DS 17: Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures (joint session TT/DS)

Superconductors with record transition temperatures up to 250 K have been discovered and confirmed in hydride materials at high pressures over the last decade, enabled by major advances in both computational and experimental approaches. Density functional theory, combined with structure search algorithms and machine learning methods, enables high-throughput predictions of novel high-pressure phases. Ab initio microscopic theories, including Eliashberg theory and superconducting density functional theory, successfully predict transition temperatures of identified phases, with several predictions now confirmed experimentally. The synthesis of novel hydrides has revealed the importance of including hydrogen quantum fluctuations in theoretical predictions. Experimentally, advances in high-pressure synthesis techniques have enabled the preparation of novel hydride phases, while electrical transport measurements, tunneling spectroscopy, and magnetic studies have established a strong body of evidence for superconductivity by probing zero resistance, the superconducting gap, and magnetic response. This focus session will emphasize these breakthroughs, highlight ongoing challenges in both experiment and computation, and provide an outlook for finding high-temperature superconductors at lower and ambient pressures.

Coordinators: Philipp Gegenwart (Universität Augsburg), Matthias Vojta (TU Dresden)

Time: Thursday 15:00–18:45 Location: HSZ/0003

Topical Talk DS 17.1 Thu 15:00 HSZ/0003

Computational searches for conventional high temperature superconductivity — •Chris Pickard — University of Cambridge

First principles methods for the prediction of the structure of materials have delivered a powerful tool for generating candidate structures for comparison with experimental analytical methods. Early studies focused on the exotic properties and structures of relatively simple systems, typically the elements and binary compounds. The promise of discovering materials with extreme properties relies on the ability of screen a wide variety of compounds.[1] I will reflect on why ab initio random structure searching (AIRSS) is particularly suited to these challenges, focussing on the dramatic acceleration that ephemeral data derived potentials (EDDPs) afford,[2] and their role in the uncovering of Mg_2IrH_6 as a feasible ambient pressure high temperature superconductor.[3]

[1] A.M.Shipley, M.J Hutcheon, R.J.Needs, Ch.J.Pickard, Phys. Rev. B 104, 054501 (2021)
[2] Ch.J.Pickard, Phys. Rev. B 106, 014102 (2022)
[3] K.Dolui, L.J.Conway, Ch.Heil, T.A.Strobel, R.Prasankumar, Ch.J.Pickard, Phys. Rev. Lett. 132, 166001 (2024)

Topical Talk DS 17.2 Thu 15:30 HSZ/0003

High-pressure synthesis of hydrides and their characterisation by single-crystal X-ray diffraction — •Natalia Dubrovinskaia[1] and Leonid Dubrovinsky[2] — [1]Material Physics, University of Bayreuth; Bayreuth, Germany — [2]Bayerisches Geoinstitut, University of Bayreuth, Germany

The sulfur-hydrogen, lanthanum-hydrogen, and yttrium-hydrogen systems have attracted significant interest following reports of near-ambient-temperature superconductivity in some of their high-pressure phases. Here, we present single-crystal X-ray diffraction studies of these systems, supported by density functional theory calculations, which reveal an unexpected chemical and structural diversity in S, La, and Y hydrides synthesised at 50*200 GPa. Syntheses were carried out in diamond anvil cells by laser heating S, La, LaH3, or Y together with hydrogen-rich precursors-ammonia borane or paraffin oil. The arrangements of heavy atoms in newly formed phases were determined from SCXRD data, while hydrogen contents were estimated using empirical relationships and ab initio calculations. Our study also uncovers the formation of previously unreported metal allotropes, carbides, and ternary compounds at high pressure. The complex phase diversity, variable hydrogen stoichiometries, and metallic nature of these high-pressure hydrides, as revealed by theory, highlight the challenges in identifying the superconducting phases and understanding electronic transitions in materials synthesised under extreme conditions.

Topical Talk DS 17.3 Thu 16:00 HSZ/0003

Electrical Transport Studies in bulk and thin-film hydride high-temperature superconductors — •Sven Friedemann[1], Sam Cross[1], Owen Moulding[1], Israel Osmond[1], Xiaojiao Liu[2], Annette Kleppe[2], Oliver Lord[3], and Jonathan Buhot[1] — [1]HH Wills Physics Laboratory, University of Bristol, UK — [2]Diamond Light Source Ltd., Didcot, UK — [3]School of Earth Sciences, University of Bristol, UK

Superconductivity is not restricted to low temperatures! Indeed, transition temperatures up to 260 K have been demonstrated by multiple groups in H_3S, LaH_{10}, and YH_9, at very high pressures. This is a success story of both theory and experiment. Theory has mastered accurate predictions of new superconductors and has been crucial to guide experimental efforts. Experiments have mastered many technical challenges. Together, these efforts open pathways to realise higher transition temperature at low pressures.

