TT 62: Focus Session: High Temperature Superconductivity in Hydrides

The discovery of superconductivity at 203 K in H_3S was a big surprise although it was predicted theoretically. While unstable at ambient conditions H_3S is a result of the dissociation of H_2S for an applied pressure in excess of 100 GPa in accordance with structure predictions. The transition temperature can be estimated with high accuracy by Density Functional Theory for superconductors. The symposium comprises results from experimental and theoretical studies.

Organizer: Rudi Hackl (WMI Garching)

Time: Thursday 9:30–12:45 Location: H20

Invited Talk TT 62.1 Thu 9:30 H20

Conventional high temperature superconductivity: from A15 to MgB_2 to H_3S — •Igor Mazin — NRL, Washington, DC

I will review, mostly for the benefits of the younger generation, the history of the half-century long quest for the room-temperature superconductivity, concentrating on the conventional electron-phonon mechanism. I will outline several stages, characterized by different paradigmes, which can be tagged in a Potterian way thus:

(1) A-15 and the concept of an upper bound on T_c
(2) V.L. Ginzburg and the concept of a negative dielectric function
(3) MgB_2 and the concept of doped covalent bonds
(4) H_3S and the room temperature superconductivity
(if the room is in Antarctica).

I am dedicating this talk to the memory of my teacher, Vitaly Ginzburg, on occasion of his 100th birthday.

Invited Talk TT 62.2 Thu 10:00 H20

Conventional superconductivity at 203 K at high pressures — Alexander Drozdov[1], •Mikhail Eremets[1], Ivan Troyan[1], Vadim Ksenofontov[2], and Sergii Shylin[2] — [1]1Max-Planck-Institut fuer Chemie, Hahn-Meitner-Weg 1, 55128 Mainz, Germany — [2]Institut fuer Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universitet Mainz, Staudingerweg 9, 55099 Mainz, Germany.

A search for high, room temperature conventional superconductivity is promising as the Bardeen-Cooper-Schrieffer (BCS) theory in the Eliashberg formulation puts no apparent limits on T_c. Materials with light elements are especially favorable as they provide high frequencies in the phonon spectrum. However only a moderately high T_c = 39 K has been found in this search in MgB_2. We systematically studied metallic hydrogen and covalent hydrogen dominant compounds and found the record T_c of 203 K at pressure 140 GPa in sulfur hydride [1]. We proved occurrence of superconductivity by the sharp drop of the resistivity to zero; the decrease of T_c with magnetic field; the pronounce isotope shift of T_c in D_2S which evidences of a major role of phonons in the superconductivity; and the magnetic susceptibility measurements. The X-ray diffraction data confirmed that the superconductive phase has the predicted bcc structure. This phase can be considered as an atomic hydrogen superconductor stabilized by sulfur.

[1] A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov, S. I. Shylin, Nature **525**, 73 (2015)

Invited Talk TT 62.3 Thu 10:30 H20

Crystal Structure of 200 K-Superconducting Phase in Sulfur Hydride System — •Mari Einaga[1], Masafumi Sakata[1], Takahiro Ishikawa[1], Katsuya Shimizu[1], Mikhail Eremets[2], Alexander Drozdov[2], Ivan Troyan[2], Naohisa Hirao[3], and Yasuo Ohishi[3] — [1]KYOKUGEN, Graduate School of Engineering Science, Osaka university, Machikaneyamacho 1-3, Toyonaka, Osaka, 560-8531, Japan — [2]Max Planck Institut fur Chemie, Hahn-Meitner-Weg 1, 55128 Mainz, Germany — [3]JASRI/SPring-8, 1-1-1, Sayo-cho, Sayogun, Hyogo 679-5198. Japan

Superconductivity with the critical temperature T_c above 200 K has been recently discovered by compression of H_2S (or D_2S) under extreme pressure [1]. It was proposed that these materials decompose under high pressure to elemental sulfur and hydride with higher content of hydrogen which is responsible for the high temperature superconductivity. In this study, we have investigated that the crystal structure of the superconducting compressed H_2S and D_2S by synchrotron x-ray diffraction measurements combined with electrical resistance measurements at room and low temperatures. We found that the superconducting phase is in good agreement with theoretically predicted body-centered cubic structure, and coexists with elemental sulfur, which claims that the formation of $3H_2S \rightarrow 2H_3S + S$ is occured under high pressure [2].

