell. Sample characterization was achieved using synchrotron single-crystal X-ray diffraction of the polycrystalline samples. Results include the formation of novel binary compounds as well as new allotropes of the halogens.

Plenary Talk

Diamond anvil cell research at the European XFEL

Rachel J. Husband[1]
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In recent years, the development of innovative techniques utilizing the unique properties of X-ray Free Electron Lasers (XFELs) has opened up new opportunities to explore extreme conditions science using diamond anvil cells (DACs). In particular, time-resolved measurements exploiting the unique bunch structure of the European XFEL, in which bursts of ultra-short, hard X-ray pulses are delivered at MHz repetition rates, have enabled the investigation of material response to dynamic heating, cooling, and compression on timescales up to hundreds of microseconds with an unparalleled temporal resolution. Further leveraging the unique properties of the XFEL source, the high peak brilliance of individual X-ray pulses has been exploited to directly heat samples via rapid energy deposition on sub-picosecond timescales, while subsequent pulses probe the structural response in a pump-probe fashion.

Such experiments are routinely performed at the High Energy Density (HED) instrument at a dedicated DAC platform comprising MHz X-ray diffraction, streaked optical pyrometry, and X-ray phase contrast imaging probes for the study of material behavior at high temperatures induced by X-ray or IR laser heating, or during rapid compression at intermediate strain rates using dynamic DAC drivers. Following the first community assisted commissioning experiment in 2019, the DAC platform has been used in over 20 experiments performed by a diverse set of international user groups.

In this talk, I will present an overview of the DAC platform at HED, focusing on its state-of-the-art capabilities. In addition, I will highlight recent scientific results from a range of user groups who have taken advantage of the time-resolved capabilities to address an expansive set of scientific goals including the mapping of phase diagrams of weakly scattering materials, investigating chemical reaction and phase transition kinetics, and determining physical properties such as thermal conductivity at extreme conditions.

(Invited) How to Predict the Refractive Index of a Silicate Glass at High Pressure Based on The Chemical Composition?

Xiangdong Li[1], Konstantin Solovev[1], Björn Winkler[2], Sergio Speziale[1], and Sergey Lobanov[1]
[1]GFZ Helmholtz Centre for Geosciences, Telegrafenberg, Germany, [2]Institute of Geosciences, Goethe University Frankfurt, Germany

The physical properties of silicate melts under high-pressures are of primary importance for understanding deep Earth structure and evolution. Silicate glasses are often used as convenient, but not necessarily appropriate, analogues of silicate melts in high-pressures experiments in order to assess the physical properties and structure of melts in the Earth's mantle. We will report on direct measurements of the optical refractive indices (nsam) of seven silicate glasses, Mg2SiO4 (Fo), MgSiO3 (En), CaSiO3 (Wo), CaMgSi2O6 (Di), CaAlSi2O8 (An), NaAlSi3O8 (Ab) and Ab25An25Di50, up to 140 GPa. The evolution of the normalized refractive index (nsam/n0, where n0 is the refractive index of a given glass at 1 atm) with pressure shows a clear dependence on the chemical composition of the glass. Specifically, the relative increase of the index with pressure is greater for glasses with higher SiO2 and/or Al2O3 contents. More generally, the free space in the structure of a given glass at 1 atm, which can be estimated from its chemical composition, determines the refractive index of that glass at high pressure. Accordingly, we propose a universal model for predicting the refractive index of silicate glasses at high pressure from their chemical composition. We will also provide a structural interpretation of the observed changes in the refractive indices of the seven glasses studied in this work, based on the measurements of Raman spectra and DFT computations.

(Invited) Optical photothermal infrared spectroscopy of h-BN in diamond anvil cell

Francesco Capitani[1], Beatrice D'Alo[1,2], Paolo Postorino[2], Gergely Nemeth[1], and Ferenc Borondics[1]
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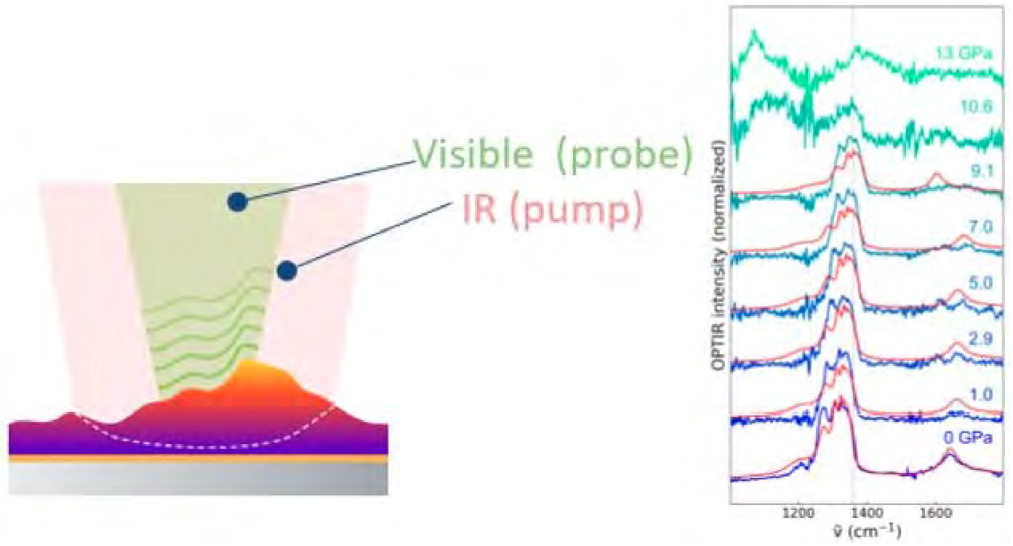
Fourier-transform infrared (FTIR) spectroscopy is a widespread experimental technique present in many scientific laboratories. Coupled to an IR microscope, it allows performing hyperspectral measurements of a plethora of samples at ambient and extreme thermodynamic conditions providing spatially resolved physical and chemical information. In the last 35 years, synchrotron IR radiation has enabled diffraction limited FTIR micro-spectroscopy, even in diamond anvil cells (DACs) in the multi-megabar regime [1]. However, the diffraction limit at long IR wavelengths (10-100 μm) limits focusing light to a micrometric spot size [2].

To overcome this limitation, the coupling of IR radiation with an atomic force microscope (AFM) has allowed unprecedented spatial resolution down to tens of nanometers [2]. However, these techniques require physical contact between the AFM tip and the sample's surface, clearly incompatible with DACs.

Optical Photothermal IR (O-PTIR) spectroscopy, an emerging technique, can achieve a sub-micrometer resolution by using two radiation sources: a pulsed IR laser, acting as a pump, and a continuous-wave probe laser in the visible range (Fig.1, left panel) [3]. As O-PTIR is a fully optical technique and does not require contact with the sample, it becomes an excellent candidate to achieve high spatial resolution at IR wavelengths inside a DAC at very high pressures.

Here we explore the potential of O-PTIR for high-pressure studies, by investigating the hexagonal to wurtzite phase transition in h-BN at high-pressure [4], as a proof-of-concept. We show that we can successfully measure O-PTIR spectra of h-BN up to 10 GPa, where an abrupt spectral change signals the phase transition to wurtzite as expected, as shown on the right panel of Fig.1. By raster scanning the sample at a single IR wavelength we achieved sub-diffraction limit IR imaging. Finally, we discuss the current limitations and the perspectives to obtain higher signal-to-noise ratio and spatial resolution.



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All-optical PVT EOS measurements in the diamond anvil cell

Reece O'Beirne[2], John Proctor[2], Ivan Holmes[1], and Matthew Errington[1]
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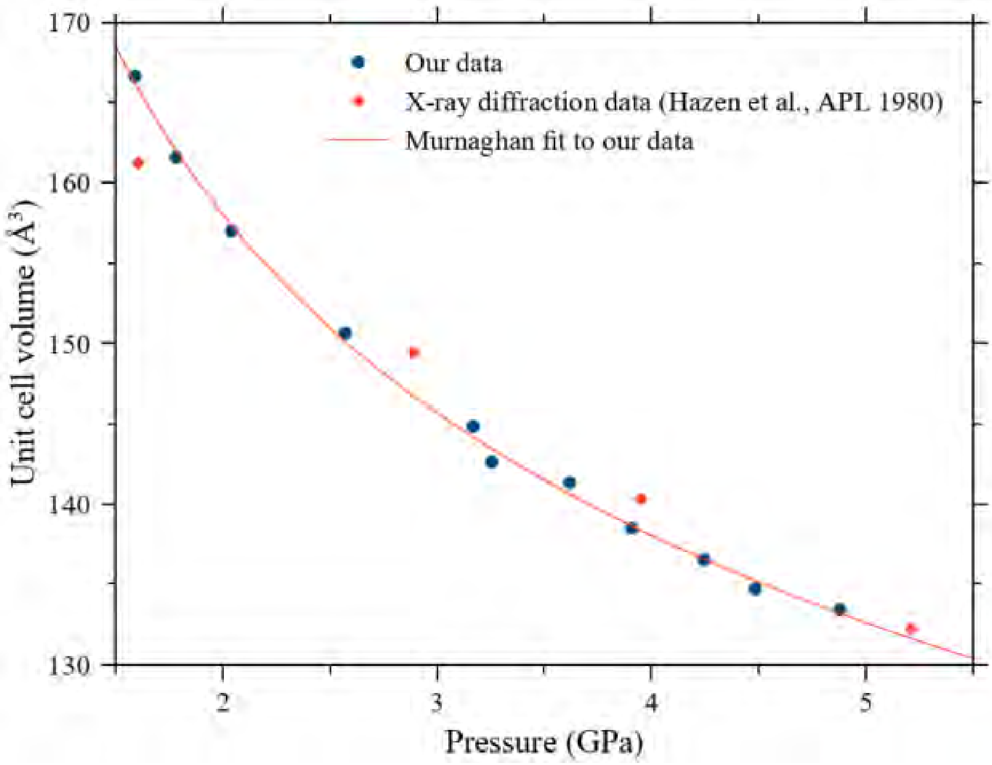
We recently presented a novel all-optical method for the determination of the PVT EOS of transparent fluids and solids in the DAC[1]. The key applications of this work are the determination of the PVT EOS of fluids at GPa pressures over a wide temperature range, and of solids which do not easily form a single crystal or powder to enable PVT EOS determination using X-ray or neutron diffraction (for instance, CH4).

Here, we present improvements to our methodology to reduce the error in our volume measurements from ± 2.7% to ± 1%, and several PV and PVT EOS, which we have recently determined. In particular, we recently measured the PVT EOS of CH4 phase 1 at 295 K. To our knowledge, the only existing measurements in the literature are four single-crystal X-ray diffraction datapoints[2]. In our recent experiment (shown below), we obtained 11 datapoints, allowing an EOS to be fitted with well-constrained fit parameters for the first time.



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High pressure reflectance characterization of YAB from mid infrared to the visible

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Yttrium aluminum borate, YAB, is an oxide with remarkable mechanical, thermal and nonlinear optical properties which has been used as a host in visible and UV lasers [1-2], and proposed as a phosphor.[3] It is a weak birefringent material with the fundamental absorption edge situated near 170 nm.[4] We have performed high pressure optical measurements from the midinfrared to the visible part of the spectrum in order to characterize the pressure evolution of the ordinary and extraordinary refractive indexes as well as the more energetic phonon modes.

Plano-parallel c- and a-cut YAB single crystals of several thicknesses were used. The crystals were loaded in a DAC with Ne as pressure transmitting medium and a ruby chip as a pressure sensor. One of the sample surfaces was gold coated. The other surface was in contact with the diamond. In this way we enhanced the reflectance signal and avoided interferences from the pressure chamber. Visible and NIR spectra were acquired in a home-made optical bench. MIR spectra were obtained by using a Bruker IFS125HR spectrometer, adapted to work with a DAC.

Outstandingly, the relative change in the refractive indexes (at 16000 cm-1) from 0 to 10 GPa is found to be only 0.3%, one order of magnitude smaller than the volume reduction in the same pressure interval, as determined by XRD. Infrared reflectance spectra display features from 600 to 1500 cm-1 corresponding to phonon modes which have been classified by symmetry. The spectra could be modelled and the phonon pressure coefficients obtained.

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Measurement of the refractive index of samples in the diamond anvil cell using white light transmission microscopy only

John Proctor[1], and Reece O'Beirne[1]
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We recently demonstrated the measurement of the PVT EOS of disordered materials in the DAC using the combination of optical microscopy, white light transmission spectroscopy and confocal laser microscopy [1]. The most challenging part of this measurement is the need to determine the refractive index of the thin film of material that comprises the sample in the DAC. In ref. [1] we achieved this by combining white light transmission spectroscopy with confocal laser microscopy. In this procedure the confocal laser microscopy measurement is the largest source of error. It is also the most time-consuming measurement, and vastly reduces the data density that can be achieved in an experiment to measure a PVT EOS.

However, in another scientific field (growth of thin films by chemical vapour deposition) a different approach has been taken [2], which allows the refractive index and film thickness to be determined using white light microscopy alone (the “Swanepoel method”). Here, we adapt the Swanepoel method to measure the refractive index and thickness of samples in the DAC using white light microscopy only. We demonstrate that measurement of these properties within an error of ± 1% is feasible. To achieve this, it was necessary to obtain the absolute value of the proportion of incident light transmitted through the DAC. This allows an analysis using the Fresnel equations and established theory of transmission of light through thin films [3] from which the sample thickness and refractive index can be separately obtained. We will present this analysis, and the design of the optical spectroscopy apparatus that makes such measurements possible.

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Session 3b: Geoscience and planetary science

(Invited) Insights into the fate of volatile species during the planetary life cycle from dynamic compression experiments

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Refractory elements like Si, Mg and Ca have similar abundances in the bulk silicate Earth relative to chondrites. However, for many elements with lower condensation temperatures – and thus higher volatility – estimates of the chemical abundances in the Earth are orders of magnitude lower than those found in chondrites. What happened to these elements during the evolution of the Earth? One hypothesis is that volatile elements were lost to space during the violent, high-energy processes of planetary accretion, formation and differentiation. There is evidence that there may be hidden reservoirs deep in the Earth's interior for some of these apparently depleted chemical species. For example, this has been know of He-3 for decades. More recently, there is significant evidence for primordial water retained in the deep Earth.

To understand how primordial volatile atomic species may be retained at the extreme pressures and temperatures of planetary interiors we have performed shock-ramp compression and shock-release using the Z Machine at Sandia National Laboratories. Shock-ramp experiments melt the sample with an initial shock at 100-130 GPa, and then isentropically compress the molten silicate to 200+ GPa. Shock-release experiments measure the acoustic velocity of molten silicates up to 200 GPa. With complementary insights from molecular dynamic simulations, these experimental data determine the compressibility of silicate melts containing water and other volatile species at a range of pressure and temperature conditions aiding our understanding of the atomic mechanisms that control chemical cycling of volatile species throughout the planetary lifecycle.

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Twin domain switching in neighborite (NaMgF3) during oscillating deformation: potential implications for intrinsic seismic attenuation of the lower mantle

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Bridgmanite is the most abundant mineral of the lower mantle, and due to its orthorhombic perovskite crystal structure is prone to twinning under deviatoric stress. Twinning as a deformation mechanism has a number of potential effects within the Earth's lower mantle. For example, twin domain switching is an anelastic attenuation mechanism. It may explain enhanced seismic wave attenuation under eastern Eurasia, where lower mantle quality factors

(Q) for P- and S-waves are on the order of 3000 and 1300, respectively, much higher than the global average given by PREM (~800 and 300, respectively).

It is therefore essential to understand twin domains in bridgmanite, to gain physical insights into the dynamic processes in the lower mantle. However, since bridgmanite is stable under pressures well above 22 GPa, detailed investigation on this mineral in a large volume press is currently very difficult. Here we report a preliminary study on intrinsic attenuation of an isostructural analogue to bridgmanite – neighborite (NaMgF3) – at ESRF beamling ID06 through oscillation experiments. Using the rotating custom-built 2D Pilatus 900k-W CdTe long-aspect ratio detector, at the sample-detector distance of ca. 4 m, we could completely resolve the characteristic triplet (200, 112, and 020) of NaMgF3 as well as other normally-overlapping pairs of peaks. Radiographic imaging and ultrasonic techniques were used simultaneously to resolve small strain. As the first feasibility study, we show that intensities of the 200 and 020 lines exhibit reversable switching as a result of flipping twin domains at an oscillating strain amplitude of ~ 10-4 s-1, with oscillation periods of 1200 – 3600 s.

Thermal conductivities of solid and molten silicates: Implications for dynamos in mercury-like proto-planets

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Remanent magnetization and active magnetic fields have been detected for several telluric planetary bodies in the solar system (Earth, Mercury, Moon, Mars) suggesting the presence of core dynamos active at the early stages of the planet formation and variable lifetimes. Among the factors controlling the possibility of core dynamos generation, the dynamics of the surrounding silicate mantle and its associated thermal properties are crucial. The mantle governs the heat evacuation from the core and therefore the likeliness of an early thermally driven dynamo. In the case of planets with a thick mantle (associated with supercritical Rayleigh numbers), the core heat is efficiently removed by mantle convection and early thermally-driven dynamos are likely. At the opposite, planets with a thin mantle (associated with subcritical Rayleigh numbers) might evacuate their inner heat by diffusion only, making early thermally-driven dynamos difficult. Within the Solar System, Mercury is a potential example of such a regime. Its small mantle thickness over the planet radius ratio might be inherent to its small orbital semi-axis and hence, might be ubiquitous among the terrestrial objects formed close to their star. To constrain the likeliness of a thermally driven dynamo on “Mercury-like” planets (i.e. with large Rc/R), we present new thermal diffusivity measurements of various solid, glassy and molten samples. We applied the Angstrom method on cylindrical samples during multi-anvil apparatus experiments at pressures of 2 GPa and temperatures up to 1700 K. Thermal diffusivities and conductivities were estimated for solid and partially molten peridotites, with various melt fractions, and for basaltic and rhyolitic glasses and melts. Our study demonstrates that melts have similar thermal properties despite a broad range of composition investigated. The melts reveal much lower thermal conductivities than the solids with almost an order of

magnitude of decrease: 1.70 (±0.19) to 2.29 (±0.26) W/m/K against 0.18 (±0.01) to 0.41 (±0.03) W/m/K for peridotites at high temperatures and various melts respectively. Partially molten samples lie in between and several predictive laws are proposed as a function of the melt fraction and solid/melt texture. Using our results into forward calculations of heat fluxes for dynamo generation for Mercury-like planets, we quantify the effect of mantle melting on the occurrence of thermally driven dynamos. The presence of a mushy mantle and partial melting could significantly reduce the ability of the mantle to evacuate the heat from the core and can prevent, shut or affect the presence of a planetary magnetic field. The buoyancy and fate of molten material in such bodies can thus influence the magnetic history of the planet. Future observations of Mercury-like planets accreted near their star and the detections of their magnetic signatures could provide constraints on their inner state and partial melting histories.

Structural changes in $CaSiO_3$ glass up to lower mantle pressures

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The physical properties of silicate melts at temperature and pressure conditions of the Earth's mantle have a fundamental influence on the chemical and thermal evolution of the Earth. However, direct investigations of melt structures at these conditions are experimentally very difficult or even impossible with current capabilities. In order to still be able to obtain an estimate of the structural behavior of melts at high pressures and temperatures, amorphous materials have been widely used as analogue materials.

Here we present the structural response of CaSiO3 glass as a proxy for deep-mantle melts up to 108 GPa via total X-ray scattering experiments. The measurements were carried out at beamline P02.2 at DESY, Germany, utilizing the newly commissioned Soller Slit configuration. Due to the pronounced size contrast between Ca2+ and Si4+, the Si–O correlations are readily resolved in the pair-distribution function—something that is impossible in other three component silicate glasses, like $MgSiO_3$ where the Mg–O and Si–O peaks overlap at a larger pressures.

We observe smooth pressure-induced changes in the structure factor and pair distribution function, along with a clear increase in Si–O coordination from four-fold to six-fold within the first 50 GPa. This behavior will be examined in detail, with emphasis on mechanistic differences relative to pure SiO_2 and in comparison with other reported results for silicate glasses under similar pressure conditions.

(Invited) High-pressure behavior Fe-O-H system in the deep Earth's interior

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The high-pressure behavior of hydrous minerals under extreme high-pressure and high-temperature conditions has garnered increasing attention in recent years. Water significantly influences the chemical and physical properties of mantle minerals, affecting melting temperatures, sound velocities, and material viscosity. Water is continuously delivered to the Earth's interior through hydrous phases in subducting slabs, where it participates in numerous chemical reactions with mantle constituents.

Iron oxyhydroxide ε-FeOOH (Py-phase) and the recently discovered pyrite-FeO2Hx ($x \leq 1$) are considered potential candidates for transporting water and hydrogen to the lowermost mantle [1,2]. The formation of pyrite-FeO2Hx at the core-mantle boundary, possibly resulting from reactions between water released from subducting slabs and the iron core, has been proposed as a potential origin for ultralow-velocity zones and seismic anomalies at the core-mantle boundary [3].

In this study, we applied methods of single-crystal X-ray diffraction in laser-heating diamond anvil cells (DACs) to investigate high-pressure behaviour, chemical reactivity and thermal stability of compounds belonging to Fe-O-H system. Recent advancements in multi-grain single-crystal XRD enable the detection of phases in minor quantities and the reliable determination of their crystal structures. We discuss the chemical processes that occur between iron oxides/oxyhydroxides and aqueous fluids under conditions corresponding to the deep interiors of the Earth.