We present combined structural and electrical transport studies of hydride high-T_c superconductors based on our development of *in situ* synthesis, x-ray diffraction, and transport measurements in diamond-anvil pressures cells including thin-film methods for electrodes and superconducting samples. We present the characterisation of clean-limit superconductivity in H_3S and the discovery of the new superconductor La_4H_{23}. We demonstrate superconductivity in thin films of LaH_{10} with a $T_c = 250$ K consistent with bulk LaH_{10}. Our results open new avenues to study hydride high-T_c superconductors with thin-film methods.

15 min. break

Topical Talk DS 17.4 Thu 16:45 HSZ/0003

Near room-temperature conventional superconductivity in hydrogen-rich compounds at high pressures: Experimental evidences — •Vasily Minkov — Max Planck Institute for Chemistry, Mainz, Germany

The pioneering discovery of superconductivity in hydrogen sulfide (H3S) with a record Tc of 203 K at 150 GPa by M. Eremets et al. had a profound impact on the field. It validated the concept of high-Tc conventional superconductivity in hydrides and triggered an intense wave of research. Subsequent studies revealed that other hydrides - such as LaH10 and YH9 - exhibit Tc values approaching 250 K, bringing the field closer than ever to room-temperature superconductivity. Despite the experimental challenges associated with micrometer-sized samples confined in diamond anvil cells, superconductivity in these compounds has been demonstrated using multiple independent techniques. Electrical four-probe measurements provide clear resistive transitions, while recent advances in high-pressure magnetometry enable direct detection of magnetic field screening and flux expulsion. We have further developed a method to probe trapped magnetic flux in hydrides at high pressure. The distinct behavior of trapped flux generated under ZFC and FC conditions provides strong evidence for superconductivity. Furthermore, the recent adaptation of electron tunneling spectroscopy to extreme pressures offers microscopic insight into the pairing mechanism and enables direct characterization of the superconducting gap structure in the high-temperature hydride superconductors.

Topical Talk DS 17.5 Thu 17:15 HSZ/0003

Predictive T_c Calculations in Hydride Superconductors — •Christoph Heil — Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria

The discovery of high-T_c superconductivity in compressed hydrides has sparked a surge of theoretical predictions, yet reported critical temperatures for identical structures can differ by tens of Kelvin or more. These discrepancies reflect differences in how lattice dynamics, electronic structure, and Coulomb repulsion are treated. In this talk, we will present first-principles workflows designed to make Tc calculations both more transparent and more predictive.

We combine anharmonic lattice dynamics with full-bandwidth isotropic and anisotropic Migdal-Eliashberg calculations (IsoME and EPW) that retain the full electronic density of states, and we incorporate Coulomb repulsion via screened interactions obtained from first principles rather than an empirical μ^*. This framework allows us to systematically compare different approximation levels and to quantify how each approximation affects T_c.

Using case studies from high-pressure hydrides, we will demonstrate when simplified treatments remain adequate and when anharmonic effects, full-bandwidth electrons, and first-principle determination of Coulomb screening become essential for quantitative accuracy. I will provide practical guidelines for reliable, reproducible T_c predictions and discuss how rigorous superconductivity calculations complement crystal-structure prediction efforts in the search for new superconductors.

DS 17.6 Thu 17:45 HSZ/0003

^{1}H-NMR investigations of bulk superconductivity in superhydrides using Lenz lenses — •F. Bärtl[1,2], D. Zhou[3], T. Helm[1], S. Luther[1], H. Kühne[1], J. Wosnitza[1,2], and D. Semenok[3] — [1]HLD-EMFL, HZDR, Dresden — [2]IFMP, TUD, Dresden — [3]HPSTAR, Beijing

The discovery of near-room-temperature superconductivity at ultrahigh pressures in superhydrides has kindled intensive research activities in the past years. However, the need to use diamond-anvil cells (DACs) for the synthesis and study of such superconductors limits the number of available experimental techniques. Nuclear magnetic resonance (NMR) spectroscopy is a key technique to study the bulk properties of superconducting materials, but it usually requires sample masses of several milligrams. Here, we present our ^{1}H NMR measurements of several superhydride preparations, using Lenz lenses, which act as magnetic-flux transformers in the NMR experiment and enable the investigation of samples with masses in the microgram range in the sample chamber of DACs. We observe several features that evidence the bulk nature of the superconducting transition in the superhydrides, the most prominent being the suppression of the ^{1}H nuclear spin-lattice relaxation rate $1/T_1T \propto D(E_\mathrm{F})^2$. Furthermore, we report on the systematic occurrence of a rate enhancement in the regime of the superconducting transition, which is reminiscent of a Hebel-Slichter-like peak.