[1] A. P. Drozdov *et al.*, arXiv: 1412.0460 (2014),
A. P. Drozdov *et al.*, Nature **525**, 73 (2015)
[2] M. Einaga *et al.*, arXiv: 1509.03156 (2015).

15 min. break

Invited Talk TT 62.4 Thu 11:15 H20

Strong-Coupling Electron-Phonon Superconductivity in H_3S — •Warren E. Pickett[1] and Yundi Quan[2] — [1]University of California Davis, Davis CA, USA — [2]Beijing Normal University, Beijing, China

The superconducting phase of hydrogen sulfide at $T_c = 200$ K observed by Eremets' group at pressures around 200 GPa is simple bcc Im-3m H_3S. Remarkably, this record high temperature superconductor was predicted beforehand by Duan et al., so the theory would seem to be in place. Here we will discuss why this is not true. Several extremes are involved: extreme pressure, meaning reduction of volume;extremely high H phonon energy scale around 1400 K; unusually narrow peak in the density of states at the Fermi level; extremely high temperature for a superconductor. Analysis of the H3S electronic structure and two important van Hove singularities (vHs) reveal the effect of sulfur. The implications for the strong coupling Migdal-Eliashberg theory will be discussed. followed by comments on ways of increasing T_c in H_3S-like materials.

Invited Talk TT 62.5 Thu 11:45 H20

High-pressure phases of S, Se, and P hydrides and their superconducting properties: Predictions from ab-initio theory — •E. K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The quest for novel high-temperature superconductors in the family of hydrogen-rich compounds has recently been crowned with the experimental discovery of a record critical temperature of 190 K in a hydrogen-sulfur compound at 200 GPa. In the present contribution, we investigate the phase diagram of the H-S system, comparing the stability of H_nS (n = 1,2,3,4) by means of the minima hopping method for structure prediction. Our extensive crystal structure search confirms the H_3S stoichiometry as the most stable configuration at high pressure. Superconducting properties are calculated using the fully ab-initio parameter-free approach of density functional theory for superconductors. We find a T_c of 180 K at 200 GPa, in excellent agreement with experiment. We also show that Se-H has a phase diagram similar to its sulfur counterpart. We predict H_3Se to be superconducting at temperatures higher than 120 K at 100 GPa. We furthermore investigate the phase diagram of PH_n (n = 1,2,3,4,5,6). The results of our crystal-structure search do not support the existence of thermodynamically stable PH_n compounds, which exhibit a tendency for elemental decomposition at high pressure. Although the lowest energy phases of $PH_{n=1,2,3}$ display T_c values comparable to experiment, it remains uncertain if the measured values of T_c can be fully attributed to a phase-pure compound of PH_n.

Invited Talk TT 62.6 Thu 12:15 H20

New sulfur hydride H_3S and excellent superconductivity at high — •Tian Cui — State Key Laboratory of Superhard Materials, College of physics, Jilin University, Changchun, P. R. China

It is predicted theoretically that molecular hydrogen would dissociate into an atomic phase with metallic properties at high pressures. Metallic hydrogen is believed to be a room-temperature superconductor. However, metallization of hydrogen is still debates in laboratory. As an alternative, hydrogen-rich compounds are extensively explored since their metallization can happen at relatively lower pressures by means of chemical pre-compressions. Here, a new sulfur hydride H_3S

that hardly occur at atmospheric pressure was predicted to be formed at high pressure by two main ways. We also found two intriguing metallic structures with R3m and Im-3m symmetries above 111 GPa and 180 GPa, respectively. Remarkably, the estimated T_c of Im-3m phase at 200 GPa achieves a very high value of 191-204 K, reaching an order of 200 K. Further calculation shown that the H atoms play a significant role in superconductivity. The experimental discovery of superconductivity with a high T_c = 203 K in H-S system at high pressure has verified our theoretically predicted results. Furthermore, the predicted R3m and Im-3m structures have been recently confirmed experimentally by synchrotron XRD.