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(Invited) Pyramidal inversion in $Ba(IO_3)_2 \cdot H_2O$

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Pyramidal inversion is a stereochemical phenomenon describing the interconversion between two equivalent pyramidal configurations of the same chemical species. Using IO_3^- as a model trigonal pyramidal unit, we report the observation of this inversion in the solid state under hydrostatic pressure, in single crystals of barium di-iodate monohydrate, $Ba(IO_3)_2 \cdot H_2O$, without any accompanying chemical reaction or guest molecule exchange. The inversion is revealed by high-pressure single-crystal synchrotron X-ray diffraction, through the emergence of charge density on the previously unoccupied side of the IO_3 pyramid at pressures above 5 GPa. The proportion of inverted pyramids increases with pressure, from 2.5% at 5 GPa to 17.5% at 15 GPa. Density functional theory calculations show that the original and inverted configurations are nearly degenerate in energy, supporting the pressure-induced interconversion. Possible factors enabling this phenomenon in barium iodate monohydrate are examined, with hydrogen bonding involving water molecules suggested to play a significant role.

SiV centers of diamond as quantum sensors under pressure

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Understanding the fundamental properties of matter under extreme conditions is essential in various fields of physics, from planetary science to quantum behavior of electrons in high-density solids. Among these topics, hydrogen and its compounds have raised particular theoretical interest. In 1935, Wigner and Huntington predicted the existence of metallic hydrogen—a phase [1] that would exhibit superconductivity at room temperature. It took nearly a century to confirm part of this prediction experimentally. In 2020, a team led by Paul Loubeyre at CEA observed the transition from insulating molecular hydrogen to metallic hydrogen at a pressure of approximately 425 GPa (4.25 Mbar) using a diamond anvil cell (DAC) at 80 K at Synchrotron SOLEIL [2]. Achieving such extreme pressures poses significant challenges, and probing the fundamental properties of matter under these conditions requires innovative techniques. Our team has developed methods leveraging defects in diamond to explore these extreme environments [3].

Specifically, we have utilized nitrogen-vacancy (NV) centers to probe the superconducting transition of mercury-doped cuprates [4]. We are now focusing on group-4 vacancies (G4V) in diamond [5]. In this poster, I will discuss the new experimental platform we developed for G4V magnetic field sensing at extreme conditions. Specifically, I will present the high-resolution spectroscopic measurement at liquid helium temperature of the fine structure of SiV centers that we plan to study under pressure using a DAC.

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Effect of uniaxial pressure on transport properties of MnTe

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Semiconductor properties can be tuned by strain, as it is known with conduction band valleys which are degenerate in bulk silicon. The degeneracy is lifted in thin layers, where lattice mismatch with substrate induces biaxial strain. A rather unusual situation occurs in MnTe where, in bulk, two groups of valence band maxima occur at similar energies (i.e. unlike in silicon, this is no degeneracy guaranteed by crystal symmetry but rather an "approximate accidental degeneracy" occurs): one of the groups is close to the A-point and another to the Gamma point (GPG) of the Brillouin zone [1].

Based on accurate ab initio calculations (using QSGW [2]), it has been predicted that by slight changes of lattice constants, the group close to A can be pushed down in energy so that GPG prevails. We report transport measurements on bulk MnTe subject to uniaxial pressure with the aim of confirming the prediction. Four regimes of temperature-dependent resistivity are observed [3] and in the second lowest (approximately 10 to 50 K), we find that the activation energy (Ea) strongly depends on applied pressure. We interpret this in terms of Ea (which is identified as the acceptor level) being different for GPG than what is known for ambient pressure where the valence band maxima close to the A-point are believed to prevail. Magnetotransport and role of magnetic order in MnTe will also be discussed along with alternative scenarios.

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Neutrons don't lie: The case of ReO_3 under pressure

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ReO3 is a well-known 5d-oxide with cation-deficient perovskite structure. It has been studied under pressure by x-rays and neutron diffraction [1-8], but the conclusions are highly confusing: Whereas neutron diffraction report consistently a transition from the ambient-pressure Pm3m phase to an Im3 phase at ~0.5 GPa [1,2,3] which might be stable to 8 GPa [4], x-ray data claim a transition to a monoclinic C2/c structure at ~ 3 GPa and to a R3c phase at 10 GPa [5]. Other x-ray studies [4] do not find evidence of a C2/c phase but instead a direct transition from the cubic Im3 to R3c [6,7] at 6-9 GPa, or even a phase mixture of Im3, C2/c and R3c structures [8], depending on the pressure transmitting fluid.

Here we present a comprehensive neutron and x-ray powder diffraction study of ReO3 under hydrostatic pressure which solves this long-standing enigma [9]. We show that the only stable phase between 1 and 15 GPa is the one with Im3 symmetry, thus confirming earlier non-hydrostatic neutron data [4] obtained at ISIS and extending them to higher pressures. We show that the observation of other structures is due to an alteration of the sample by high-intensity synchrotron radiation and that these effects disappear when the x-ray flux is sufficiently reduced. The structural pressure dependence will be reported which demonstrate a densification of ReO3 by a void-filling mechanism.

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Full energy structure of the Cr^{3+} activator in $Cs_2(Ag,Na)InCl_6$ double halide perovskite hosts under pressure

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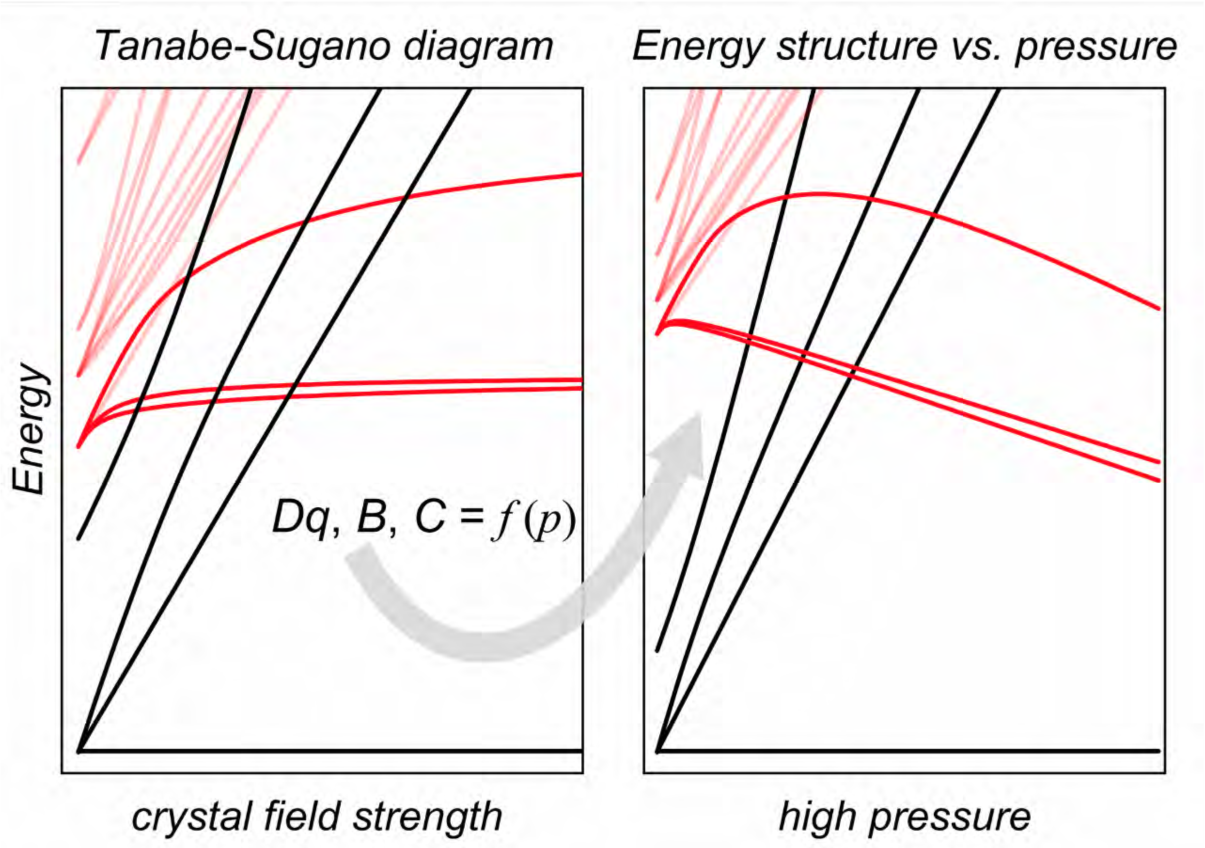
Pressure is one of the means by which one can alter the spectroscopic properties of optical materials activated with transition metal (TM) ions. The energies of electronic transitions of a d^n TM ion is described by an appropriate Tanabe-Sugano (TS) diagram, and the effect of pressure can be intuitively understood as increasing the interaction strength with coordinating ions (crystal filed strength, Dq), i.e. moving right on the TS diagram. In reality, the effect of pressure cannot be reduced just to increasing crystal field strength since pressure also affects the mutual electrostatic iteraction of the d^n electrons in the TM ion. This is described by Racah parameters B and C, which can be obtained experimentally based on a few optical transition measurements.

In this work I report the effect of pressure on radiative transitions in double halide perovskites $Cs_2(Ag,Na)InCl_6$ activated with Cr^{3+} (d^3), by means of high pressure photoluminescence (PL) and photoluminescence excitation (PLE) spectroscopy. In these materials, a spectacular change between broadband to narrow line emission in the PL spectrum occurs at elevated pressure, resulting from crossover between the $^4T_2$ and ^2E states in the TS diagram. Similar effect was observed by for the first time by Dolan et al. in an analogous fluoride material [1].

In this research I am going one step further – utilizing high pressure PLE spectroscopy, I gain access some of the higher excited states of the system. This allows me to determine all three parameters: crystal field strength Dq, Racah parameters B and C, relevant to the energetic structure of the system. Finally, on the basis of pressure dependence of the parameters, the pressure evolution of all energy levels of the Cr^{3+} dopant is determined, following the approach described in my previous publication [2]. In effect an energy diagram of all the crystal field levels of Cr^{3+} dopant in halide perovskite matrix is constructed, which can be understood as the true TS diagram of the system, where abstract parameter Dq is replaced by pressure.



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(Invited) X-ray Raman scattering spectroscopy elucidates the microscopic structure of water at high pressure

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Water exhibits numerous thermodynamic and structural anomalies that are not yet fully understood. Hence, the precise microscopic structure of water has been a subject of intense debate. Our collaborative teams have contributed to the understanding of this enigmatic liquid with a focus on the X-ray Raman scattering (XRS) spectra of the oxygen K absorption edge with corresponding molecular and spectral simulations.

XRS is a particularly useful tool for obtaining near-edge spectra of light elements under extreme conditions. In XRS, a hard X-ray photon scatters inelastically from the electrons in the sample. The spectra of the scattered photons provide information analogous to soft X-ray absorption and can access core-level X-ray spectra sensitive to the local atomic environment of the atom. XRS is bulk-sensitive and readily allows for studies in complex sample environments, e.g., a diamond anvil cell.

We have examined the oxygen K-edge XRS spectra of compressed water at temperatures from ambient [1] to supercritical [2] conditions, as well as ice phases Ih, VI, and VII [3]. The results illuminate the mechanism of compressibility of liquid water at ambient temperature, by interstitial water molecules squeezing into an otherwise persistent fluctuating tetrahedral hydrogen-bonded network [1]. Distortions of the hydrogen-bond network increase dramatically toward the supercritical regime [2]. Ab-initio computational molecular dynamics and spectral simulations align closely with the experiments, allowing for quantitative conclusions. I will highlight XRS's capabilities and showcase our studies on the microscopic structure of water.

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Dynamic diamond anvil cell for time-resolved study: Application on Water

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Dynamically compressed and statically compressed matter can exhibit different behaviours. Such differences may be related to mechanisms of phase transitions, nucleation kinetics [1], or competition between metastable states [2]. We have developed a dynamical Diamond Anvil Cell to probe compression rates ranging from those obtained by quasi-static second timescale to dynamic nanosecond timescale pressure ramps. Three time-resolved measurements have been developed: angular dispersive X-ray diffraction on the ID09 beamline; optical imaging using a Phantom camera; and fluorescence and Raman spectroscopy.

Initial work on the dynamic compression of water has been focused on solidification of the metastable overcompressed fluid [3]. Recently, we performed a systematic study of dynamically decompressed ice VII. The d-DAC enables a controlled isothermal decompression ramp. The essential output is summarized in the figure below (Fig1). The boundaries of the phase diagram of H2O are dramatically shifted. For high compression rate ice VII can be recovered at ambient pressure. The strong shift of the melting line of water questions fundamental issues of how a solid melt.

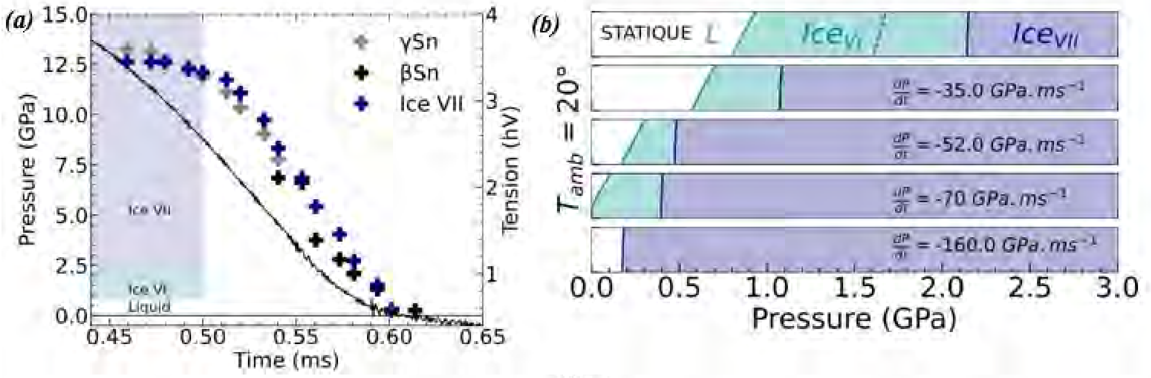

Fig 1.

***(a)** The configuration of the dDAC bench for time-resolved X-ray diffraction on ESRF's ID09 beamline enables the acquisition of micro-structural information with a temporal resolution of up to 250 kHz. An example of a decompression process is presented, demonstrating the metastability of ice VII at high decompression rates. Phase identification is obtained from diffraction patterns, and pressure is determined using lattice parameters and the Birch-Murnaghan equation of state.*

***(b)** Evolution of the water diagram phase close to ambient in function of the compression rate, data from the dDAC bench and ID09. This study highlights a new paradigm in dynamic exploration of phase diagrams with transition line displacements, du to competition between thermodynamic stability and kinetics nucleation of phase*

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High-Pressure Structural Invariance in Liquid Bismuth Across the Melting Curve

Shir Ben Shalom[1], Neta Ellert[1], Laura Henry[2], Moran Emuna[3], Yuri Kirshon[1], Pierre Piault[2], Andrew King[2], Nicolas Guignot[2], Yaron Greenberg[3], Eyal Yahel[3], and Guy Makov[1]
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Elemental metal liquids often retain the structural characteristics of their corresponding solid phases, exhibiting locally favored arrangements similar to their solid-state order. Bismuth (Bi) exhibits remarkable structural and thermodynamic behavior under pressure, including transitions between five low-symmetry solid allotropes and anomalous melting curve- where the melting temperature initially decreases before increasing. Several studies have also proposed the existence of pressure-induced transitions in the liquid state. Despite extensive research at ambient pressure, the structure of liquid Bi under high pressure remains poorly characterized, limiting our understanding of its phase behavior.

In this study, we investigate the structure of liquid Bi in the 1-4 GPa pressure range, just above the melting line, across multiple solid phase transitions. Energy-dispersive X-ray diffraction (EDXRD) measurements were performed at the PICSHE beamline of the SOLEIL synchrotron. The collected data were used to derive the structure factor, S(Q), and the pair distribution function, g(r), at each pressure point. The position of the first peak in the radial distribution function shifted by ~1% from the origin despite increasing liquid density, while the second peak shifted by 0.01 nm towards the origin. The coordination numbers of the first and second shells increase with increasing pressure. Analysis using the Quasi-Crystalline Model (QCM) reveals that the short-range order in liquid Bi remains largely invariant across the pressure range and retains features of a distorted Bi-I–like structure, with only a minor variation in the α angle. Despite melting from different solid phases, these results reveal a surprising structural persistence in liquid Bi. Our findings show that the solid-liquid structural correlation observed in some elemental metals does not hold for bismuth.

Is there a Liquid-Liquid transition in realgar (As_4S_4) under Extreme Conditions? A Comprehensive Synchrotron study

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The possibility of having two or more liquid phases of the same substance, separated by a first-order liquid-liquid transition (LLT) where density discontinuously changes, has been discussed as early as the 1970's [1] and has been strongly debated in the case of supercooled water in the last 4 decades [2]. Experimental studies have clearly established the existence of first-order transitions in a few liquid systems, such as phosphorus [3,4] and sulfur [5]. However, our understanding of the LLT remains relatively primitive, and experimental realizations remain scarce and, in most cases, heavily disputed. In this context, the AsS system appears as a promising candidate for LLT according to recent literature [6-8]. Indeed, experiments [6] have revealed sharp and strong changes in the structural and dynamics properties of the AsS melt as pressure is increased. This led to the proposition that the AsS liquid undergoes two major transformations: first, from a molecular to a polymeric liquid around 2 GPa, and second, to a metallic liquid around 5 GPa. Moreover, according to two recent computer simulations using ab-initio molecular dynamics (AIMD) [7,8], a discontinuous volume jump occurs at the molecular-to-polymeric liquid transition.

Motivated by these findings, we have systematically investigated liquid As_4S_4 using synchrotron-based in situ x-ray absorption, x-ray diffraction (XRD), x-ray radiography and tomography in the Paris–Edinburgh press. This set of various techniques enabled us to obtain the first measurements of the density of liquid AsS along various isotherms up to 6 GPa, as well as to explore the liquid structure and viscosity of AsS as a function of pressure and temperature. Furthermore, we measured the melting curve of AsS, and estimated the density changes along the melting line. The results will be shown in this presentation and discussed in relation with the proposed liquid-liquid transition.

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The Frenkel line of nitrogen and an empirical equation for the coordination number of real fluids

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Over the past decade there have been numerous studies investigating the Frenkel line, a crossover, originally in the supercritical state, between a non-rigid and a rigid fluid capable of sustaining shear waves. Part of the interest in this is sustained by the fact that the Frenkel line is correlated with maxima of solubility/solvent potency of the fluids, suggesting these supercritical fluids may be better tuned for practical applications such as drilling and industrial processing.

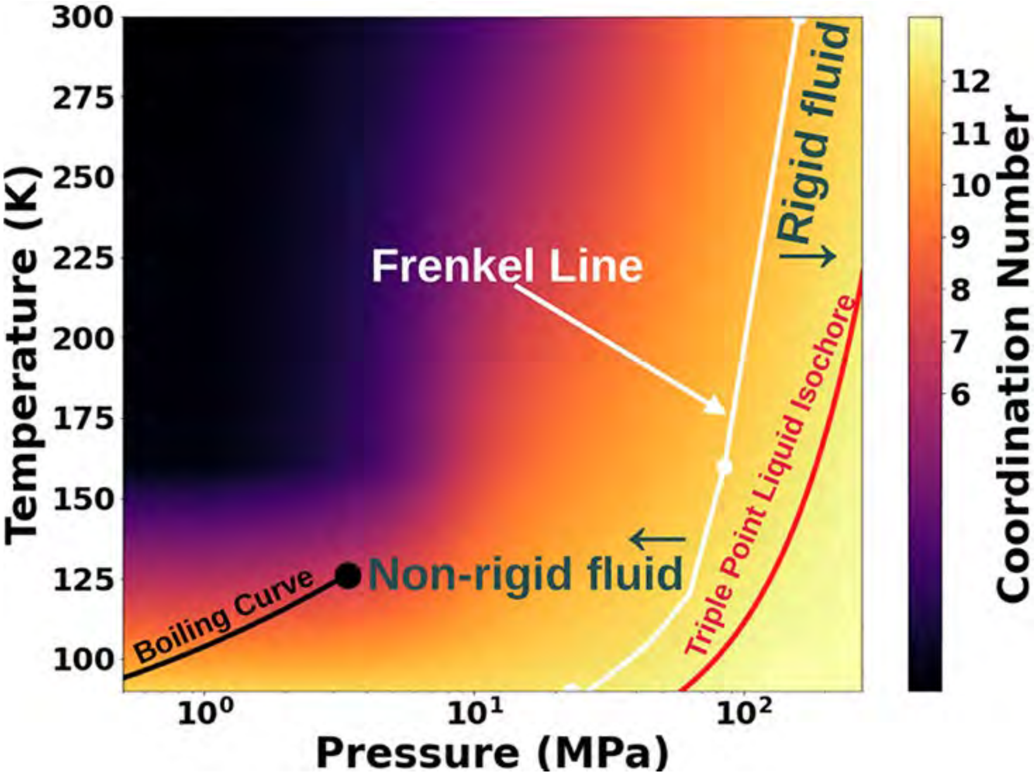
The original proposals discovered the line by means of computer simulation, most commonly with Lennard-Jones and soft sphere fluid models, and used changes in the particles' velocity autocorrelation function as an identifying feature. On the experimental front, several groups have located the line in a wide range of real supercritical fluids, from Ne and Kr to CO2 and water.

Over the last few years we have undertaken a campaign to study the Frenkel line in N2, by means of neutron diffraction, Raman spectroscopy and modelling, across a wide range of temperatures and pressures spanning both the subcritical, regular liquid regime and supercritical one. To this end, we have developed a machine-learned interatomic potential (MLIP) for molecular nitrogen that is capable of reproducing all experimental findings to date.

Here we present the latest and final chapter in this campaign, having determined the structure of N2 at 90 K (0.7 Tc) across a wide range of densities from the vicinity of the boiling curve to close to the melting line. Even at these conditions we were able to locate the Frenkel line, resolving a long-standing open question about its origin in the phase diagram, and introduce a new structural order parameter to identify the crossover which shows the changes less subtly than previously-used ones such as the coordination number.

Moreover, we were able to show using our MLIP that the structural changes correlate directly with dynamical ones as evidenced by the velocity autocorrelation function, directly relating the structural and dynamical properties of the fluid on either side of the Frenkel line.