DS 17.7 Thu 18:00 HSZ/0003

Above-room-temperature superconductivity in substituted LaH_x superhydride — •Stanley Tozer and Audrey Grockowiak — Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, 01069 Dresden, Germany

We have synthesized a higher order La-based superhydride with initial superconducting transition temperature of 294 K that, when heated, morphed into a higher order system with a T_c ^{onset} of 556 K and a transition width of approximately 120 K [1]. The x-ray and the electrical transport data support one another with regard to the pressure measured, and the inhomogeneous nature of the synthesis that resulted in a substituted higher order La-based superhydride in close proximity to FIBed electrodes with a broad multi-phase, irreversible transition and non-zero background resistance below T_c. The electric leads embedded in our 'crucible' probe a pathway through this inhomogeneous growth, a very small portion of which is the superconductor of interest. We have used informed growth to reproduce the initial result in a range of pressures lower than allowed for the binary LaH_{10}. A multi-probe approach is being implemented to address growth-to-growth variations and follow the transformation of the initial 294 K superconductor. This will provide an understanding of this new class of superconductor that begs the question as to the upper limit of superconductivity in the superhydrides and whether BCS theory can describe them.

[1] A.D. Grockowiak et al., Electronic Materials 2, (2022)
[2] doi.org10.3389/femat.2022.837651

DS 17.8 Thu 18:15 HSZ/0003

Search for Room-temperature Superconductivity in the La-Sc-H System — •Dmitrii V. Semenok[1], Ivan A. Troyan[2], Di Zhou[1], and Viktor V. Struzhkin[1,3] — [1]Center for High Pressure Science & Technology Advanced Research, Bldg. 8E, 10 Xibeiwang East Rd, Beijing, 100193, China — [2]private — [3]Center for High Pressure Science & Technology Advanced Research, 1690 Cailun Rd, Bldg 6, Shanghai 201203, China

One of the highlights of 2025 in the field of hydride superconductivity was the announcement of the experimental discovery of room-temperature superconductivity in the fully ordered ternary polyhydride P6/mmm-$LaSc_2H_{24}$ at around 260 GPa [1]. We performed a DFT analysis of intermetallic compound formation in the La-Sc system with a view to modifying the synthetic procedure, and calculated parameters of the superconducting state of the isostructural P6/mmm-La_3H_{24} and P6/mmm-Sc_3H_{24} at 300 GPa. Attempts to experimentally reproduce the synthesis of $LaSc_2H_{24}$ from the $LaSc_2$ alloy (with a careful selection of the homogeneity region of this alloy's composition) at 264-280 GPa have not yet resulted in the detection of any traces of superconductivity between 255 K and 295 K in the corresponding hydride. In my report, I will show the results of additional experimental attempts to reproduce [1], planned for January-February 2026.

[1] Y. Song et al., arXiv: 2510.01273 (2025).

DS 17.9 Thu 18:30 HSZ/0003

Computational modeling of disordered hydride superconductors — •Pedro Nunes Ferreira[1], Luiz Tadeu Fernandes Eleno[2], and Christoph Heil[1] — [1]Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, 8010, Graz, Austria — [2]Departamento de Engenharia de Materiais, Escola de Engenharia de Lorena, Universidade de São Paulo, Lorena, Brazil

Designing and optimizing novel hydride superconductors requires methods that accurately treat realistic chemical disorder. In this talk, I will present an ab initio thermodynamic framework, the extended generalized quasichemical approximation (EGQCA), tailored to the modeling of superconducting alloys, especially high-T_c superhydrides. EGQCA enables the prediction of any computationally accessible property, such as T_c and electron-phonon coupling, as a function of composition using only a small set of supercell calculations, making it particularly well suited for complex hydrogen-rich materials. I will illustrate its capabilities with applications to high-T_c superhydrides at high pressure, as well as defective hydrides stabilized at ambient pressure. Finally, I will discuss how EGQCA opens the door to high-throughput design and screening of disordered superconductors, with the potential to significantly advance hydride superconductivity research.