Finally, when combined with our previous studies, we were able to formulate an empirical equation that describes the evolution of the coordination number of N2 as a function of density across the entire region of the phase diagram inhabited by the fluid. This equation is general and readily transferrable to other chemical species, from noble gases to simple molecules.



EHPRG Award

When crystallography meets planetary science: insights into large icy moons of Jupiter and Saturn

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Search for potential habitable environments beyond the Earth is a central challenge in modern planetary science and astrobiology. To date, icy moons of Jupiter and Saturn are the only extra-terrestrial planetary bodies where the presence of liquid water has been discovered in the form of subsurface oceans. These oceans are nowadays the most appealing astrobiological targets and have become the focus of interdisciplinary research, as well as of ongoing and upcoming space missions. A unique aspect of extra-terrestrial ocean worlds is the influence of high pressure on their physical state and thermochemical evolution. On the large ocean worlds like Ganymede, Titan, and Callisto, pressures at the base of the hydrosphere can achieve up to 1.7 GPa. While a variety of salts and volatiles are expected to be dissolved in the interior of large icy moons, some of these compounds can be stable in the form of salt hydrates or gas clathrate hydrates at relevant conditions. Formation and destabilization of these hydrates govern the chemical exchange in the interior, with a major impact on the chemical evolution and astrobiological potential of subsurface oceans. The current contribution overviews the collaborative work of crystallographers and planetary scientists of the last years dedicated to 1) in situ high-pressure X-Ray diffraction studies of potential extra-terrestrial minerals, and 2) implications of the experimental results to the evolution of the large ocean worlds. Methodological approach and the advantages of using of in situ single-crystal X-ray diffraction will be discussed. Case studies on salt hydrates and clathrate hydrates will be presented, followed by a discussion of open questions and ongoing research activities.

Financial support provided by the Agence Nationale de la Recherche (ANR) through the project CAGES (“High pressure clathrate hydrates in large ocean worlds”, ANR-23-CE49-0002, PI A. Pakhomova) is acknowledged.

(Invited) Phase Stability and Stimulated Reactivity of Methane

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Methane plays a crucial role in both fundamental and applied sciences and is a major constituent in the interiors of outer solar system planets such as Uranus and Neptune, as well as in Earth's deep interior. Its physical state under extreme conditions is governed by high pressures and temperatures, making the high-pressure–high-temperature phase diagram of methane central to disciplines including physics, chemistry, planetary science, and geology. As the simplest hydrocarbon, CH_4 exhibits rich polymorphism, forming a variety of crystalline structures that have been extensively studied in a wide pressure and temperature range (1–4). Despite extensive investigation, its phase diagram—particularly the relationship between solid phases and the fluid state—remains less well-resolved than that of other simple molecular solids (5–11). In addition to its structural complexity, methane's chemical reactivity under extreme conditions has garnered significant interest, with previous studies demonstrating decomposition only at very high temperatures and pressures (6, 10–12).

Using diamond anvil cell experiments with resistive heating and optical spectroscopy, we explore methane’s phase diagram to 45 GPa and 1100 K, refining its high-temperature phase boundaries and revealing a melting curve significantly higher than previously reported(13). We further investigate methane’s chemical stability up to 160 GPa at room temperature, and under milder pressures when exposed to external stimuli such as light or reactive species like molecular nitrogen (N_2) (14). In its pure form, methane remains chemically inert under compression at room temperature; however, this changes dramatically when excited with powerful light sources or combined with N_2, especially under high-pressure or high-pressure–high-temperature conditions. These findings revise our understanding of methane’s chemical resilience and open new perspectives on C–H chemistry with implications for prebiotic processes and nitrogen-rich planetary environments.

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(Invited) The emptied hydrate: from the high pressure synthesis to the recovered functional material

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The investigation of the pure water phase diagram has often unravelled exciting discoveries. The already complex polymorphism of ice is furtherly enriched if we consider the solid mixture of water and gases at high pressure. In particular, several solid stoichiometric and non-stoichiometric phases of the mixture H2O-H2 have been characterized in the latest years [1], some of which, being metastable at ambient pressure and low temperature (77 K), can be recovered and handled in laboratory.

Surprisingly, three of these, i.e., the sII clathrate together with the C0 and C2 phases, show a metastable behaviour even in the absence of a molecular guest in the water framework. They are obtained by keeping the hydrate under vacuum in the temperature range 110-160 K, yielding in this way the pure ice polymorphs XVI [2], XVII [3] and Ic [4,5], respectively. Here we report our studies concerning the high pressure synthesis and characterization of the C0 hydrate and its emptied counterpart, i.e., ice XVII [6,7], mainly performed through Raman and neutron scattering experiments. We also discuss the properties of the other emptied hydrates discovered to date, in the new perspective of considering these materials relevant for technological applications [7], as well as in the astrophysical context [8].

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Large compositional variability in water-ammonia solid mixtures at high pressure and temperature

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Water and ammonia are two major components of the mantle of the giant icy planets Neptune and Uranus, as well as several moons of Jupiter and Saturn. The pressure and temperature conditions inside these celestial bodies of very different diameter and composition is so vast that it is crucial to obtain experimental data on water/ammonia mixtures of various compositions and over a large range of pressure (P) and temperature (T) conditions to constrain their interior structures. At ambient pressure, ammonia and water form 3 stoichiometric compounds (xH2O:yNH3): ammonia monohydrate (AMH,1:1), ammonia hemihydrate (AHH, 1:2) and ammonia dihydrate (ADH, 2:1). These 3 hydrates, when compressed at low temperature above ~10 GPa and then annealed to 300 K, crystallize into a simple bcc structure [1], similar to that of the high pressure ice VII phase of water. We have demonstrated that this structure is the host of a disordered ionico-molecular alloy (called DIMA phase) where NH4+ and OH- coexist with NH3 and H2O molecules [2]. Recently, we have also shown that a “plastic” version of the bcc DIMA phase can also be observed along the melting line line at high T [4,5,6] in AMH and AHH and that the orientational disorder drives site disorder [6].

In this work, by studying the melting and freezing behaviour of the 2:1 mixture under high pressure and temperature by XRD and Raman spectroscopy, we report here the existence of plastic ADH at high T and also the discovery of a new class of ammonia hydrates with non-stoichiometric compositions, intermediate between pure water and ammonia hemihydrate [7]. A large variability in the composition of these hydrates is observed with P and T, which is made possible by fast molecular diffusion through their plastic network. Our works also highlight an increased solubility of ammonia in water ice at high P-T, which should be taken into consideration in interior models of icy planets and satellites.

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High Temperature properties of methane-hydrogen inclusion compounds

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Hydrogen and methane are two of the most abundant molecules in the universe, and analysing their dynamics under high temperature and pressure conditions is fundamental to our understanding of the interior evolution of planets [1]. Experimental studies augmented with Density Functional Theory (DFT) calculations established the pressure-induced formation of a series of methane-hydrogen van der Waals compounds [2], but their dynamic properties have so far remained unstudied. These can represent qualitative differences between DFT structure optimisations (which neglect rotational degrees of freedom) and experiments (where rotational states can be found to very low temperatures) [3].

In this work, we performed ab initio molecular dynamics (AIMD) simulations at pressures up to 220 GPa and temperatures up to 3600 K. We investigated a range of methane-hydrogen compositions, as well as pure methane and hydrogen. We studied phase transitions, local structure, and species lifetimes.

These simulations allowed us to construct pressure-temperature phase diagrams of all compounds and to precisely determine their melting and dissociation lines. We also analysed the interesting dynamics in the methane-hydrogen compounds as these two lines converge and determined the onset conditions for carbon-carbon bond formation.

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Quantum Diamond Magnetometry : High-Pressure Sensing for High-Tc Superconductivity

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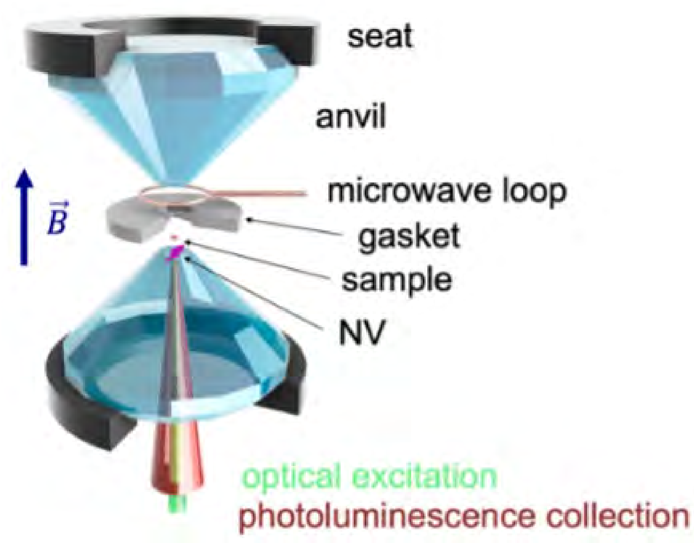
High pressure enhances quantum properties of materials, such as the superconductivity of cuprates [1], nickelates [2], and super-hydrides [3]. The diamond anvil cell (DAC) is the workhorse for high-pressure studies but sets constraints on the methods for in-situ characterization. By implanting NV centres on the tip of a diamond anvil, we achieve local measurements and enhanced resolution of phase transitions [4], complementing structural determination which can be independently done using X-ray diffraction [5].

This approach, validated above the megabar [6], enables the study of superconductivity of pressure-synthesized hydrides. Although the high-pressure high-temperature synthesis of these super-hydrides has been significantly improved in the past years, determining the stoichiometry of the compound remains a challenge since the hydrogen atoms are invisible in the X-ray diffraction pattern.

The coupling of nuclear spins in the material within the DAC to the electronic spins of NV centres on the anvil tip suggests the possibility of using nuclear magnetic resonance (NMR) for detecting protons in the pressurized sample. Previously NMR has been used to observe nuclear spin precession at a few kilobars [7] and symmetry breaking in solid hydrogen [8]. Nevertheless, the sensitivity of the spin precession detection, based on an external pick-up coil, remains poor. We leverage NV centres as quantum probes, coupled to nuclear spins, to develop NMR at micrometre scale [9, 10].



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High-Pressure Synthesis and Characterization of the Novel Potassium Superhydride KH9

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Through high pressure diamond anvil cell experiments, we report the synthesis of two novel potassium superhydrides (KH9-I and KH9-II) and investigate their structural and vibrational properties via synchrotron X-ray powder diffraction and Raman spectroscopy, complemented by density functional theory (DFT) calculations. Above 17 GPa at room temperature, KH-II and H2 react to form KH9-I; this reaction can be accelerated with temperature. KH9-I possesses a face-centered-cubic (fcc) potassium sublattice with a slight rhombohedral distortion (space group R-3m). Compression above 78 GPa converts KH9-I to another polymorph, KH9-II, which adopts a primitive simple hexagonal potassium sublattice (space group P6/mmm) and remains stable up to at least 100 GPa. Both KH9 polymorphs exhibit ionic character, comprising K+ and H− ions, along with quasi-molecular H2 units, resulting in rich Raman activity. [1]

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Ternary Sulfur Hydride Compounds

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Ternary hydride compounds have attracted considerable recent interest for hosting high-temperature superconductivity under pressure[1,2]. In such ternary systems, the addition of a third element can serve to help maximise the superconducting properties over binary systems by tuning the electronic properties and/or decreasing the pressures required for stabilising high-Tc phases. Sulfur has been previously observed to form high-temperature superconducting hydride phases, with a maximum critical temperature (Tc) of 200K at 160 GPa[3]. By doping the SH3 system, in this work we perform X-ray diffraction and electrical transport measurements at pressures between 90 and 160 GPa to investigate methods of suppressing the structural instabilities that are detrimental to high-Tc superconductivity.

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Formation of Molybdenum Deuteride at High Pressure: A Neutron Diffraction Study

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The structure of molybdenum deuteride ($MoD_{1.35}$) was studied using time-of-flight neutron powder diffraction under pressures up to ~6 GPa. The sample was synthesised in situ by reacting molybdenum powder with deuterium gas, introduced via an offline high-pressure gas-loading technique, and compressed using a Paris–Edinburgh press. Above ~4 GPa, diffraction data revealed the formation of a hexagonal deuteride phase. Rietveld refinements confirmed the P63/mmc symmetry, with full occupancy of octahedral sites and partial occupancy of tetrahedral sites, and determined the over-stoichiometric deuterium content as 1.35(4). The refined atomic positions and interatomic distances provide insight into D–Mo interactions and the origin of non-stoichiometry.

High Pressure Synthesis of Cesium Superhydrides

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With the recent advances in the utilization of the diamond anvil cell technique for hydrogen compression, a series of new materials with unusually high hydrogen content (superhydrides) have been discovered. Some of them, such as bcc-CaH6 [1], bcc-YH6 [2], hcp-YH9 [3] and fcc-LaH10 [4], can be synthesized at pressures above 150 GPa, and they demonstrate high temperature superconductivity with Tc>200K. Previously, we demonstrated that rubidium superhydrides, RbH9 and RbH5, are stabilized at the much lower pressures of 8.7 and 21 GPa, respectively [5].

Ab initio crystal structure prediction calculations that utilize density functional theory (DFT) have predicted that cesium should form superhydrides at pressures as low as 2 GPa [6]. Here, we studied the Cs-H system in laser-heated diamond anvil cells with X-Ray diffraction and Raman spectroscopy under high hydrogen pressure up to 100 GPa. We observed a formation of a series of cesium superhydrides, determined their composition, crystal structures, V(P) equations of state, and pressure domains of stability. DFT calculations allowed us to propose tentative arrangement of hydrogen atoms in the crystal structures. All cesium hydrides turn out to be insulators with rich Raman activity, indicating a presence of quasimolecular H2 units and H3- anions.

The work was supported by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program (Grant Agreement No. 948895, MetElOne).

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Imaging magnetic fields using NV centers as quantum sensors - study of the magnetic transition of UH3 under high pressure

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NV centers are point defects of diamond composed of the association of a nitrogen atom (N) and a vacancy (V). They emit photoluminescence, with a varying intensity depending on the spin state of the center. By combining a microwave and an optical excitation, it is possible to determine optically the positions of the NV centers energy levels, which are related to its local environment. It is therefore a multifunction quantum sensor, allowing in particular to perform magnetic measurements.

In order to use the NV centers at high pressure, it is necessary to adapt to the restrictions associated with the diamond anvil cell (DAC), a tool allowing to reach pressures higher than the megabar. By creating NV centers using nitrogen ion beams focused at the surface of one of the anvils, it is possible to place these sensors near the sample, directly inside the DAC. We developed an optical magnetometry setup for high pressures, which lets us reconstruct the complete vector magnetic field around the sample at a micrometric scale. [1]

The non-hydrostatic stress at a standard diamond anvil tip limits the use of NV centers to about 40 GPa. By drilling a micro-pillar at the surface of the anvil, it is possible to restore quasi-hydrostatic pressure favorable for NV centers, and thus extend their use up to 130 GPa. [2]

This technique offers a new diagnostic to study the magnetism of materials under high pressure. In this project, we choose to study the magnetic transition of UH3, from ferromagnetism at low temperature to paramagnetism at high temperature, to better understand 5f magnetism in actinides. Since UH3 is stable at ambient pressure, we first synthesized the samples in H2 loading and performed X-ray diffraction before selecting and placing the best ones in a NV-DAC. We then used NV magnetometry to follow the evolution of the Curie temperature of UH3 with pressure, up to about 20 GPa so far, decreasing from 174K at ambient pressure with a rate of about 2K per GPa as expected from the low pressure results observed up to 3.2 GPa in the literature. [3]

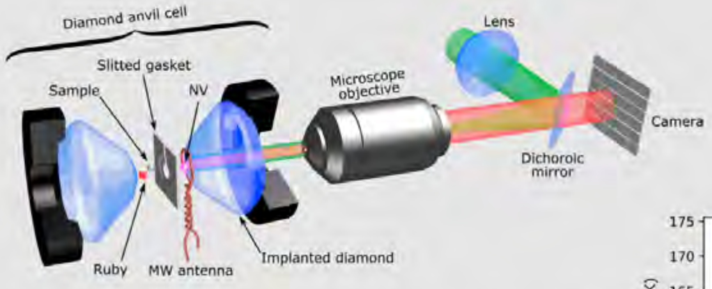

Fig 1. Measurement setup used for high pressure NV magnetometry. [1]

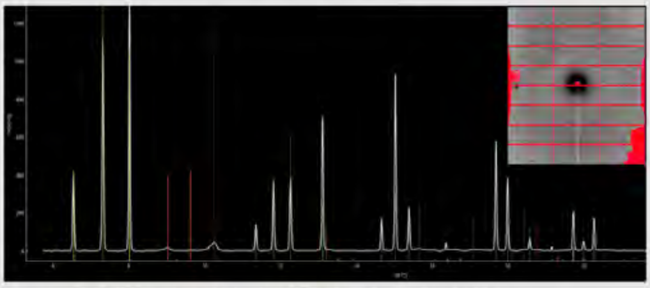

Fig 2. XRD pattern obtained at 2GPa of UH_3 (green lines) with traces of the rhenium gasket (orange lines).

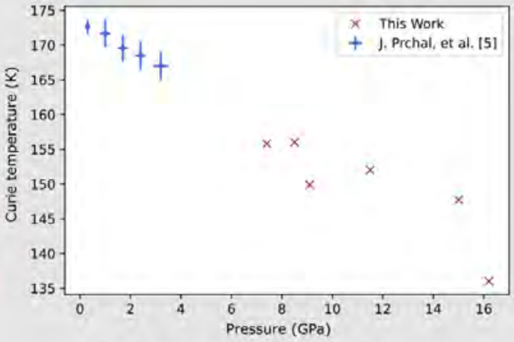

Fig 3. Evolution of Curie temperature with pressure.

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High-pressure modulation of breathing kagome lattice: Lifshitz transitions and evolution of the electronic structure

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Kagome metals, characterized by their triangular crystal lattice, are known to host a rich variety of phenomena, including electronic correlations, density wave orders, non-trivial topology, and magnetism. These materials have become a prominent platform for exploring the interplay between these features and their influence on various physical properties. Our study explores how high pressure affects the kagome ferromagnet Fe_3Sn_2, with particular emphasis on changes in its electronic and crystal structures, as well as the relaxation dynamics of charge carriers.

At ambient pressure, Fe_3Sn_2 exhibits a slightly distorted kagome lattice with a breathing mode. Applying pressure suppresses this modulation, with a reversal occurring at pressures exceeding 15 GPa. This suppression induces a series of electronic transitions affecting the Fermi surface. We detect them utilizing broadband infrared spectroscopy and ultrafast pump-probe measurements. In addition to these electronic Lifshitz transitions, we observe that the relaxation times of photoexcited charge carriers approach values typical for systems with an undistorted kagome lattice when the breathing mode is suppressed. We further investigate the pressure-dependent effects on electron-phonon coupling using coherent phonon spectroscopy and Raman scattering.

Our findings reveal significant structural and electronic transformations under high pressure, offering new insights into the phase diagram of Fe_3Sn_2. These results highlight potential pathways for tuning both the electronic and vibrational properties of kagome metals, emphasizing the importance of combining multiple high-pressure techniques to capture the intricate behavior of these materials under extreme conditions.

Session 6a: Central Facilities

(Invited) Developing the High Pressure Science Programme at the ISIS Neutron and Muon Source

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The advantages of neutron radiation for diffraction experiments, compared to those of X-rays, have been well documented. Less well known is the potential for performing neutron diffraction experiments at the extreme conditions of high pressure.

PEARL – the dedicated high pressure neutron diffraction instrument at ISIS – was designed around the Paris-Edinburgh press and has, for the past 20+ years, formed a significant part of the high pressure user programme at the ISIS facility.

Beyond the PEARL instrument, we have been pushing the pressure regime accessible (beyond gas pressures) on other diffraction instruments at the ISIS source including, SXD the single crystal instrument, SANDALS the liquid amorphous instrument, HRPD the high resolution powder diffractometer and WISH the dedicated long wavelength diffractometer enhanced for magnetic and large unit cell diffraction measurements. For all these instruments both the PE press is being utilised and other new clamp cell devices to go beyond the 1 GPa pressure range. This is vastly increasing the range of chemistry, geology and physics it is possible to investigate at the extremes of pressure and temperature.

The talk will initially describe the current and developing capabilities of the PEARL instrument in terms of pressure and temperature range. I will then provide examples of the science uitlising diffraction data obtained on PEARL and other diffraction instruments at ISIS from a broad range of materials. On-going developments which will push the pressure and temperature capabilities beyond that currently available to the user programme again across the suite of ISIS diffraction instruments will also be presented.

(Invited) Dynamic compression experiments at the HED-HiBEF scientific instrument at European XFEL

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Coupling modern light sources to high-power long-pulse lasers allows to access electronic and atomic structures of materials at an unprecedented level of structural, spatial and temporal resolution during dynamic compression experiments.

In the past couple of years, several dynamic compression set-ups have been realised at the High Energy Density – Helmholtz-international Beamline for Extreme Fields (HED-HiBEF) scientific instrument at European XFEL which offers a 10 Hz 100 J optical laser drive system, namely the DiPOLE 100-X laser.

First experiments with DiPOLE100-X in 2023 made use of a set-up optimised on X-ray diffraction using two large area VAREX4343CT flat panel detectors in interaction chamber 2 at HED-HiBEF at a photon energy of 18 keV (1, 2, 3). In 2024, the photon energy range was extended to 24 keV for experiments using this set-up which extended the momentum-transfer range of structure factor data from 8.8 to 12.0 Å-1.

In 2024, the first spectroscopy experiments for dynamic compression were realised in interaction chamber 1 of HED-HiBEF. Besides experimental set ups for X-ray Raman spectroscopy, resonant inelastic X-ray scattering, stochastic correlation X-ray spectroscopy and plasmon dispersion measurements, the set up included a van Hamos spectrometer with four Ge220 crystals (4) which allowed to study spin state of Fe bearing materials under dynamic compression. The excellent reproducibility of DiPOLE100-X allowed to access states in systems of low signals by accumulation of multiple spectra of repetitive DiPOLE100-X shots. The set-up included X-ray diffraction capabilities using a Jungfrau detector downstream of the sample.

All these experiments were coupled with the typical shock diagnostics VISAR and SOP which were continuously optimised in performance for the different set-ups (5).

Currently, first in-house experiments are planned which aim to combine imaging of materials and small angle X-ray scattering under shock compression in a transversal geometry.

In this contribution, we will give an overview of the three experiments and focus on possible new applications for Earth Science materials.

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[2] J. Wark et al., JAP (2025) DOI: 10.1063/5.0256844
[3] D. Kraus et al., Nature (2025) DOI: 10.1038/s41586-025-09035-6
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Acknowledgements
We acknowledge the European XFEL in Schenefeld, Germany, for provision of X-ray free electron laser beam time at the Scientifc Instrument HED and would like to thank the staff for their assistance. The authors are indebted to the HIBEF user consortium for the provision of instrumentation and staff that enabled these experiments. We thank the participants of community proposals #2740, #6656 and #6659 for continuous support and discussions which considerably helped to optimise the set-ups at HED-HiBEF. We acknowledge funding of the Federal Ministry of Education and Research of Germany (Project 05K19PE2). CC acknowledges financial support by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) via project AP262/3-1 and STE1079/10-1 (project number 521549147).

Developing Neutron Techniques at Extreme Conditions: the High Pressure Neutron Diffractometer at China Spallation Neutron Source (CSNS)

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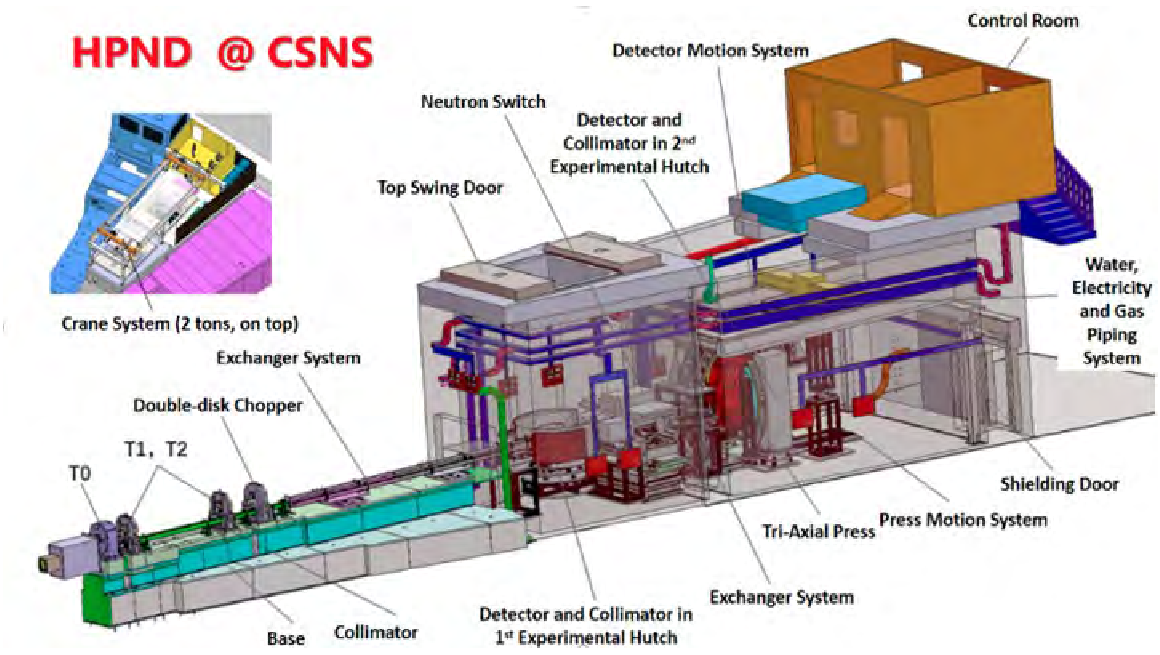
The development of neutron techniques under extreme conditions is invaluable to condensed matter physics, crystal chemistry, materials science, and earth and planetary sciences. In situ neutron diffraction experiments at high-pressures (HP) provide unique opportunities to investigate materials under these harsh conditions. As one of the cornerstone research platforms within the Shenzhen Materials Genome Large-Scale Facilities project, the high-pressure neutron diffractometer has been designated as Beamline BL-15 at CSNS and is currently callibrating HP sample enviroments with neutrons by the Southern University of Science and Technology (SUSTech) and CSNS. The beamline is expected to be commissioned in 2025, with neutron diffraction and imaging as its primary techniques in conjunction with various sample environments under extreme conditions. Its main design parameters are as follows: 1) the d-spacing range (90° detector in the single frame mode): 0.5 – 5 Å; 2) the resolution: $\Delta d/d \leq 0.6\%$ (90° detector); and 3) the neutron flux at the sample position: $> 5 \times 10^6$ n/s/cm^2 @ 100 kW. The extreme sample environments include: 1) high-pressure (P) and temperature (T) [P (max) = 20 GPa, T (max) = 1300 K); 2) low-T and high magnetic field [B (max) = 9 T, T (min) = 4 K]; and 3) high-P percolation (pore pressure ≤ 150 MPa, confining pressure ≤ 200 MPa, deviatoric stress ≤ 300 MPa, and sample temperature: 270 K ≤ T ≤ 370 K). The high penetrating power of neutrons presents great advantages in designing pressure cells with various types of high strength metals, alloys, and ceramics. A suite of pressure devices, such as true triaxial multi-anvil press, piston cylinder, P-E cell, gas/liquid high-P cell, portable cubic press, and ZAP cell, etc., will be used to provide extreme P-T conditions and the flexibility of switching experimental systems between the portable and transferable devices. The high-P facility is augmented by simultaneous multi-mode in situ measurements for physical parameters such as mechanic, thermal, acoustic, optical, and electrical properties under extreme conditions.

High-P neutron facility at CSNS will provide scientists with a new venue to carry out frontier interdisciplinary research under comprehensive extreme sample environments of high pressure, high/low temperature, and/or high magnetic field. Similar techniques have been successfully used to study the equations of state, structural phase transitions, and thermomechanical properties of metals, ceramics, and minerals. We have previously conducted researches using neutron diffraction technique on the formation/decomposition kinetics of methane, CO2 and hydrogen hydrate clathrates, and hydrogen/CO2 adsorption of inclusion compounds such as metal–organic frameworks (MOFs). High-P neutron facility at CSNS is expected to have a positive impact on the basic science research in physics, chemistry, materials science, energy science, and earth and planetary sciences, and therefore create ample opportunities for new discoveries in science and technology.



High-pressure research at the HPCAT beamlines following the APS Upgrade

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After a year-long upgrade to the Advanced Photon Source (APS-U), the HPCAT high-pressure research beamlines received their first X-ray photons in July of 2024. The APS-U project has seen a complete rebuild of the APS storage ring to incorporate a state-of-the-art multi-bend achromatic lattice, boosting the brightness and coherence of X-rays generated by the synchrotron (in August of 2024, the APS measured a world-leading 45 pm·rad electron-beam emittance), and users experiments at HPCAT have already begun benefitting from the improved source.

HPCAT services the high-pressure community through its 5 beamline end stations, each of which are dedicated to enabling synchrotron X-ray techniques to experiments at high pressure. Diffraction techniques include micro-focused monochromatic diffraction for powder and single-crystal samples in a wide variety of sample environments, micro-white-beam Laue diffraction, and small-angle scattering. Spectroscopic techniques include X-ray absorption (XANES and EXAFS) and emission, X-ray Raman, inelastic scattering, and nuclear forward scattering. A dedicated Paris-Edinburgh press beamline offers radiographic imaging and energy-dispersive diffraction. Work is ongoing to commission Bragg coherent diffraction imaging, phase contrast imaging, and nano-focus diffraction with high resolution, leveraging the properties of the new X-ray source.

We will discuss the immediate impacts of APS-U on synchrotron high-pressure experiments at HPCAT, with supporting highlights from user experiments at the upgraded beamlines, as well as prospects for future developments at HPCAT that best position the high-pressure community to capitalise on the new APS-U X-ray source.

Structural investigations of iron by X-ray heating and Diamond Anvil Cells at European Free Electron Laser

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The X-ray heating technique in combination with a DAC has been explored in numerous studies at the High Energy Density Instrument of the European XFEL to investigate structural changes at over megabar pressures and up to melting temperatures. The fast nature of the experiments yielding information on the structure evolving with temperature on nanosecond to microsecond time-scales demonstrated detectability of metastable and hard-to-detect new phases. We apply this approach to relatively well-known systems such as iron (proposal 3063 involving multiple institutions (Univ Lille, Sorbonne Univ, Univ Grenoble Alpes, Univ Freiburg, EuXFEL, CEA, Carnegie Institution for Science, DES/y, Univ Edinburgh, Stony Brook Univ, Univ of Chicago, Univ Oxford; PI: S. Merkel and G. Morard) to benchmark our experiments and to explore the phase diagram well above the megabar pressures, which opens a new range of opportunities for high pressure research.

(Invited) High-pressure data quality in today's data-centric world

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The FAIR data principles [1] are essential for the efficient and effective reuse of data, promoting knowledge discovery and innovation, ensuring that research data is Findable, Accessible, Interoperable, and Reusable. While the FAIR guiding rules have improved data openness and reusability, they do not guarantee the accuracy, reliability, or representativeness of scientific data. FAIR data is not necessarily quality data, but data quality as a package (including dimensions indicators, assessment and agreed alignment) should be FAIR.

As it is widely known, high-pressure data are often incomplete and of relatively poor quality. This can be attributed to such factors as the interaction of probing radiation with the pressure vessel, restricted access to the sample and the limited range and reliability of instruments when recording transient events at extreme conditions in dynamic compression techniques. However, the precision of pressure measurements has improved significantly over the years, impacting important aspects like the proper calibration of pressure reference points and the determination of key physical quantities, such as the bulk moduli. A rigorous error analysis is another critical component of data quality. Noteworthy, many publications still focus solely on statistical uncertainties within a single experiment, neglecting the systematic uncertainties associated with the pressure standard.

In this presentation, I will address several key questions: What benchmarks can be used for data quality assessment in the high-pressure field? What dimensions are necessary for validating data quality? How can we enhance data quality

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Synthesis of chemically simple carbonates at moderate pressures and temperatures

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“Conventional” sp^2-carbonates hosting [CO_3]-building blocks are ubiquitous in nature as they are the major source of carbon in the biosphere, hydrosphere, in soils and in the Earth's crust [1]. In the recent decades the family of carbonates has been extended by the discovery of sp^3-carbonates with [CO_4]-units, which are typically obtained at high p,T-conditions (> 70 GPa, > 1500 K) (summarized in [2]). Another significant observation was that, at around 20-30 GPa, carbonates can react with CO_2 to form novel pyrocarbonate units ([C_2O_5]) [3,4]. A similar result occurs when an oxides reacts with CO_2 [5].

Here, we applied Raman spectroscopy and single crystal XRD complemented with DFT calculations in order to study the formation of novel carbonates in laser-heated diamond anvil cells (LH-DACs). We demonstrate that chemically simple sp^2-carbonates such as Be[CO$_3$] (Fig. 1), Al$_2$[CO$_3$]$_3$ or Fe$_2$[CO$_3$]$_3$ can be synthesized by a reaction of a corresponding oxide (BeO, Al$_2$O$_3$, or Fe$_2$O$_3$) with CO$_2$, even if carbonates hosting these cations were not previously known [5-7]. Some of them can be recovered at ambient conditions. In addition, some of these sp^2-carbonates may be considered as potential hosts of carbon in the Earth's mantle.

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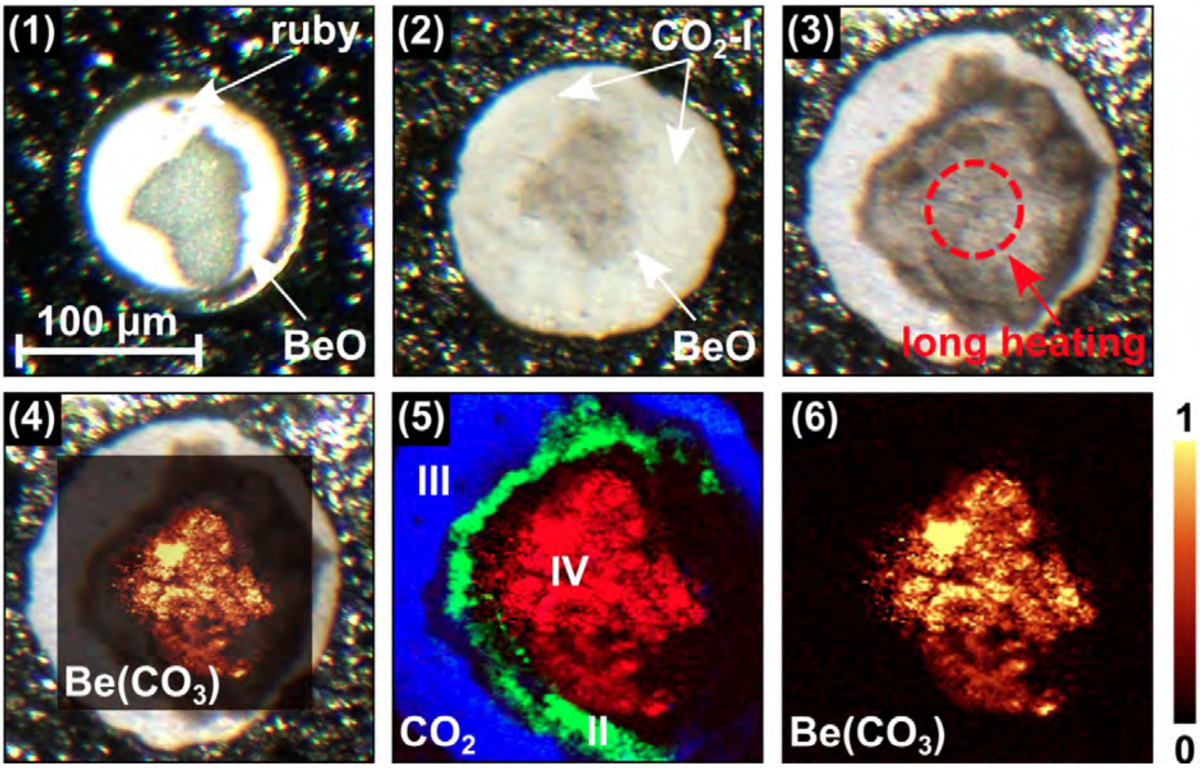

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Plenary Talk

The iron phase diagram at multiple timescales

Sébastien Merkel[1], Ginestet Hélène[1], EuXFEL 2700, 3063, 5700, and 6659 community proposals[2], ESRF ES::1538 proposal[3]
[1]Univ Lille, France, Lille, France, [2]EuXFEL, France, [3]ESRF, France

The iron phase diagram at high pressure and temperature is still discussed despite numerous experimental and simulation studies. Indeed, discrepancies still exist on the melting curve and the existence of a high pressure and high temperature cubic phase is debated. New techniques must be developed to address those issues.

This work re-addresses the high pressure phase diagram of iron using 3 independent time-resolved techniques: X-ray heating at femtosecond timescales at the European XFEL (EuXFEL), laser-heating at microsecond timescales at the ESRF, and laser-driven shock compression at the EuXFEL.

The EuXFEL provides extremely intense X-ray flashes repeated up to every 220 ns. The facility, coupled with the High Energy Density (HED) instrument, allows heating, melting, and crystallizing iron samples repeatedly and probe for its crystal structure as the sample cools from its previous state over experiment durations of up to 80 microseconds. Here, we use this procedure to follow Fe samples under static pressures in the diamond anvil cell, and study the state of Fe as it cools from the previous pulse, either in the solid or the liquid state, in 220 ns.

At ESRF, we use laser pulses of 10 to 40 ms seconds on Fe samples in diamond anvil cells, and explore the structure and state of the sample during the high temperature phase, and as it cools to ambient temperature.

Finally, the EuXFEL can be synchronized with the DiPOLE 100-X laser, enabling X-ray diffraction experiments during dynamic compression. Those experiments allow the collection of high-quality in situ X-ray diffraction data and visar measurements of shocked and off-Hugoniot Iron.

Here, I will present results from those 3 sets of experiments and discuss how pressure, temperature, timescale, and thermodynamic path can affect what we believe we know regarding the high pressure phase diagram of iron.

(Invited) A New X-ray Transparent Internally Heated Pressure Vessel for High-Pressure and High-Temperature in-situ view experiments

Barbara Bonechi[1], Margherita Polacci[1], Mike Burton[1], Richard Brooker[2], Fabio Arzilli[3], Eric Lahera[4], Alain Prat[4], Jean-Louis Hazemann[4], Giuseppe La Spina[5], Elisa Biagioli[1], Benoit Cordonnier[6], Robert Atwood[7], Sebastian Marussi[8], and Peter Lee[8,9]
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A novel X-ray transparent Internally Heated Pressure Vessel (IHPV) has been developed to enable synchrotron X-ray radiography and microtomography experiments under high-temperature (up to 1250 °C) and high-pressure (up to 200 MPa) conditions, providing an in-situ view of dynamic processes. This innovative system, tested and used at Diamond Light Source (UK) and European Synchrotron Radiation Facility (France), advances the study of magmatic and volcanic processes.

The IHPV allows real-time visualization and quantification of crystallization, degassing, bubble formation, chemical mixing, and immiscibility in multiphase materials. Previous studies were limited to shallow conduit depths (<500 m), but this apparatus enables investigations at 2-7 km depths, where critical eruptive processes occur. Applications extend beyond geosciences to material sciences and the engineering remit.

Two experimental setups were tested: (1) very fast X-ray radiography to capture vesiculation and degassing during magma ascent, achieving high temporal resolution (25 frames per second), and (2) fast X-ray microtomography to observe crystallization and bubble growth under controlled cooling at crustal storage pressures (20-100 MPa). The ability to perform 4D imaging (3D + time) significantly enhances quantitative analysis of magma crystallization kinetics, bubble nucleation, and growth, refining numerical models of eruption dynamics and improving volcanic hazard assessment.

This X-ray transparent IHPV is a breakthrough for experimental geosciences, enabling in-situ real time investigations across an unprecedented range of pressure and temperature conditions. Its application extends beyond Earth Sciences to metallurgy, ceramics, and composite materials, where in-situ high-resolution imaging of dynamic phase transitions is essential for advancing materials research.

Pressure gradients inside the hydrostatic cavity of DACs loaded with silicone oil and methanol-ethanol 4:1 as pressure transmitting media

Samuel Martin, Javier Cobo, Adrian Sansiseñena, and **Ignacio Hernandez**[1]
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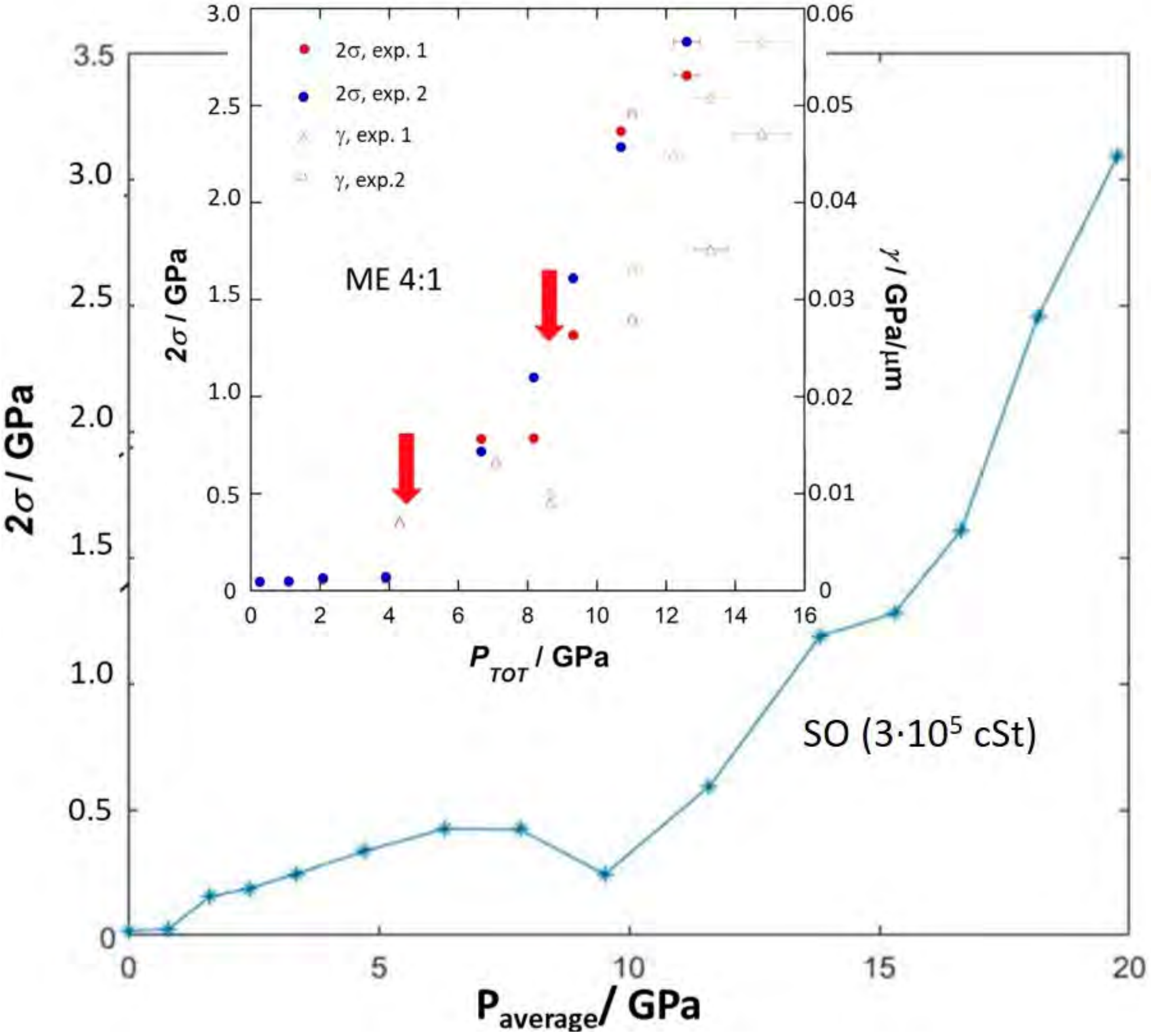
A vast number of high pressure experiments traditionally involve methanol-ethanol (ME 4:1), or silicone oil (SO) as pressure transmitting media. These materials are liquids at ambient conditions but solidify at given pressures, as studied by different authors [Angel 2007]. This fact necessarily affects the hydrostaticity of the conditions inside the pressure cavity formed by the gasket and diamonds [Klotz 2009, Dunstan 1989].

We have employed a simple method based on Raman spectroscopy for studying the pressure distribution along the cavity as a function of the (average) pressure, and the hole and gasket geometry. Thereby, we have quantified the onset of the loss of hydrostaticity and the expected value of the errorbars when employing ME or SO as pressure transmitting media up to 20 GPa.

We find that, even though not observable through changes in the ruby luminescence, ME loses hydrostaticity at pressures as low as 5 GPa, and the average pressure gradients are in the order of 0.05 GPa/μm at 15 GPa. Also, both SO and ME behave similarly in terms of pressure dispersion in the range 4-20 GPa, for given gasket geometry.



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Imaging in (Laser-Heated) Diamond Anvil Cells: From Phase Diagrams to Material Properties

Bernhard Massani[1], Stewart McWilliams[1], Zena Younes[1], Earl O'Bannon III[3], Alex Patsoukis-Dimou[1], Olivia Sabine Pardo[3], Emma Ehrenreich-Petersen[2], Ri Cao[1], Zsolt Jenei[3], Hanns-Peter Liermann[2], Nico Giordano[2], and Konstantin Glazyrin[2]
[1]University Of Edinburgh, UK [2]Deutsches Elektronen-Synchrotron (DESY), Germany, [3]Lawrence Livermore National Laboratory (LLNL), USA

'Observing stuff' is most likely the first scientific method ever used and well predates Newton's famous apple. Imaging techniques have long been used for scientific use and cover a huge variety of techniques. However, imaging in laser-heated diamond anvil cells (LH-DACs) largely has been limited to transparent samples. Recent advances in X-ray Phase Contrast Imaging (XPCI), however, also allow the observation of opaque materials under static high pressure in diamond anvil cells [1].

For many physically relevant materials large discrepancies in the melt curves (depending on the experimental approach) exist, with iron being the most prominent example [2-4]. As a fairly new approach, we use time-resolved imaging to directly observe the solid-liquid and solid-solid phase transition in laser heated samples in the diamond anvil cell along with simultaneous X-ray diffraction and optical radiometric temperature measurements. This technique was benchmarked with experiments on the uncontroversial high-pressure melting of platinum [5], and used on a variety of other samples from simple metals to geologically relevant materials such as Olivine. As such, XPCI offers a new insight into phase transitions of (opaque) materials under static high pressure.

Furthermore, we will give an outline of the possibility to study material properties such as the dynamics in the melt as well as other transport properties by the direct observation of their response to heating.

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Optimized Sample Geometry for X-ray Diffraction Experiments under Laser Heating in Diamond Anvil Cells.S

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The diamond anvil cell (DAC) combined with laser heating is a powerful tool for investigating phase diagrams of materials under extreme pressure-temperature (P–T) conditions. However, this method present significant limitations. In particular, strong thermal gradients within the sample chamber make the interpretation of diffraction data challenging, as illustrated by ongoing controversies regarding the melting curves of some metals. Moreover, laser heating is ineffective for materials with poor optical absorption, such as rare gases or simple molecular compounds.

We have developed a geometry in which the sample is enclosed in a boron-doped diamond (BDD) capsule. This opaque, high-thermal-conductivity material enables efficient absorption of laser energy and ensures a homogeneous temperature distribution. Our measurements show significantly reduce thermal gradients in the region probed by the X-rays, enabling precise determination of phase transition lines and associated thermodynamic properties.

This approach is illustrated with measurements on gold, nitrogen, and water over a wide P-T range.

(Invited) Study of high pressure properties of geomaterials using time-resolved diagnostics

Guillaume Morard[1]
[1]IMPMC-CNRS, France

Free Electron Lasers represent a cutting-edge generation of large-scale facilities, generating exceptionally brilliant X-ray pulses. These pulses can be coupled with Diamond Anvil Cells (DACs) or High-Power Lasers to conduct time-resolved studies of materials under extreme conditions. Moreover, the ESRF-EBS introduces a novel high brilliance beam, enabling innovative time-resolved methodologies.

Shock compression achieves high pressure-temperature (P-T) conditions but only for a few nanoseconds. Utilizing short X-ray pulses of a few femtoseconds enables the probing of highly homogeneous samples under extreme conditions. I will present our recent research on Fe spin state measurements in liquid olivine and liquid FeO, as well as the liquid structure of MgSiO3 exceeding 200 GPa or liquid Fe and Fe alloys at 200 GPa.

Furthermore, the MHz to kHz frequency range of the X-ray beam now permits tracking phenomena occurring in DACs at microsecond timescales. Coupling this high repetition rate with pulsed lasers enables the tracking of melting relations in the cell for homogeneous samples before chemical migration ensues. I will discuss partial melting of Fe alloys, and also recent advancements in X-ray heating of Fe, which allows for the deduction of phase diagrams and thermal conductivity when combined with in situ measurements and Finite Element Modeling.

(Invited) From between diamonds to the centres of planets – large scale impacts from tiny samples

Helen Maynard-Casely[1]
[1]Australian Centre for Neutron Scattering, Australia

We live in a bubble in terms of pressure, thinking that 1 atmosphere (10,000 Pa) is normal (and probably just as well for the continuation of humanity). But in our solar system, there are large swathes of matter that exist elevated pressures, which has shaped each of the terrestrial, gas giant and dwarf planets differently. In this general interest talk I will relate how space-based observations have posed questions that high-pressure science has endeavoured to answer – explaining how we know what materials to explore and under what conditions. From this several applications can be discussed, from how high-pressure science has given hope for habitability on Ganymede, though to explaining gravitational fields around the gas giants. In the case of Uranus and Neptune, the scarcity of space-based information means that high-pressure science is, in part, taking the lead in suggesting phenomena that could be observed by future space-based missions. Lastly, the vast increase in observed exoplanets means that the application of high-pressure science is by no-means limited to our own solar system and very much a growing business.

(Invited) Crystallising phase relations of Earth's outer core

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The origin of the geomagnetic fields has been discussed in relation to chemical differentiation in the outer core. Seismological, cosmochemical, and mineral physics studies indicate that the Earth's core is mainly composed of iron with some amounts of impurities to account for a 4–7% density deficit compared to pure iron at the relevant pressure and temperature conditions. The conventional idea is that crystallisation of the inner core would power the geodynamo as it enriches impurities at the base of the outer core which leads to gravitational instability and drives convection in the outer core. Despite years of research since the first proposition by Birch (1952), what chemical system does the inner core crystallise out of is yet to be determined even among a small number of candidate impurities: Si, S, O, C, and H, and therefore we have not fully understood the mechanism to drive the geodynamo. While melting/crystallising phase diagrams for Fe-impurity binary systems have been repeatedly proposed, those diagrams for 330 GPa at the inner core-outer core boundary included extrapolation of experimental data to a great extent and consistent comparison between different systems is challenging.

In this talk, I will present recent updates on the phase relations of Earth's core-forming materials from our group; we have established a self-consistent thermodynamic model for the binary systems Fe-O, Fe-Si, Fe-S and Fe-C, which is applicable to 370 GPa and 7000 K and all the systems were based on consistent pressure scales. From thermodynamic calculations, seismologically observable properties of liquid Fe-alloys were compared with the outer core profiles. We then determined the composition of a solid Fe-alloy which would crystallise out of each binary outer core. The conclusion is that none of the above binary systems works for both the outer and inner cores simultaneously.

Engaging Students in High-Pressure Physics Through Sapphire Anvil Cell Experiments

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The adaptation and integration of modern physics achievements into education is a rather popular endeavour [1, 2]. However, high-pressure physics seems to be lagging behind in this area. This work addresses this gap by presenting an example of how to involve both high school and undergraduate students in high-pressure physics using a sapphire-anvil cell (SAC).

The SAC is of the piston–cylinder type, with anvils shaped as proposed in [3]. Typically, it generates pressures of around 2 GPa, although in some experiments it has reached 9.5 GPa. The sample diameter of approximately 0.55 mm is manageable even for students with relatively little experience in practical physics experiments.

A common student experiment involves visually observing the crystallisation of liquid samples at room temperature and high pressures. For instance, water crystallises at pressures above 0.9 GPa.

Another experiment involves observing phase transitions between different solid states of a substance, each characterised by distinct visible-range absorption spectra. Based on the author’s experience, sulphur is a particularly illustrative example.

Drawing on well-documented, highly reproducible phase transitions from the literature, students construct a calibration curve that correlates the torque applied by a dynamometric wrench with the pressure inside the SAC. The dynamometric wrench is used to tighten the nut that applies force to the anvil.

Moreover, in addition to its educational applications, the SAC can be used by students to investigate samples for which the literature provides little or no data. In doing so, they can gain new insights into the behaviour of substances under high pressure, thus conducting what might be called exploratory research.

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(Invited) How plastic water is?

Livia Eleonora Bove[1,2,3]
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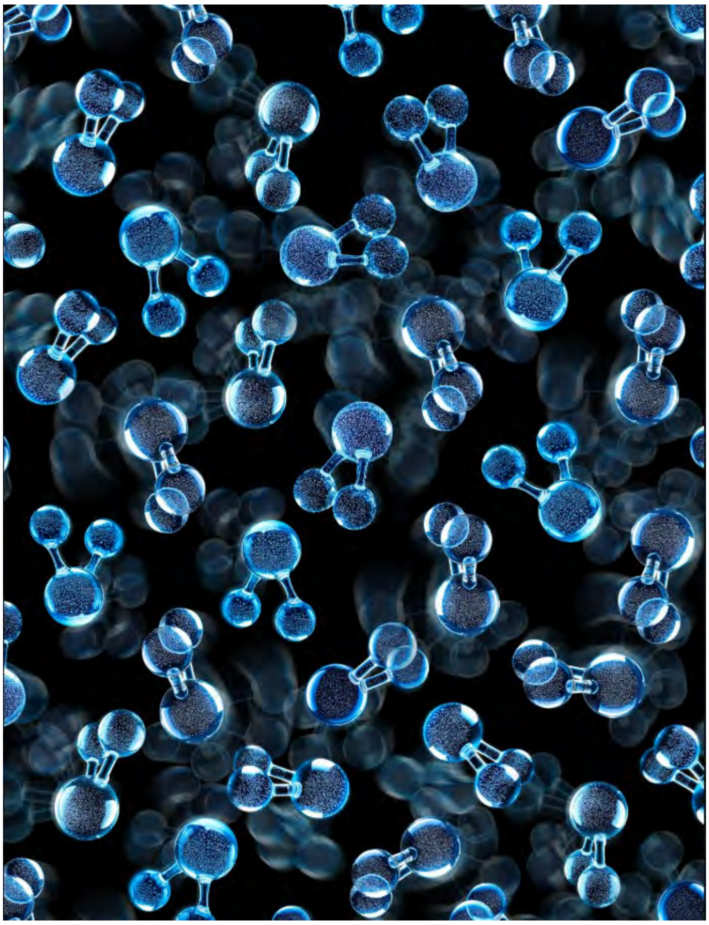
Over the past decade, computer simulations [1–3] have predicted the existence of a novel and intriguing phase of water, termed "Plastic water." This phase was expected to emerge along the melting line between liquid water and ice VII, as well as in water mixtures under extreme pressure–temperature (p–T) conditions [4]. In this phase, water molecules remain organized in a regular crystalline lattice while retaining the freedom to reorient, resulting in a hybrid state between that of a solid and a liquid. While plasticity is commonly observed in crystals of globular molecules like methane—where rotational motion persists within the crystal at high temperatures prior to melting—its occurrence in water ice is highly unusual.

Beyond plastic ice, theoretical studies predict several exotic high-pressure phases of water with similar (bcc-type) streuctures but profoundly different proton dynamics: quantum tunneling in the symmetric phase, molecular reorientation in plastic ice, long-range proton diffusion in the superionic phase, among them. High-pressure quasielastic neutron scattering (HP-QENS) offers a uniquely sensitive probe of these dynamic processes, enabling direct observation and experimental confirmation of these elusive phases.

Our recent HP-QENS experiments under high pressure have unveiled varying degrees of plasticity in high-pressure ice phases [5], water–ammonia ice mixtures [6], salty ices [7], methane and hydrogen-filled ices [8,9], and confined amorphous ice [10]. In this talk, I will discuss how plastic water arises in diverse environments and under varying p–T conditions, how plasticity is linked to the “glassy” behavior of water, and the implications of the existence of plastic ices for the geodynamics of icy moons.



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Can we compute high-pressure melting curves without knowledge of the crystalline structure?

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In many cases, finite-temperature crystalline structures are unknown, and determining them significantly complicates melting temperature calculations. A method that eliminates the need for prior knowledge of crystalline structures can accelerate, simplify, and streamline the prediction of melting curves from first principles. In this presentation, we will describe such an approach, which combines first-principles calculations with machine-learned potential molecular dynamics simulations. The method has been tested on several systems, and the results will be discussed.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and was supported from LDRD project with tracking code 23-ER-042.

Melting at Extreme Conditions: X-ray diffraction Meets Phase-Contrast Imaging

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Melting is generally very well studied at ambient pressures. However, how does the situation change when you conduct your studies at pressures exceeding the GPa level? How are the kinetics different, how does the compression rate influence melting, and if a pressure marker is included does this influence the results by adding potential nucleation sites? Lastly, of course, how can you accurately and precisely determine the melting temperature/condition at high pressures? All of these questions can – and will be – answered using a hierarchical approach where X-ray diffraction (XRD) probes the atomic structure and X-ray phase-contrast imaging reveal the melting behavior of the system in question. We will present different case studies on both gallium and platinum to unravel the secrets of melting kinetics at extreme conditions in the diamond anvil cell (DAC). This is done with the help of conventional XRD methods as well as principal component analysis and machine-learning assisted segmentation of images. These studies have been carried out using either the conventional DAC combined with laser-heating or using the dynamic diamond anvil cell (dDAC). In addition, results from the newly developed laser-heated dDAC will be presented.

This work has been performed at the Extreme Conditions Beamline, P02.2, at PETRA III, DESY, Hamburg, Germany.

Grain-size, grain-growth and melting under extreme conditions: A novel approach to melt identification

Tara R McElhinney[1], B. J. Heinen[2], O. T. Lord[2], K Vlasov[2], E-M. Rogmann[2], E. Fanesi[2], D. Daisenberger[3], and S. A. Hunt[1]
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Constraining melting temperatures of Fe at high pressure is pivotal in understanding the dynamics of planetary cores. The melting curve of most metals at high pressure remains poorly constrained. This variability reflects both the experimental challenges and the variety of techniques used to determine melting under extreme conditions. Common melt diagnostics in diamond anvil cells (DAC) include the laser speckle technique, liquid diffuse scattering, temperature plateaus, and resistance jumps. Each produces distinct and highly variable melting curves, where diffuse scattering has produced melting temperatures up to 500K higher than those from laser speckle in Ti. The lower laser speckle melting curve has been interpreted to be the result of dynamic recrystallization (DRX); however, measuring the microstructure is difficult close to melting at high pressures. There is an absence of understanding of high homologous temperature behaviour in metals, producing further uncertainty in the interpretation of melting.

Experiments here are carried out on Ti using internal resistive heated DAC (IR-DAC) at Diamond Light Source between 21-41 GPa. Peak intensities are used to independently measure grain-size and detect melting. A significant reduction in peak intensities marks the onset of DRX at 60-85% of the melting temperature, coinciding with those reported from the laser speckle method. The onset of melting produces a rapid drop in peak intensities and a plateau below the background. Melting points produced using this technique are consistently within error of those from resistance jumps and temperature plateaus.

(Invited) Life under extreme conditions

Judith Peters[1,2,3]
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The impact of external conditions on different bio-systems are as varied as their adaptation mechanisms. The main question is what happens when a biological system is submitted to extreme conditions and what makes it stable with respect to them. Concerning membranes, they play an important role for membrane permeability and fluidity. They are able to metabolically adapt their lipid composition, which is known as homeoviscous adaptation. The understanding of their physico-chemical properties is very important to get insights into the possible architecture of protomembranes at the origin of life. Recent advances of our understanding of different membrane types will be presented 1-3.

Proteins are known to be in their native state inside certain limits of temperature and pressure. Such state is generally a folded one and both temperature and pressure can denature and unfold a protein. The investigation of the full (T, p)-plan is laborious, as many parameters as compressibility, expansivity, heat capacity and others influence it and they cannot be measured by a sole technique. We will show which methods can be used and what is our actual knowledge on adaptation mechanisms of proteins 4.

Life cells are the most complex systems and their characterisation is puzzling. We will focus on recent studies of extremophilic bacteries and archaea to give hints on the factors which permit to such cells to thrive under high temperature and high hydrostatic pressure conditions 5,6.

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(Invited) From Snails to Fitting High-Pressure Raman Data

David Dunstan[1]
[1]Queen Mary University of London, UK

Too many gardeners believe it is necessary to control snail populations by killing them, because if they are merely removed, they come back. I tested this (using Tippex spots) and Monte Carlo modelling confirmed it, while refuting the need to kill them – they come back only slowly [1]. My co-author introduced me to Maximum Likelihood methods and the Bayesian Information Criterion for more effective quantitative model selection. I now use these and the related Occam Factor and the Bayes Factor [2,3] in the analysis of high-pressure experimental results. Two case studies are presented. The pressure dependence of III-V semiconductor band-gaps is shown to be correctly fitted not by a polynomial in pressure but by a linear dependence on density [4]. The fitting of Raman spectra of carbon nanotubes under high pressure is being improved by quantitative model selection [4], aiming ultimately at automatic fitting and selection of the best fit.

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Plenary Talk

Will hydrogen-based superconductors come out of the DAC?

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[1]University of The Basque Country, Spain

Over the past decade, the discovery of superconductivity above 200 K in hydrides under megabar pressures—such as H_3S and LaH_{10}—has marked a transformative milestone in condensed matter physics. These findings have firmly established that electron-phonon mediated high-temperature superconductivity is achievable under extreme conditions. However, whether similar mechanisms can yield high critical temperatures (Tc) at ambient or near-ambient pressures remains an open and compelling question.

In this talk, I will explore the prospects of realizing high-Tc superconductivity at ambient pressure, guided by recent predictions based on machine learning techniques [1,2]. I will also present a new family of perovskite-like hydrides [3] that are thermodynamically stable—and thus potentially synthesizable—at moderate pressures around 25 GPa. Remarkably, these compounds remain metastable upon decompression to ambient pressure and exhibit superconducting transitions near 100 K, driven by the stabilizing influence of quantum anharmonic effects. These results open promising avenues for the design and synthesis of high-Tc superconductors operable at or near ambient conditions.

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Molecular orbital theory for bonding in high-pressure boron and hydrogen clusters

Harry Morgan[1,2], and Anastassia Alexandrova[2]
[1]University of Manchester, UK [2]UCLA, USA

Pressure is a fascinating tool for studying multicentre covalent bonding interactions in ionic materials. Under ambient conditions, a successful approach to the bonding in cluster-based materials, such as MB6 hexaborides with their octahedral [B6]2- anions, is to use analogies to molecular clusters, in that case [B6H6]2-. Materials under pressure often form clusters entirely unknown in gas-phase chemistry as atoms aggregate to reduce volume; we might therefore assume that gas-phase bonding theories are not applicable to these clusters. However, in this talk I will show that in fact gas-phase MO theory correctly predicts structural trends at 150 GPa. I will illustrate the approach with two case studies, one on the superhydrides LaH10 and EuH9, and one on the hexaborides MB6 (M = Ca, Sr, Ba). Simple electron counting models supported by density functional theory calculations can simplify the interpretation of complex structural trends through properties including atomic charges, pairwise bond strengths, and σ and π bonds. In the hydrides we have demystified the elegant, symmetrical hydrogen sublattices by identifying the ionic and covalent interactions that underpin them.[1] In the hexaborides we have shown that the B24 oligomers and even B6n polymers formed under pressure nonetheless obey the Wade-Mingos rules for borane cluster bonding, and that a deviation from those rules in BaB6 can be explained by metal-assisted B-B π bonding.[2]

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(Invited) Pressure-Induced Multicenter Bonding in $CsIO_3$: A New Perspective on Main-group Perovskite Formation Mechanism

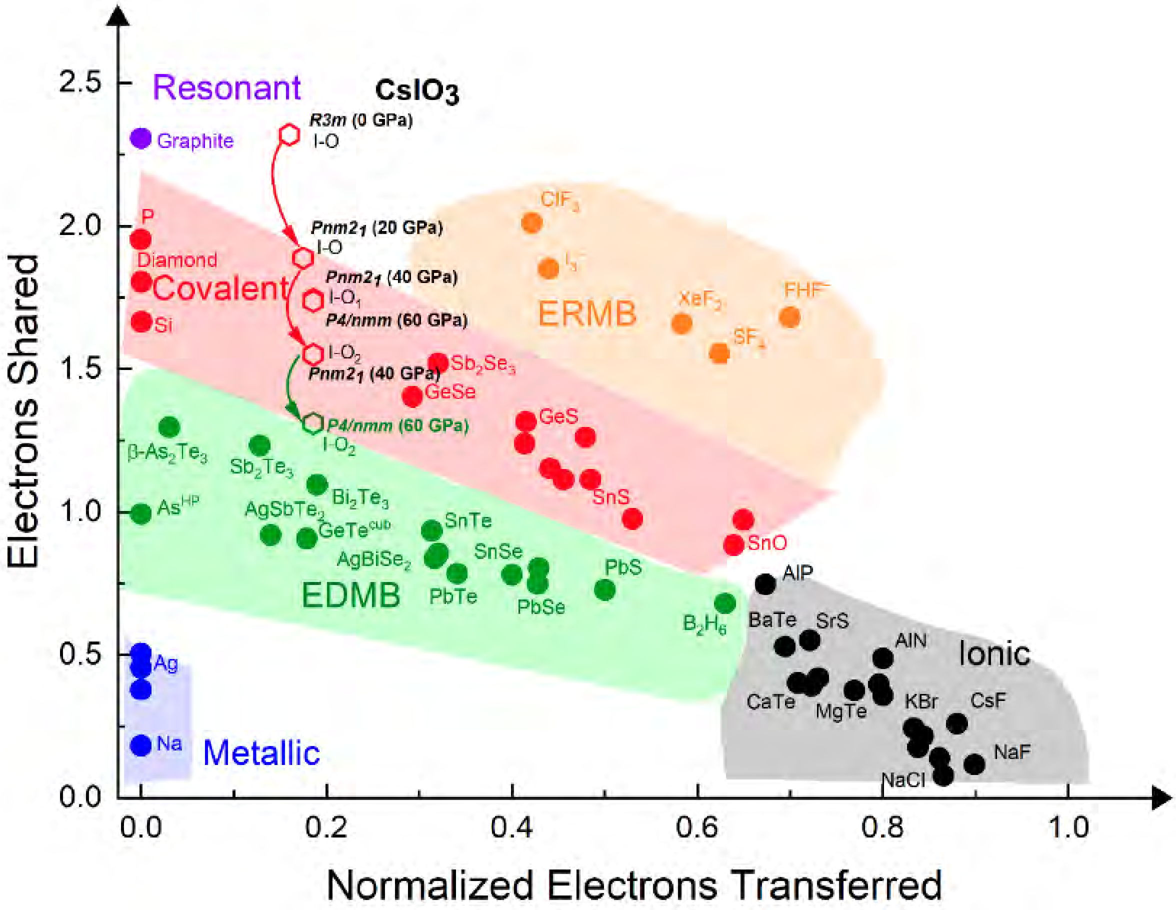
Hussien H. Osman[1,2,3], Jose Luis Rodrigo-Ramón[2], Shafi Ullah[1], Enrico Bandiello[1], Daniel Errandonea[2], Óscar Gomis[1], Tania García-Sánchez[1], Pablo Botella[2], Robert Oliva[4], Plácida Rodríguez-Hernández[5], Alfonso Muñoz[5], Catalin Popescu[6], Frederico Alabarse[7], and **Francisco Javier Manjón**[1]
[1]Universitat Politecnica De Valencia, Spain, [2]Universitat de València, Spain, [3]Helwan University, Egipt, [4]Geosciences Barcelona (GEO3BCN), Spain, [5]Universidad de La Laguna, Spain, [6]ALBA-CELLS, Spain, [7]Elettra Sincrotrone Trieste, Italy

Perovskites of the ABX_3 and BX_3 types are pivotal materials in solid-state chemistry due to their broad range of physical properties and technological applications. However, despite extensive studies, the true nature of the B–X bonding framework—critical to the structural stability and functional properties of these materials—remains debated.

In this work, we explore the pressure-induced evolution of chemical bonding in cesium iodate ($CsIO_3$), combining theoretical simulations with recent experimental insights. We reveal that the

$[IO_3]^-$ polyanions undergo a progressive pressure-induced polymerization process (PPP) along three dimensions, ultimately leading to a tetragonal perovskite phase characterized by [IO5+1] structural units above 50 GPa. Crucially, this transformation marks a shift from conventional resonant delocalized I–O bonding in IO_3 units at room pressure to the emergence of electron-deficient multicenter bonds (EDMBs) in [IO5+1] units above 50 GPa.

The implications of our results extend beyond $CsIO_3$: our findings suggest that the stabilization of perovskite structures in BX_3 and ABX_3 compounds under pressure, such as AIO3 (A= K, Rb, Cs, Tl, NH4+), is driven by 3D polymerization of BX3 units and the formation of EDMBs in BX6 octahedra. This new bonding model provides a consistent framework for understanding phase transitions and bonding anomalies in perovskites with main-group elements. These insights enrich the fundamental understanding of chemical bonding under pressure and open new paths for designing functional materials based on multicenter interaction principles.



Machine learned interatomic potential study of NH_3-H_2O-CH_4 mixture under extreme pressures and temperatures

Gracie Chaney[1], Thomas T. Thevenet[1], Arthur France-Lanord[1], and Flavio Siro-Brigiano[1]
[1]Sorbonne University, Villejuif, France

It is believed that the interiors of icy giants, such as Uranus and Neptune, are composed of a mixture of water, methane, and ammonia subjected to extreme temperatures and pressures. Laser-shock and Diamond Anvil Cell experiments on these mixtures have found evidence of nanodiamonds and ionized water under such extreme conditions.[1,2] However, the specific chemical reactions underlying these formation of hydrocarbons and nanodiamonds in ionized water are still unknown.

Previous computational work used machine-learned interatomic potentials (MLIPs), trained on ab initio data, to predict the reaction mechanisms leading to nanodiamond formation from water–methane mixtures.[3] These simulations showed that, under high-temperature and high-pressure conditions, water transforms into a superacid that induces methane protonation and catalyzes hydrocarbon formation toward nanodiamond synthesis.

In this work, I will present our results that build upon the previous study, using MLIPs to predict the reactions in water–methane–ammonia mixtures with varying ammonia concentrations at 3000 K and under high pressures. We particularly focus on the effect of ammonia on the superacid character of the mixture and on the degree of ionization of water. This is done by characterizing the free energy of proton transfer from ammonia to CH_4 and water, directly from unbiased DFT-MD simulations.

We observe an interesting effect of ammonia in the mixture: it is able to "sequester" protons from water, thereby reducing iwater acidity by lowering the population of H_3O^+ ions. Despite this behavior, our results indicate that the superacid character of water persists even in the presence of ammonia.

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Session 9b: Theoretical and computational methods

(Invited) Elastic constants with anharmonic corrections using quasiparticle theory

Ernesto J Blancas[1], and Alberto Otero-de-la-Roza[1]
[1]University Of Oviedo, Spain

The prediction of elastic constants (Cij) of materials under extreme conditions of pressure and temperature is important for developing the geochemical and geophysical models of planetary interiors. The experimental determination of Cij under these conditions is highly challenging, as strain needs to be coupled with extreme conditions of pressure and temperature. Due to that, the computational prediction of Cij is essential. In the past, density-functional theory (DFT), ab initio molecular dynamics (AIMD) and the quasiharmonic approximation have been used to compute Cij at arbitrary pressure and temperature. However, at high temperatures, QHA results can become unphysical, while AIMD is typically more complex to use and computationally expensive. In this work, we explore the use of the recently implemented quasiparticle approximation (QP) [1], proposed by Allen[2], to calculate thermodynamic properties at high temperature. In the QP approach, nth order force constants are used to derive volume- and temperature-dependent entropies, which are fitted with a Debye-like model to generate the rest of the thermodynamic properties. In this talk, we present the extension of the QP framework to the calculation of Cij at no additional cost, leveraging the Born-Huang connection between interatomic force constants and Cij [3]. In particular, the phonon frequencies are used to calculate sound velocities (via the Christoffel equation) from which Cijs are obtained by solving an inverse problem [4]. The different methods for obtaining Cij are evaluated in simple and geologically relevant systems.

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Formation of new hydro-carbonitrides under pressure: kinetics versus thermodynamics

Andreas Hermann[1], Ross Howie[1], Dominique Laniel[1], and Miriam Peña Alvarez[1]
[1]The University of Edinburgh, UK

For technological applications, materials synthesised under high-pressure (and high-temperature) conditions must be recoverable to ambient. Compounds that are expected to form covalently bonded high-pressure phases are promising in this regard, hence the continued search for polymeric nitrogen allotropes, or studies of diamond formation from molecular precursors.

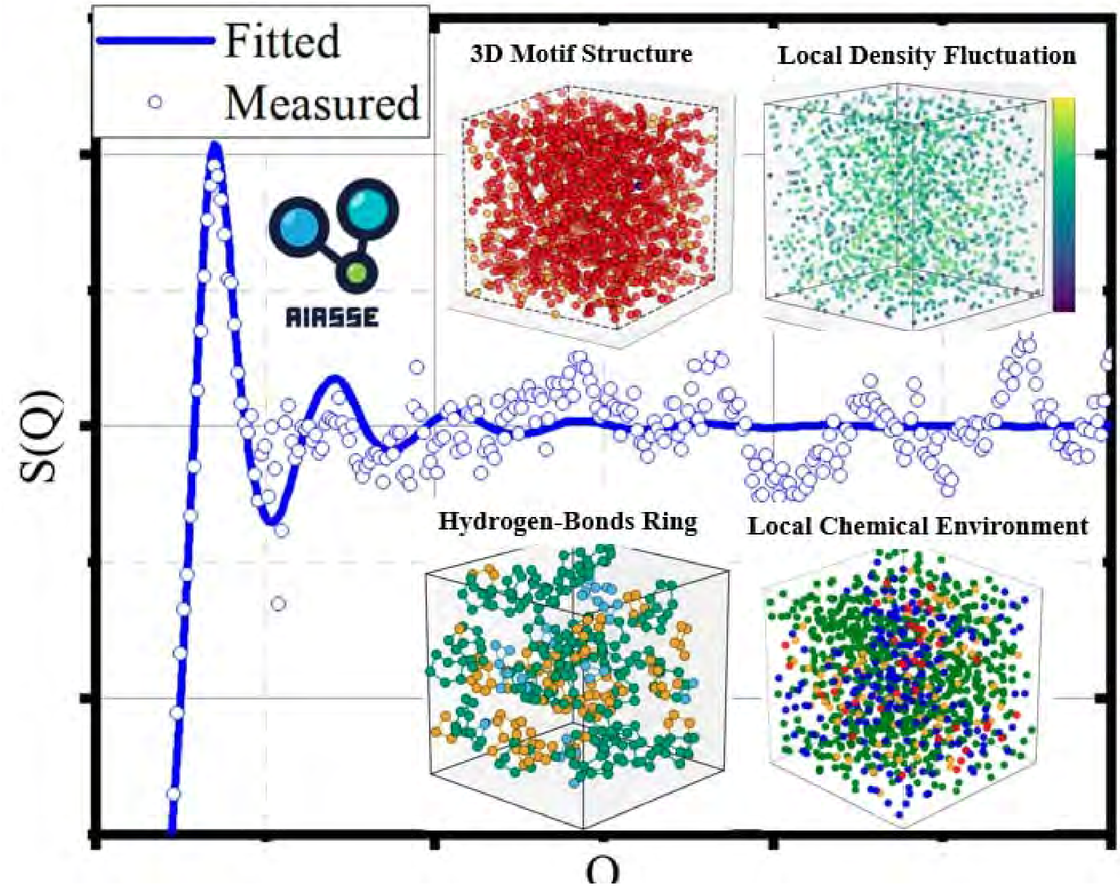
Here, we present an overview of our recent work on H-C-N hydro-carbonitrides. These include initially purely computational studies of the CH_4-N_2 and H-C-N-O phase spaces, which predicted various high-energy density and polymeric compounds. Subsequently, our computations accompanied experimental studies to help explain the formation of a series of van der Waals compounds; oligomerisation; and network structure formation following laser heating of the samples.

Density functional theory based total energy calculations and molecular dynamics simulations are used to establish phase relations and (meta)stability of compounds, and utilise diffraction and spectroscopy data to determine compositions and crystal structures.

AIASSE - Ab Initio Augmented Structure Solving Engine: A Hybrid Approach to Atomic and Electronic Structure Characterization of Disordered Materials

Ayobami D. Daramola[1], Cipirian G. Pruteanu[1], and Graeme J. Ackland[1]
[1]Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, UK

We present a hybrid computational methodology that self-consistently integrates empirical potential–based Reverse Monte Carlo (EPSR) refinement of neutron and X-ray total scattering data with ab initio molecular dynamics simulations rooted in Density Functional Theory (DFT). This approach bridges experimental observations with first-principles theory, offering a coherent multiscale view of disordered materials—from large-scale bulk structural correlations to atomic-scale dynamics and electronic properties. Implemented in a unified software framework, our method enables direct, on-the-fly feedback between experimental refinement and quantum mechanical calculations. We validate this approach through case studies on dense fluid krypton, amorphous SiO_2 glass, low-density amorphous ice, and water–methanol mixtures, illustrating its ability to uncover structure–property relationships and emergent phenomena in complex systems.



Powder-Diffraction-Based Structural Comparison for Crystal Structure Prediction Under Pressure

Alberto Otero De La Roza[1]
[1]University of Oviedo, Spain

Crystal structure prediction (CSP) is a computational method for the prediction of the thermodynamical stable phase (or the energy landscape) from the stoichiometry or the molecular diagram of a compound. CSP is a hard problem because it involves a global search over the space of all possible structures, and it is computationally very demanding. It would be beneficial to be able to use experimental information, such as powder X-ray diffraction (XRPD) patterns, to inform and speed up the CSP search for the stable structure. This is particularly important in the field of high-pressure experimental X-ray diffraction experiments, where the powder data available is generally not of enough quality to allow the unequivocal determination of high-pressure crystal structures. To assist CSP, it is necessary to compare calculated structures with experimental patterns but, for achieving this, two problems need to be solved: i) lack of vibrational effects (and errors from the DFT method) may cause deformations in the unit cell relative to experiment, shifting peak positions, and ii) experimental patterns have peak shapes and widths that are directly not calculable from the structure. In this work, we present a crystal similarity index (VCGPWDF) for comparing structures with experimental patterns that allows for lattice deformations of the former [1]. VCGPWDF is simple, efficient, fully automatic, and does not require indexing of the pattern. It gives meaningful results even if the experimental pattern is of very low quality. The development of VCGPWDF opens the door for XRPD-assisted CSP searches aimed at the solution of structures under high pressure.

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P1: Dispersion of the KCl refractive index at high pressure

Reece O'Beirne, and John Proctor
[1]Materials & Physics research group, University of Salford, UK

Using the combination of white light transmission spectroscopy and confocal laser microscopy[1], we have measured the dispersion of the KCl refractive index in the visible, near-IR, and near-UV regions up to 7 GPa. To verify the accuracy of our experimental measurements, we also determine the PV EOS. Our volume measurements agree with the known EOS[2] within error, demonstrating that our all-optical method can now determine the volumes for a PV EOS to ± 1.6%. To measure the dispersion, we found it essential to automate most of the data analysis using Python. We also present our methodology and code for this automated data analysis.

[1] J.E. Proctor et al., Physics of Fluids 36, 087145 (2024).
[2] A. Dewaele et al., Phys. Rev. B 85, 214105 (2012).

P3. High-Pressure Phase Evolution of Bi–Ga Alloys Driven by Polymorphism, Anomalous Melting, and Liquid Miscibility Gap

Shir Ben Shalom[1], Moran Emuna[2], Yaron Greenberg[2], Eyal Yahel[2], and Guy Makov[1]
[1]Ben Gurion University of The Negev, Israel, [2]Nuclear Research Centre Negev, Israel

The high-pressure states of the elements can significantly impact the phase diagrams of their alloys due to polymorphism in the solid state and anomalies and slope changes in the melting curve. Here, we investigate the effect of these characteristics on a model system, the monotectic Bi-Ga system, in which both Ga and Bi have anomalous melting curves and several solid phases. We constructed a thermodynamic model for the high-pressure phase diagrams of the Bi-Ga binary system up to 10 GPa. Our results reveal a strong correlation between the high-pressure phase diagrams of elemental Bi and Ga, which display solid phase transitions and anomalous melting curves, and the shape of the Bi–Ga alloy phase diagram. In addition, at higher pressures, the liquid miscibility gap in this system disappears, and the phase diagram changes from a monotectic to a eutectic type at a pressure of 8 GPa. Electrical resistance measurements in a Paris-Edinburgh press under high pressure and temperature conditions were used to identify the phase lines experimentally. Very good agreement was found between the measured transitions and the calculated phase diagram up to 6 GPa. For example, the anomalous behavior of the monotectic temperature and the liquidus line was calculated and validated experimentally.

This study presents a combined computational and experimental investigation that comprehensively characterizes the pressure-dependent Bi–Ga phase diagram up to 6 GPa and proposes its extension to 10 GPa. The high-pressure behavior of the pure elements plays a critical role in understanding the complex phase relations in their alloy system. Additionally, the work highlights the effectiveness of thermodynamic modeling in interpreting experimental data for binary systems, where acquiring complete datasets often demands considerable effort.

P5. Melting curve of Phosphorus: Evidence for a solid-liquid-liquid triple point

Hermann Muhammad[2], Mohamed Mezouar[2], Gaston Garbarino[2], Laura Henry[3], Tomasz Poreba[2], Max Gérin[2], Matteo Ceppatelli[4,5], Manuel Serrano-Ruiz[5], Maurizio Peruzzini[5], and **Frédéric Datchi**[1]

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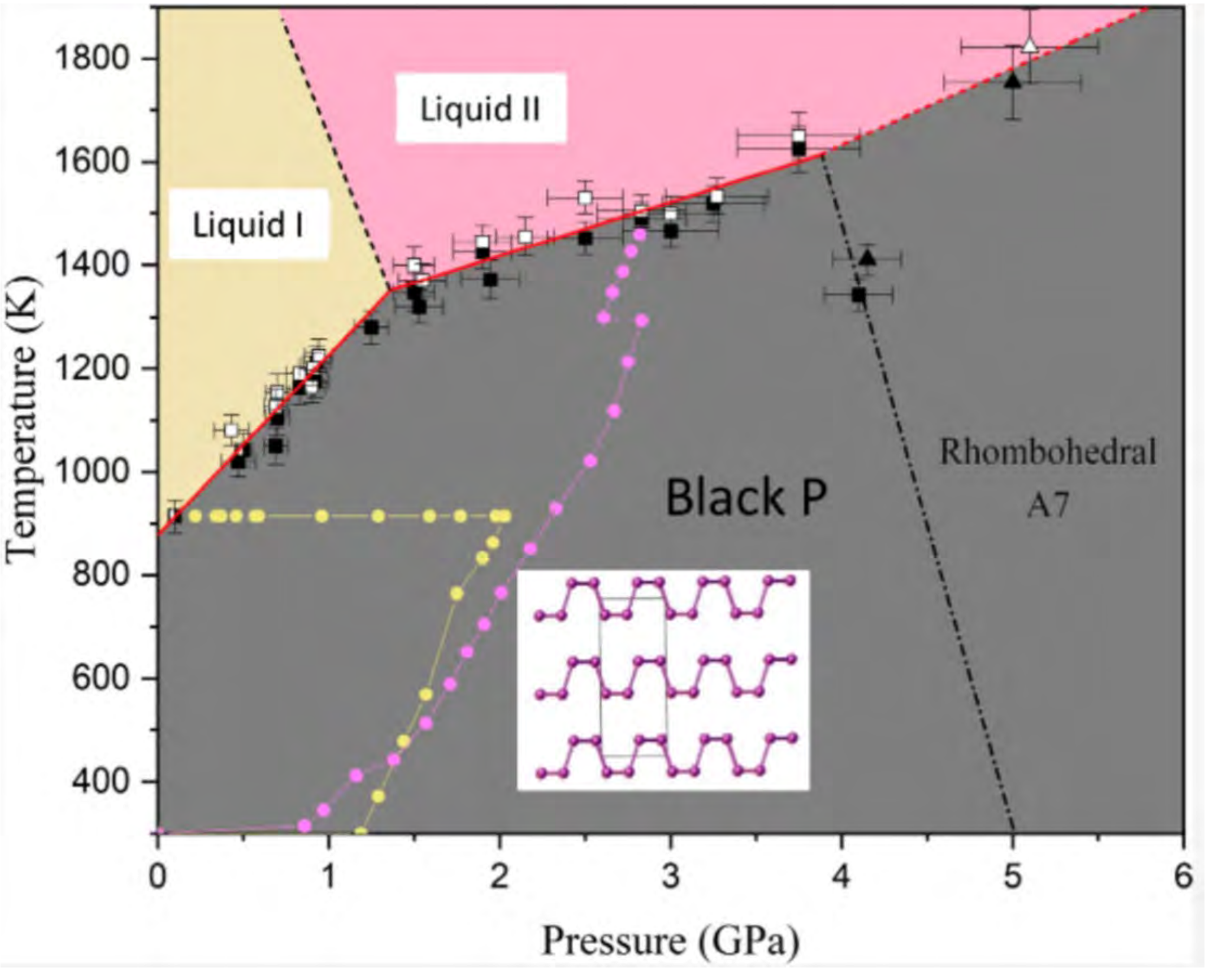
Black phosphorus (bP) is a crystalline material that can be seen as an ordered stacking of two-dimensional layers, which results in outstanding anisotropic physical properties. The knowledge of its pressure (P)-temperature (T) phase diagram, and in particular, of its melting curve is fundamental for a better understanding of the synthesis and stability conditions of this element. Despite the numerous studies devoted to this subject, significant uncertainties remain regarding the determination of the position and slope of its melting curve. Here we measured the melting curve of bP in an extended P, T region from 0.10(3) to 5.05(40) GPa and 914(25) to 1788(70) K, using in situ high-pressure and high-temperature synchrotron X-ray diffraction [1]. We employed an original metrology based on the anisotropic thermoelastic properties of bP to accurately determine P and T. We observed a monotonic increase of the melting temperature with pressure and the existences of two distinct linear regimes below and above 1.35(15) GPa, with respective slopes of 348 ± 21 K/GPa and of 105 ± 12 K/GPa. These correspond to the melting of bP towards the low-density liquid and the high-density liquid, respectively. The triple point at which solid bP and the two liquids meet is located at 1.35(15) GPa and 1350(25) K. In addition, we have characterized the solid phases after crystallization of the two liquids and found that, while the high-density liquid transforms back to solid bP, the low-density liquid crystallizes into a more complex, partly crystalline and partly amorphous solid. The X-ray diffraction pattern of the crystalline component could be indexed as a mixture of red and violet P.



[1] H. Muhammad et al, J. Phys. Chem. Lett. 2024, 15, 8402–8409

P7. Heat capacity and other thermodynamic properties of hcp-CrH

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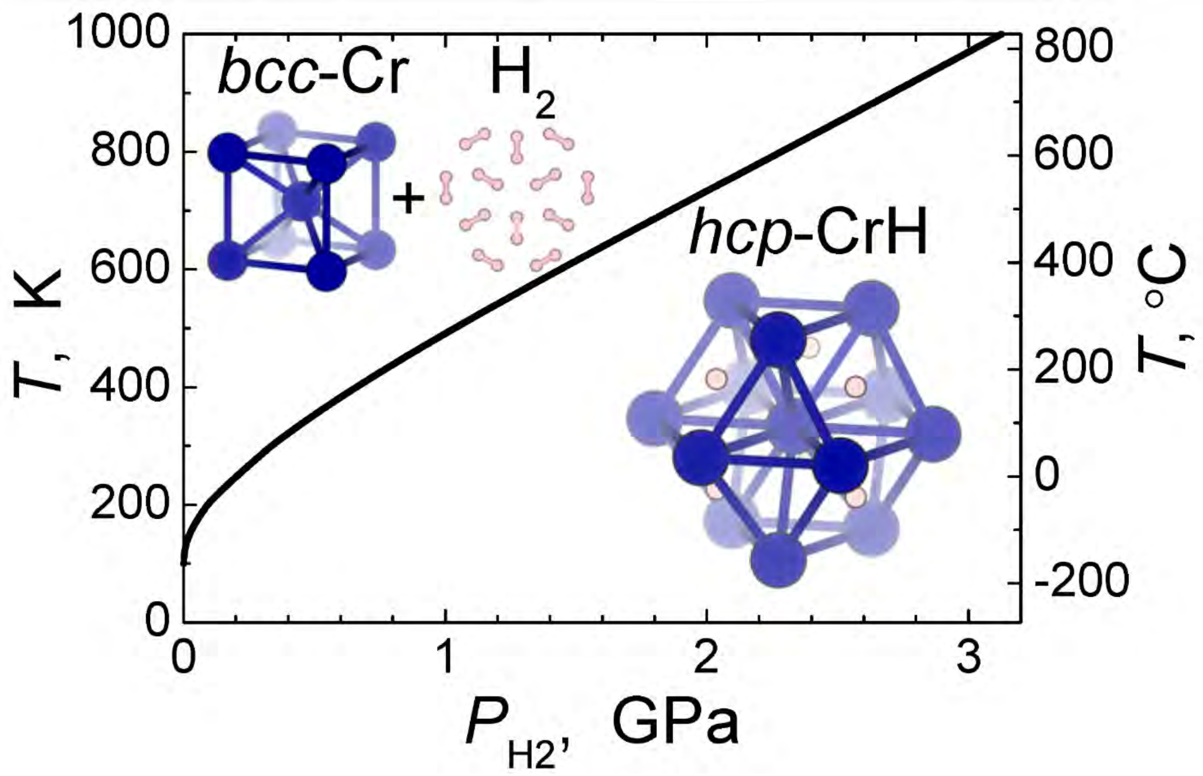
Polycrystalline samples of chromium hydride CrH with a hexagonal close-packed (hcp) metal lattice were synthesized at a hydrogen pressure of 7.4 GPa and a temperature of 873 K, rapidly cooled to 100 K, recovered to ambient pressure and studied by differential scanning calorimetry at temperatures from 120 to 220 K [1]. The calorimetric study and density functional theory calculations helped to determine the isobaric heat capacity C_P of hcp-CrH at temperatures up to 1000 K and to clarify the shape and position of its acoustic phonon band and the coefficient of electronic heat capacity. Using the obtained C_P(T) dependence of hcp-CrH for the calculation of its Gibbs energy gave the line of the Cr + (1/2)H_2 = CrH equilibrium in the P-T diagram of the Cr–H system. The position of this line corroborated the debatable opinion that the pressure of thermodynamic equilibrium is much closer to the pressure of hydride decomposition than to the pressure of its formation.



The work was funded by the Russian Science Foundation under project no. 23-22-00361 and by the Horizon 2020 program of the European Union (Grant no. 948895, MetElOne).

[1] M.A. Kuzovnikov et al, Int. J. Hydrogen Energy 116 (2025) 507–515

Investigating the Stability of High Entropy Sulphides at High Pressures: Delineation of Solid-State Phase Transformations

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High entropy (HE) materials are synthetic materials comprised of five or more elements in a lattice of a single crystalline phase that is stabilized by entropy rather than enthalpy and show promise of significant industrial and societal importance. In particular, HE sulphides can be chemically tailored to improve performance of energy storage, electrocatalysis, and thermoelectric energy conversion materials. Assessing the stability of HE materials has largely focussed on the effect of temperature and understanding the effect of pressure on stability is required to complete the assessment. To date, only one study has investigated a single HE sulphide at high pressures. This work expands on this sole study by investigating additional HE sulphides at high pressure, (Mn,Fe,Cu,Zn,Ag,Cd,Ga,In,Sn)S and (Mn,Fe,Zn,Cd,Ga,In)S, alongside medium and low entropy sulphides – (Mn,Fe,Zn,Cd)S and (Zn,Cd)S, respectively. All sulphide samples were synthesised using a solventless thermolysis, single source precursor approach and characterised using powder X-ray diffraction post-synthesis. Samples were loaded into a diamond anvil cell with helium as a pressure medium. In-situ X-ray diffraction of the sulphides at ambient temperature and pressures up to 20 GPa was conducted at the I15 – Extreme Conditions beamline at the Diamond Light Source. The results indicate a clear solid-state transformation from a wurtzite (P63mc) to sodium chloride ($Fm\bar{3}m$) structure, where lattice distortion is most evident in the nine-metal cation HE sulphides. The phase transformations occurred within a pressure range of ~7-11 GPa and the sodium chloride structure was retained after decompressing to ambient pressure.

P11. The pressure response of the K2[Ru(bipy)(CN)4]·3H2O coordination polymer studied by Raman and photoluminescence spectroscopy

Olga Karabinaki[1], Konstantina Siapaka[2], Dimitra Kouskouki[3], Theodore Lazarides[3], Keizo Murata[4], John Arvanitidis[2], and Dimitrios Christofilos[1]
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Coordination polymers (CPs) are hybrid crystalline materials, in which organic ligands connect to metal ions or clusters to produce extended coordination networks, with varied structures and strong luminescence signal [1,2]. Among them, $K_2[Ru(bipy)(CN)_4]\cdot 3H_2O$ (bipy: bipyridine) features the $[Ru(bipy)(CN)_4]$ anion (-2), which is strongly solvatochromic, with its absorption and emission spectra being tunable over a wide range in different solvents [3]. In this work, we examine the pressure response of the crystal (triclinic P-1 space group, Z=2 [3]) by means of Raman and photoluminescence (PL) spectroscopy. Daphne 7676 oil, solidifying at ≃5 GPa at room temperature, is used as pressure transmitting medium.

Because of the complexity of the studied system, its Raman spectrum is rich, and it can be divided into different spectral regions, depending on the moieties involved in the vibrational modes [4]. On the other hand, the strong PL signal in the 1.5-2.5 eV region is composed of various components that originate from the transitions between the ^{3}MLCT (Metal-to-Ligand Charge Transfer) excited state and the vibrational levels of the ground state [5]. With increasing pressure, the majority of the Raman peaks shift to higher frequencies, reflecting the bond hardening upon volume contraction. In the pressure range 1.3-1.9 GPa, new Raman peaks appear in the spectrum, discriminated against the initial peaks due to different pressure coefficients of their frequencies. Additionally, for pressures higher than 4.5 GPa more significant changes in the pressure evolution of the Raman spectrum occur, regarding the number of the Raman peaks, their frequencies and pressure coefficients. All these changes are reversible upon pressure release and suggest the occurrence of structural transitions of the studied system. The structural transitions also affect -though to a lesser extent- the pressure evolution of the PL spectrum and particularly the profile of its high energy side.

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P13. Structural- and valence-state changes in EuT2X2

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Among the characteristics of materials containing the element europium is their magnetic state. This state depends on the valence configuration of europium, which can change due to several factors from the symmetry of the crystal structure to changes in interatomic distances. It is the distance between Eu atoms that is a significant factor for the resulting type of magnetic arrangement and is also a factor for the formation of the magnetic moment itself. As has been empirically shown several times, the valence state of europium is linked to the effective atomic size of europium. By reducing the volume of the crystallographic elementary unit cell, one may influence the valence of Eu. Studying structural changes is therefore an effective method to describe changes in the valence state of europium.

EuRu2Ge2 and EuRu2P2 are ferromagnetic intermetallics. When high pressure is applied, we could observe a change in compressibility around 8 GPa for EuRu2Ge2, which is probably related to the different elasticity in different pressure intervals. In the case of EuRu2P2, there are even two pressure points signifying change of elasticity of the crystal lattice. In case of relation to the valence state of the 4f electron shell, this would represent a step-like development of the europium valence in this compound. Although direct evidence of the valence state of europium can only be provided by a microscopic experiment like e.g. absorption spectroscopy (to be perfofrmed), the development of crystallographic parameters provides significant information about the electron states in the valence shell. The results of the study of the crystallographic parameters of these two ferromagnetic compounds under pressure will be the subject of a conference contribution.

P15. Clathrate-like CeB12 with Superior Hardness

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Metal borides, as potential new superhard materials with excellent electrical conductivity, have received extensive attention due to their robust three-dimensional covalent bond framework and diverse topological geometries. Based on first principles calculation, we use CALYPSO software to predict the structure of Ce-B compounds in the pressure range of 0-100 GPa. Three structures Pmmm CeB_4, $Pm\bar{3}m$ CeB_6, $Fm\bar{3}m$ CeB_{12} exhibit good kinetic and thermal stability under environmental pressure. Among them, the boron-richest compound $Fm\bar{3}m$ CeB_{12} has a high density of B-B covalent sublattice, and thus exhibits a high Vickers hardness of 38.9 GPa, which is comparable to the standard of superhard materials (40GPa). By analyzing the bonding properties and electronic structure of CeB_{12}, it is found that the B-B covalent sublattice network leads to the metallic behavior of CeB_{12}, and the B-B interaction dominates the structural stability. This study will enrich innovative research in the theoretical design of novel superhard compounds with good electrical conductivity.

P17. Comparing DFT calculated P-V equation of states of high-pressure hydrides to experimental XRD results

Milo Dixon[1]
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Recent theoretical studies suggest that certain ternary hydrides, particularly those containing alkali or alkaline earth elements along with transition metals, may exhibit high-Tc superconductivity at pressures below 100 GPa. Remarkably, Mg_2IrH_6 has been proposed as a potential high-Tc superconductor at 1 atm by several independent groups, with predicted Tc values ranging from 65 to 170 K . Theoretical calculations suggested that this phase could be synthesised by the extraction of interstitial hydrogen from the believed stable (above 15 GPa) Mg_2IrH_7. Following this, experimental studies have synthesised a hydrogen-deficient, insulating phase of Mg_2IrH_5 up to 28 GPa and it has been proposed that this phase could act as a precursor for the synthesis of the superconducting phase via the addition of interstitial hydrogen.

A problem, however, arises in distinguishing between different hydrogen stoichiometries in this system due to all structures sharing very similar lattice symmetries. Additionally, hydrogen is essentially invisible to XRD techniques when bonded to significantly heavier elements.

It is generally considered that additional substitution of hydrogen into a crystal lattice will increase the crystallographic volume. While this volume change can be measured using XRD, the precise amount by which one-part hydrogen contributes to the volume is not well understood and strongly depends on the specific system. Therefore, theoretical DFT calculations may be used to help predict the crystal volume and so extract the stoichiometry.

In this poster, I shall compare DFT calculated P-V EOS for MgH_2, IrH_3 and the Mg_2IrHx system to experimental results to indicate the reliability of theoretical predictions.

P19. Novel Chromium Silicides $MoSi_2$-type $CrSi_2$ and $PdGa_5$-type $CrSi_5$ Synthesized under High-Pressure

Takuya Sasaki[1], Koichi Takano[1], Takumi Kitahara[1], Nico Alexander Gaida[1], and Ken Niwa[1], Masashi Hasegawa[1]
[1]Department of Materials Physics, Nagoya University, Japan

Two novel chromium silicides, MoSi2-type CrSi2 and PdGa5-type CrSi5, were successfully synthesized under high-pressure conditions. These phases were synthesized at pressures higher than those for the high-pressure synthesis of Si Zintl phases and clathrate compounds. MoSi2-type CrSi2 crystallized in the tetragonal structure with a space group of I4/mmm and lattice parameters of a = 3.09422(2) Å and c = 7.54051(5) Å. PdGa5-type CrSi5 crystallized in the tetragonal structure with a space group of I4/mcm and lattice parameters of a = 5.99998(8) Å and c = 9.2363(2) Å. The enthalpy difference calculated by DFT indicates that CrSi5 becomes stable under high pressure. PdGa5-type CrSi5 is richer in Si than not only the Cr-Si system but also any other transition-metal silicides reported so far. This is comparable to the composition ratio of clathrate compounds. The Si-Si bonds in CrSi5 are covalently linked, forming an intriguing tunnel-like network. Si-rich transition metal silicides have the potential to become the third unique crystal structure group after Zintl phases and clathrate compounds.

P21. Phase transitions in ferroelectric van der Waals crystals under pressure

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[1]School of Physics & Astronomy, University of Nottingham, UK[2]Department of Physics, College of Sciences, Qassim University, Saudi Arabia, [3]Department of Physics, Loughborough University, UK

Van der Waals (vdW) crystals consist of weakly interacting atomically thin layers bound by weak vdW forces. They can be stacked and twisted in different ways to create heterostructures that can exhibit a wide range of different phenomena, including emergent properties such as interfacial ferroelectricity [1]. vdW crystals, such as α-In2Se3, can also be intrinsically ferroelectric. α-In2Se3 is a semiconductor with non-centrosymmetric vdW layers that exhibits both out-of-plane and in-plane ferroelectric polarization at room temperature [2,3]. Furthermore, it is reported to have multi-ferroic order combining ferromagnetism, ferroelectricity, and ferroelasticity [4]. The different polymorphs and polytypes phases of In2Se3 feature distinct structural and ferroelectric properties [5], which are known to be affected by pressure [6].

Here, we report on structural phase transitions in α-In2Se3 due to hydrostatic compression and decompression. We probe the behaviour of the phase transition by in situ Raman spectroscopy and imaging in a high-pressure diamond anvil cell (Figure 1). Mechanical deformations of the crystal lattice and their layer stacks (2H or 3R with hexagonal (P63mc) and rhombohedral (R3m) space group symmetry, respectively) are modelled by density functional theory, revealing a phase transition into the paraelectric β phase of In2Se3. Our investigation reveals that the behaviour of 2H-α-In2Se3 is significantly different to that of 3R-α-In2Se3 [6]. Specifically, the reversibility of the ferroelectric-paraelectric phase transition depends on the sample quality and lattice strain induced by defects and imperfections.

Understanding and controlling the coupling between the electrical and mechanical properties of ferroelectric vdW crystals is crucial for the development of technological applications, spanning from sensors and actuators, to memory and fast switching devices.

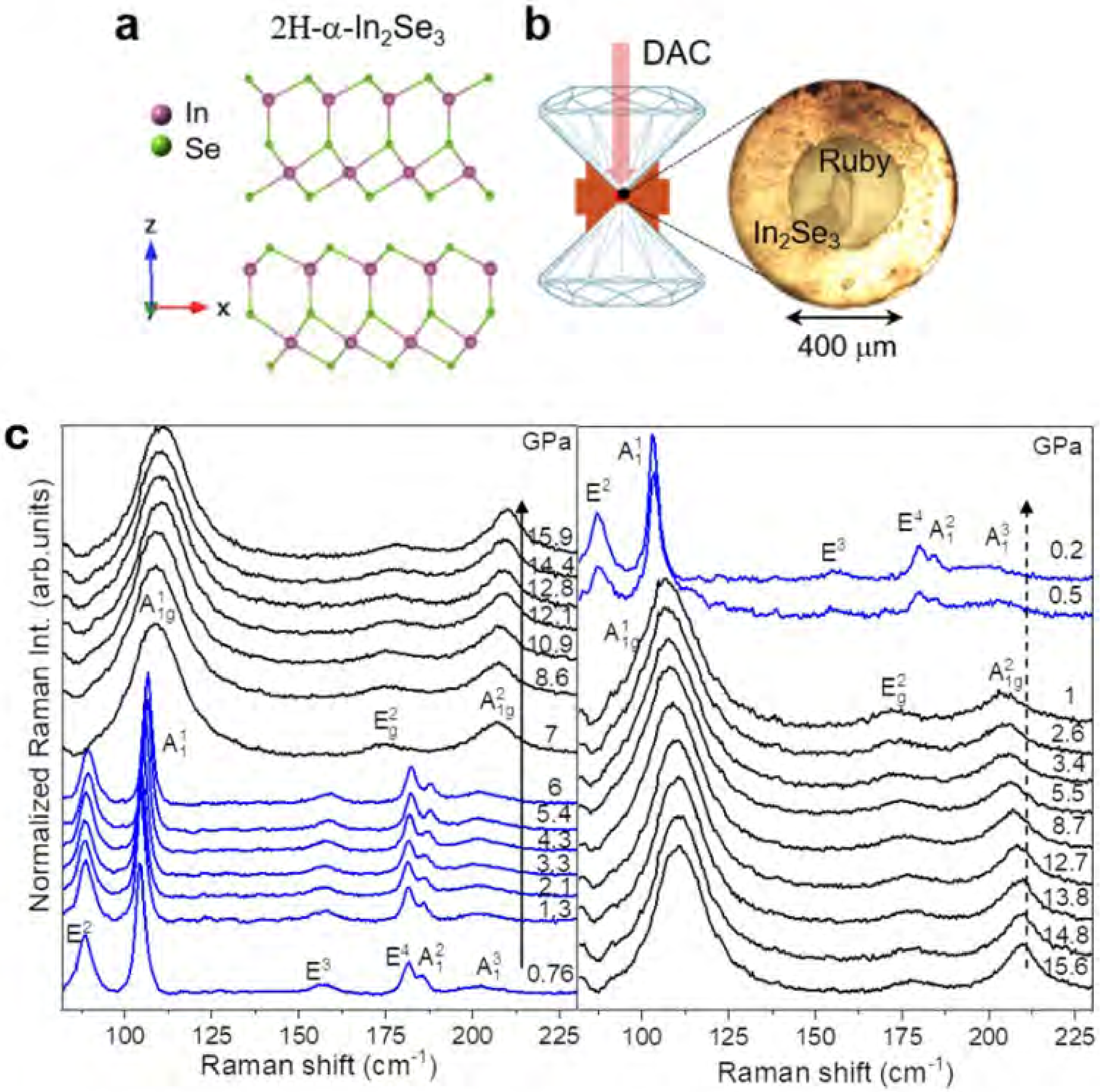

Figure 1: a) crystal structure of 2H-α-In_2Se_3; b) Raman spectroscopy inside a DAC; c) Raman mode evolution under pressure.

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[4] App. Phys. Lett. 118, 072902 (2021)
[5] Nat. Comm. 15, 10481 (2024)
[6] Inorg. Chem. 57, 8241-8252 (2018)

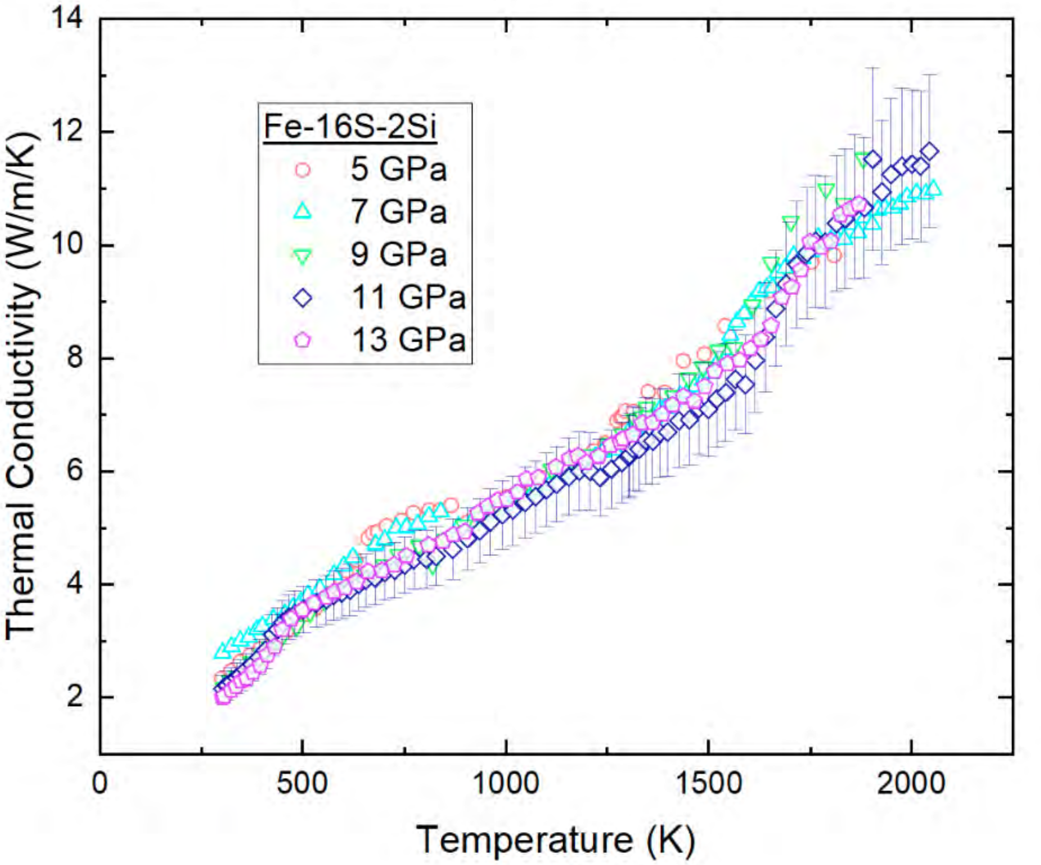
P23. Electrical Resistivity of Liquid Fe-16wt%S-2wt%Si at High Pressures with Implications for Heat Flow in Sub-Earth Exoplanets

Erin Lenhart[1], Wenjun Yong[1], and Rick Secco
[1]University Of Western Ontario, Canada

The heat flow contributing to magnetic field generation at the pressures of terrestrial planetary cores may be constrained using high-pressure experiments. To find thermal convective force in the core, thermal evolution models may be combined with adiabatic heat flow estimates, which require thermal conductivity values, which may in turn be obtained from electrical resistivity measurements. Previous electrical resistivity measurements have been performed at pressures up to 5 GPa on liquid Fe-S alloys at the eutectic composition or higher. This study provides novel measurements up to 13 GPa in the moderate 10-20wt% S compositional range of Fe alloys corresponding to the estimated core compositions of Vesta and Mars along with the maximum miscible amount of Si alloyed into the liquid. This allows for characterization of the adiabatic heat flow in the core of sub-Earth exoplanet TRAPPIST-1h, which likely formed near the frost line of its host star.

Experiments were performed in a 3000 ton multi-anvil press on Fe-16wt%S-2wt%Si powder samples. One thermocouple on each end of the sample completed a 4-wire circuit in situ, allowing voltage drop across the sample as a function of temperature to be measured into the melt at 5-13 GPa. Post-experimental recovered samples were polished to a cross-section for geometry measurement and electron microprobe analysis. Electrical resistivity was then calculated, from which thermal conductivity was estimated according to the Wiedemann-Franz Law.

For pressures of 5-13 GPa, electrical resistivity of 400-500 μΩ·cm was found in the complete melt with no discernible dependence on pressure within the error of measurement. Thermal conductivity values of 5-8 W/m/K were calculated for the region of partial melt prior to complete melting at ~1650 K. Thermal conductivity then increases to 11±0.5 W/m/K at the maximum experimental temperature of 2000K. For TRAPPIST-1h, an adiabatic heat flow at the top of the core is estimated.


Fe-16S-2Si
5 GPa
7 GPa
9 GPa
11 GPa
13 GPa
Thermal Conductivity (W/m/K)
Temperature (K)
14
12
10
8
6
4
2
0
500
1000
1500
2000

P2. New instrumentation at P02.2, PETRA III, DESY employing Soller slits for structural measurements of non-crystalline materials at extreme conditions

Christoph Otzen[1], Giuseppe Cocomazzi[1], Axel Phelipeau[1], Mario Wendt[2], Konstantin Glazyrin[2], and Clemens Prescher[1]
[1]University of Freiburg, Institute of Earth and Environmental Sciences, Germany, [2]German Electron Synchrotron DESY, Germany

Investigating the structures and behavior of materials at extreme pressures is important for the development of novel materials with superior properties such as hardness, superconductivity, energy and hydrogen storage capabilities, etc., and for improving our understanding of the geologic processes in the interior of planets. Using the diamond anvil cell (DAC) and a focused beam of synchrotron X-rays, the structures of crystalline materials can be rigorously studied at extreme pressures. On the contrary, investigating the structures of non-crystalline materials through measurements of the diffuse X-ray scattering is very challenging at high pressures in the DAC. The reason is that the diamond anvils cause an intense Compton scattering background, which is difficult to distinguish from the diffuse scattering of non-crystalline samples. However, this problem can be overcome efficiently by employing Soller slits, also known as multi-channel collimator, which can block the background signal originating from the diamond anvils and thus increase the signal to background ratio.

In this work, we present our new experimental setup at the Extreme Conditions Beamline P02.2 at the 3rd generation light source PETRA III, DESY, Hamburg, where we employ Soller slits to enable structural investigations of non-crystalline materials at extreme pressures in the DAC. The efficient performance of the setup and the high quality of collected scattering images is demonstrated by means of different glass samples. Thereby, our silicate glass samples can serve as analogue materials for high-pressure melts relevant for understanding the interior dynamics of the Earth or other planets. The new setup enhances the research capabilities at P02.2 and aims at promoting research on non-crystalline materials at high pressures.

P4. Softening of fcc and hcp metals at high homologous temperatures contribute to effective elastic softening in the inner-core

Tara R McElhinney[1], A. M. Walker[2], M. G. Pamato[3], O. T. Lord[4], I. S. Izad[5], and S. A. Hunt[1]
[1]University of Manchester, UK, [2]University of Oxford, UK [3]University of Padova, Italy [4]University of Bristol, UK, [5]University of Western Australia, Australia

A major challenge in understanding the composition and structure of the Earth's inner-core is the absence of experimental data on metals and alloys close to the liquidus. Here we address this by performing high-pressure experiments on hexagonal close-packed zinc and face-centred cubic copper up to melting, as analogues of iron. Samples together with an elastic reference, were heated through to the liquidus while simultaneously being subject to cyclic deformation at strains of 10-4 - 10-5 and frequencies of 0.1-0.3Hz. Experiments were performed in a D-DIA at 3-4 GPa. The change in length of the samples, characterised throughout the experiment by X-radiographs, were used to calculate the Eω (finite-frequency Young's modulus). Although the stress amplitude is approximately constant, above homologous temperatures of ~0.85, both samples exhibit significant softening. This softening is attributed to changes in strain accommodation mechanisms at high temperatures. The effective softening reported here suggests the inner-core may be readily deformable, and could in part explain low seismic velocities.

P6. Bonding changes in solid nitrogen under high pressure and temperature

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Nitrogen has a complex phase diagram with 15 detected solid molecular phases [1]. Understanding nitrogen's complex phase transitions under extreme conditions provides crucial insights into fundamental molecular interactions mechanisms and potential pathways for synthesizing novel high-energy-density materials with applications ranging from energy storage to planetary science.

In this study, we tracked the electronic and structural changes of nitrogen under high pressure and temperature using a novel combined setup for X-ray Raman scattering and X-ray diffraction at beamline ID20 at the ESRF, exploiting the diamond anvil cell method and further characterized the phase state of nitrogen by optical Raman spectroscopy. We employed a resistively heated diamond anvil cell to reach temperature and pressure up to 600 K at 88 GPa with the aim to investigate the θ-phase.

In the pressure regime between ambient conditions and 80 GPa, we studied the nitrogen K-edge X-ray Raman scattering spectra in the liquid phase and the solid δ-, δ*-, ϵ- and the ζ-phase. The heated sample showed a mixture of the ζ- and θ-phase.

The measurements exhibit significant changes in the nitrogen's bonding structure, indicated by corresponding variation of the π*, σ* and continuum spectral features. These changes are interpreted via calculated spectra based on ab initio molecular dynamic simulations, which reproduce observed spectral changes and reveal a hindrance of free rotations of the N2 molecules in the ϵ-phase.

This work is supported by the BMBF via the projects 05K22PE2 and 05K22OF1.

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P8. Phase Transitions of Solid and Liquid Fe-Si Alloys with Applications to Planetary Core Composition and Dynamo Processes

Ben Kalman[1], Wenjun Yong[1], and Richard A Secco[1]
[1]University Of Western Ontario, Canada

It is widely accepted that the convection of the liquid metallic outer core is the driver of the dynamo-produced magnetic field in terrestrial bodies, yet the core composition and the processes which occur within the core are difficult to study due to the extreme temperatures (T) and pressures (P). By examining the phase changes that occur with varying P, T, and composition (X), phase diagrams may be constructed for expected core mimetic compositions. The constructed phase diagrams of Fe-Si alloys along with known or modeled P,T conditions of solid/liquid phases within the cores of interest can then be used to determine likely compositions of these cores.

Experiments were conducted in a 1000-ton cubic anvil press at P up to 5 GPa and T into the liquid state. A central 5-hole BN cylinder held 5 different Fe-Si sample compositions simultaneously with a thermocouple located at the base of the BN cylinder, and was surrounded by a graphite furnace within a pyrophyllite cubic pressure cell. Fe-Si samples were prepared from pure Fe up to 33 wt% Si using mixtures of powders with known compositions. Following quenching of each experiment, the samples underwent electron microprobe analysis and along with textural analyses, these were used to map the T-X phase diagram at constant P. These phase diagrams will then be applied to the cores of small terrestrial bodies, such as the Moon, Mercury, and Vesta, to identify potential core compositions that are consistent with observational data and models that employ prescribed interior compositions and phases.

P10. Pressure-Induced Occupancy Changes in Methane Hydrate II: Implications for Planetary Ices

Miss Cerian Robertson[1], Ross Howie[1], Dominique Laniel[1], Sarah Bolton[1], James Spender[1], Hannah Shuttleworth[1], Tomas Marqueno[1], and John Loveday[1]
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Methane hydrates are important compounds for the study of water–hydrocarbon interactions. Measurements of their behaviour at high-pressure can also provide insights for both planetary science and energy storage. Methane and water are two of the most abundant components in the outer solar system, therefore it is important to understand the behaviour of methane hydrates under pressure in order to model the interiors of ice-rich planetary bodies, such as Titan, Neptune, and other icy moons/planets. Due to their ability to store large volumes of methane in their water cages under relatively mild conditions, methane hydrates have gained high interest in recent years as a potential gas storage and transport media [1].

Methane hydrate II (MH-II) is stable between 1 and 2 GPa at room temperature. It adopts a unique clathrate structure composed of three cage types, including a barrel-like cage capable of hosting multiple guest molecules [2]. While the overall structure remains unchanged across this pressure range, previous studies have reported a possible change in methane occupancy around

1.4 GPa, indicating a pressure-induced transition point without a change in the crystal symmetry [3].

We have performed Raman spectroscopy and synchrotron X-ray diffraction at this potential transition point. Results from these measurements will be presented and discussed.

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P12. Styrkja: a pressure intensifier for miniature HP-HT devices for 4D synchrotron X-ray microtomography

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Third and fourth generation synchrotron light sources with high fluxes, and beam energies enable the use of innovative X-ray translucent experimental high-pressure and temperature apparatus. In the past years, various published designs have expanded capacities for 4D X-ray microtomography for engineering and geological research aiming at performing mechanical testing, phase transformation or fluid flows through porous media. Most of these rigs use either X-ray transparent windows or vessels made of low-density materials and low-pressure flexible fluid connections to enable rotation. Consequently, their pressure capacity remains (usually <50 MPa-725 PSI) well below their laboratory off-line equivalent. In this contribution, we present Styrkja, a bespoke pressure intensifier designed to power the Mjolnir-rig suite (Fusseis et al., 2014, Butler et al., 2020, Cartwright-Taylor et al., 2022 and Freitas et al., 2024). This design enables, with pressure upgrades on the rigs themselves, to expand significantly the pressure capacity of these rigs with confining pressures up to 200 MPa/30000 PSI. Powered by low pressure fluid lines (<35 MPa-5000 PSI), this device sits on the rotational stage below the rig. It integrates all the hard tubing, gauges, valves and safety devices in a compact design making it ideal for use at synchrotron beamlines.

P14. Li-Battery Cathode Materials: Investigating the High Pressure-Temperature Phase Stability Field of Olivine-Structured Li(Fe,Ni,Mn)PO_4

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Lithium manganese (II) phosphate ($LiMnPO_4$) occurs naturally as lithiophilite, a common accessory mineral in lithium-rich granitic pegmatites, and is the manganese end member in a solid solution with the iron end member triphylite ($LiFePO_4$). Alongside lithium nickel (II) phosphate (LiNiPO4), these olivine-structured phosphates are excellent candidate cathode materials in lithium-ion batteries because of their advantageous electrochemical performance, in addition to the relatively low manufacturing costs, low toxicity, reduced environmental footprint, and high safety levels, compared to other cathode materials. Recently, theoretical and experimental works on lithium-ion battery component materials have expanded focus to high pressure (P) and low-to-high temperature (T) for two main reasons: i) to assess the stability of existing materials at non-ambient conditions for specialized applications and ii) to synthesize and characterize new stable phases that may have more advantageous electrochemical properties. In this preliminary work, we report – to the best of our knowledge – the first P-T phase diagrams of $LiFePO_4$, $LiNiPO_4$, and $LiMnPO_4$ that delineates the phase stability field of the olivine structure. High P-T experiments were conducted in a 1000-ton large volume multi-anvil apparatus and phase structures were determined using Raman spectroscopy. Future works will investigate the thermophysical properties of these materials and use X-ray diffraction to determine the structure of the high P-T phase of $LiMnPO_4$.

P16. Effect of high-pressure processed apple on human gut microbiota, phenolic metabolites and short chain fatty acids by using a dynamic in vitro colonic fermentation system

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Introduction: High-pressure processing (HPP) has been employed to increase the bioaccessibility of phenolic compounds (PC) during gastrointestinal digestion but most of them reach the colon unchanged (1). Apple is one of the most consumed fruit that are available worldwide throughout the year, so its intake represents an important source of bioactive compounds, mainly phenolic compounds (2). There are numerous scientific evidence showing that frequent apple intake has positive effects on human health (3).

The aim of the current study was to evaluate the impact of a daily intake of HPP-treated apple (400 MPa /35°C/5 min) for 14 days on human gut metabolism using a dynamic in vitro gastrointestinal digestion and colonic fermentation (DGID-CF) simulator, model that best simulates human digestion.

The gut metabolic activity was studied by analyzing the phenolic metabolites and short chain fatty acids (SCFAs), and the changes in the microbial population in the colon regions (ascending-AC, transverse-TC, and descending-DC).

Materials & Methods: Apples cv. Golden Delicious from Aragón (Spain) were prepared and processed by HPP (400 MPa/35 °C/5 min) as previously described (4). HPP-apple ingredient was submitted to DGID-CF and phenolic metabolites, SCFAs and microbiota were analyzed (5).

Results: The bioconversion of phenolic compounds of HPP-apple by gut microbiota produced a higher concentration of phenolic metabolites in DC being majority 3,4-dihydroxyphenylacetic acid and 3-(3-hydroxyphenyl)propionic acid. At the same time, a significant increase of de SCFA butyric acid was observed in the TC. These compounds have positive health effects due to their anticancer, anti-inflammatory and antioxidant properties, among others. Also, HPP-apple favor the increment on beneficial gut bacteria as Bifidobacterium spp. and Lactobacillus spp. and a decrease the level of harmful ones as Enterobacteria, total coliforms and Clostridium spp.

Conclusion: Fermentation of HPP-apple in the colon results in increased formation of metabolites with important health benefits.

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P18. Metadynamics study of kinetic pathways of coesite densification

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We study compression of coesite in the region of pressures up to 35 GPa, substantially beyond the equilibrium transition pressure to octahedral phases (8 GPa to stishovite). Experiments at room temperature showed that up to 30 GPa the metastable coesite structure develops only minor displacive changes (coesite-II and coesite-III) while the Si atoms remain 4-coordinated. Upon compression beyond 30 GPa, reconstructive transformations start, following different pathways from the complex structure of coesite. Besides amorphization, two different crystalline outcomes were observed experimentally. One is formation of defective high-pressure octahedral phases [1] and another one is formation of unusual and highly complex dense phases coesite-IV and coesite-V with Si atoms in 4-fold, 5-fold and 6-fold coordination [2]. Capturing these structural transformations computationally, however, represents a challenge. Here we show that employing metadynamics with Si-O coordination number and volume as generic collective variables in combination with a machine-learning based ACE potential [3] one naturally observes all three mentioned pathways resulting in the phases observed experimentally. We analyze the atomistic mechanisms along the transformation pathways. While the pathway to coesite-IV is simpler (Fig. 1), the transformation to octahedral phases (Fig. 2) involves two steps. First, a hcp sublattice of oxygen atoms is formed where Si atoms occupy octahedral positions but the chains of octahedra do not form a regular pattern. In the second step the Si atoms order and the chains develop a more regular arrangement. We predict that the pathway to coesite-IV is preferred at room temperature while at 600 K the formation of octahedral phases is more likely.

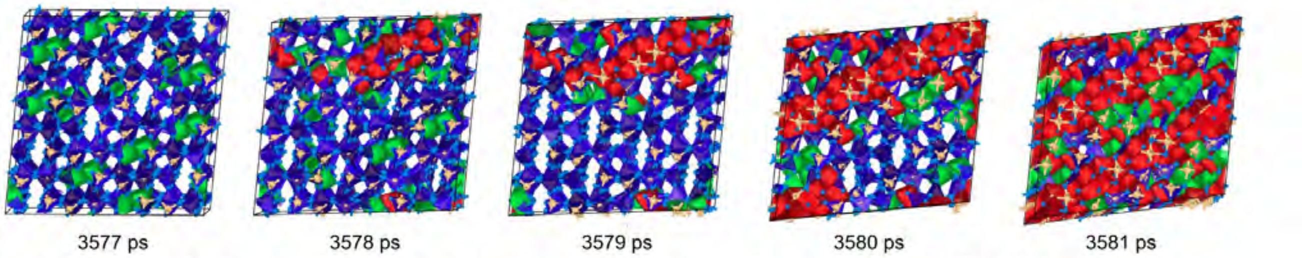

Fig. 1.:Evolution of the structure of the system during formation of the coesite-IV at p = 35 GPa and T = 300 K.

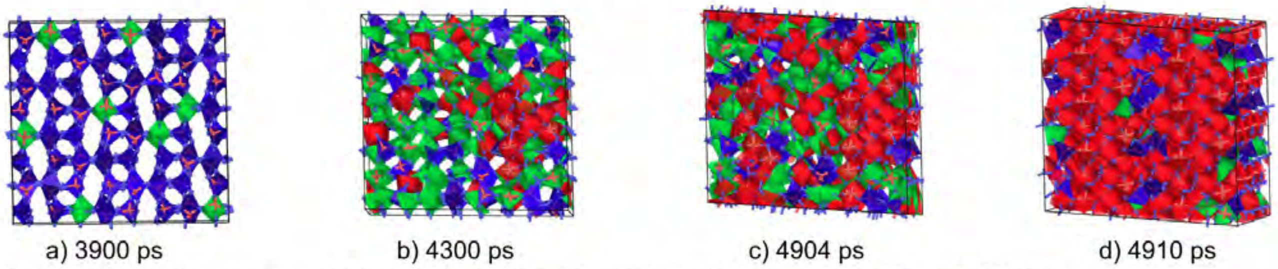

Fig. 2.:Evolution of the structure of the system during formation of the HPO phase at p = 35 GPa and T = 300 K.

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P20. High Energy Scattering Capabilities at Beamline I15

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Beamline I15 at Diamond Light Source is dedicated to x-ray diffraction experiments of materials under extreme conditions of temperature and pressure. I15 operates with a wiggler source, providing x-rays in the range 20 – 80 keV, and offers powder diffraction, single crystal and x-ray pair distribution function (XPDF) experiments. Although most high pressure (diamond anvil cell) powder diffraction experiments are carried out in the lower energy range of 20 – 40 keV (as a reasonable compromise between 2θ resolution and accessible reciprocal space range) there are intrinsic advantages to using higher energy x-rays (60 – 80 keV) for some extreme conditions experiments: i) a larger accessible reciprocal space ($Q=4\pi\sin\theta/\lambda$) range for a given experimental 2θ geometry and ii) the ability to penetrate deeper into semi-transparent sample assemblies, hence enabling collection of diffraction patterns from samples contained within other materials. The lower interaction of high-energy x-rays with materials also propagates to a reduced risk of beam damage to samples. Here we present three recent cases demonstrating the versatile high energy scattering capabilities for extreme conditions experiments at I15: 1) XPDF (total scattering) DAC experiments in radial scattering geometry using a TOMO-DAC 2) high pressure single crystal experiments on noble gas metal complexes and organic systems 3) powder diffraction experiments through an x-ray transparent triaxial hydraulic pressure rig, usually used for 4D microtomography.

P22. Digital temperature controller for the externally heated diamond anvil cell

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We present the design of a temperature controller for the externally heated diamond anvil cell (DAC), enabling precise and reliable high-temperature operation. The system uses digital feedback from thermocouples mounted on the external heater and/or near the diamond, with PID regulation applied via phase angle modulation of the heater's AC supply voltage, ensuring maximum efficiency. It maintains stable temperatures to ±0.5 °C precision indefinitely and is robust against thermocouple failure or dislodgement. This, and other safety features – including overcurrent protection, heating element failure detection, and an overtemperature cut-out circuit independent of the main control system – permit the DAC to be left unattended at high temperature overnight. The controller has been tested up to 300 °C and incorporates comprehensive electronic datalogging, including fault recording, to support experimental reliability.

P24. High Pressure Hydrogen capabilities at ISIS Neutron and Muon Facility.

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Neutrons are an excellent tool for research into hydrogen technology, at ISIS a large number of experiments are run in relation to many technologies involving hydrogen including hydrogen storage where pressuring hydrogen to high pressures in different materials is required. This has many issues including hydrogen embrittlement in materials and regulations such as Dangerous Substance and Explosive Atmosphere Regulations. This poster looks at the capabilities, requirements and challenges of conducting high pressure hydrogen experiments.

P25. Strain Dependent Optical Properties of Core/Shell Nanoplatelets

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Colloidal nanoplatelets are promising materials with tunable narrow emission bands and large photoluminescence quantum yields. In this work we utilize high hydrostatic pressure to investigate the effects of lattice strain on the optical properties of CdSe/CdZnS core/shell nanoplatelets. This work incorporates experimental photoluminescence spectra measured in a diamond anvil cell with hydrostatic pressures up to ~6 GPa, as well as comparison with theoretical models and density functional theory to investigate strain dependent bandgap shifts in colloidal nanoplatelets. This modeling allows for insight into how band structure, confinement, electrostatic effects alter the measured photoluminescence spectra.

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