

A Forum of Forward-Looking Scientific Vision: Synergy of 21st Century High-Pressure Science and Technology

A workshop, convened to explore the synergy of 21st century high-pressure science and technology, was held from April 29 to May 1, 2006 at the Advanced Photon Source of the Argonne National Laboratory. The meeting featured an extensive array of forward-looking presentations along with ample opportunities for discussions among the 112 scientists and 20 graduate students and postdoctoral researchers in attendance from the fields of physics, chemistry, materials science, biology, and earth and planetary sciences, from both academic institutions and the National Labs around the country.

The aims of the Workshop were to review the status of U. S. high-pressure research and to identify future grand challenges in the following nine thrust areas:

- *Integrated high pressure science*
- *Dense condensed-matter physics*
- *Chemical bonding under compression*
- *High-pressure materials research*
- *High-pressure petrology and mineralogy*
- *Deep Earth geochemistry*
- *Mission to the Earth's core*
- *High pressure seismology and elasticity*
- *Biological and organic systems under pressure*



Fifty-nine talks given by experts from a wide variety of disciplines within the field of high pressure research reviewed the surge of high pressure discoveries in recent years as well as the technological advances in the development of new high-pressure instrumentation and analytical probes, and raised scientific and technological issues concerning the upcoming challenges for high pressure research in the 21st century. The group discussed the great scientific potential in establishing a next-generation “synergetic consortium” that would integrate state-of-the-art high-pressure techniques, facilities, and probes, and make them readily accessible to multidisciplinary high-pressure scientists. The consortium would enable high-pressure specialists and non-specialists alike to focus on specific scientific goals which were previously hindered due to technical limitations.

In the three-day workshop, presentations focused on the synergy and interdisciplinary nature of the multiple subfields of high-pressure science and technology. On the first day, an introductory session explored the chemical and physical fundamentals of matter at high densities. These presentations set the stage for an extensive group of talks that demonstrated how both static and dynamic experiments, particularly in combination with each other, along with condensed-matter theory, can provide a means to unravel the phenomena governing the behavior of matter under extreme conditions. The second day started with an overview of recent progress in seismology and geodynamics and then identified questions to be answered and the role that high pressure mineral physics can play in sorting out some of the pressing questions in these fields. Answers to some of these problems were pursued during talks in the later sessions on high-pressure mineral sciences, in which new results, developments, and technologies were presented. The second day ended with two talks outlining current work in the area of biological

and organic systems under high pressure. On the third day, recent developments in the studies of Earth's deep interior were discussed from both experimental and theoretical viewpoints. The need for a synergetic consortium was further emphasized in these presentations, for example, to lead the development of a new generation of "designer" samples and anvils, integrated studies with various probing techniques, cooperation between theory and experiment, and coordinated educational efforts among different research groups. Besides the in-depth discussions in the APS conference room, two facility tours of the Advanced Photon Source were provided during the workshop.



The participant reception to the program was overwhelmingly positive, with many compliments on the outstanding quality of the talks and discussions. The workshop will result in a publication of a series of visionary papers in the *Proceedings of the National Academy of Sciences*, designed to illustrate the synergetic nature of the interdisciplinary field of high pressure research

The Workshop on the Synergy of 21st Century High Pressure Science and Technology was jointly sponsored by the Consortium for Materials Properties Research in Earth Sciences (COMPRES), the Carnegie-DOE Alliance Center (CDAC), and the High-Pressure Collaborative Access Team (HPCAT).

Co-Organizers: Ho-kwang Mao (*Carnegie Institution*), Guoyin Shen (*HPCAT*), Wolfgang Sturhahn (*Advanced Photon Source*), Yanbin Wang (*GSECARS*), Russell J. Hemley (*Carnegie Institution*)

Local Organizing Committee: Haozhe Liu (*HPCAT*), Veronica O'Connor (*HPCAT*), Michael Lerche (*Advanced Photon Source*)



Appendix

I. Students and postdoctoral researchers

A detailed list of students and postdoctoral researchers and their home institutions is given below:

Postdoctoral	Institution		Students	Institution
Alice Acatrinei	LANL		Chris Seagle	U Chicago
Itzhak Halevy	CalTech		Hongbo Long	Stony Brook
Jenny Jackson	GL-CIW		Kirill Zhuravlev	LANL
Steve Jacobsen	GL-CIW		Rafael Jaramillo	U Chicago
Stefani Japel	Mexico State		Resul Aksoy	Texas Tech
Svetlana Kharlamova	APS		Eric Suber	U of Illinois
Wendy Mao	LANL		Ji Feng	Cornell
Xinguo Hong	GSECARS		Rusty Cooper	UIUC
Michael Lerche	APS		Yuan-Chieh Tseng	Northwestern
Yejung Feng	U Chicago		Selvi Emre	Texas Tech

II. The workshop program and list of speakers

April 29 Saturday

8:30 – 8:45

Opening Session

APS Auditorium

8:30

Opening
Ho-kwang Mao, Carnegie Institution of Washington

8:35

Welcome
J. Murray Gibson, Argonne National Laboratory

8:45 – 10:45

Session 1: Integrated High-Pressure Science

APS Auditorium

Chair: *William A. Bassett, Cornell University*

8:45

Synergy of High-Pressure Research
Ho-kwang Mao, Carnegie Institution of Washington

9:15

The Chemical Imagination at Work in Very Tight Places
Roald Hoffmann, Cornell University

9:45

Electronic Structure of Materials under High Pressure
Chi-Chang Kao, Brookhaven National Laboratory

10:15

Planetary High Pressure Physics Inside and Outside Our Solar System
David J. Stevenson, CalTech

11:00 – 12:30

Session 2: Dense Condensed-Matter Physics - I

APS Auditorium

Chair: *Malcolm F. Nicol, University of Nevada at Las Vegas*

11:00

Current Problems in High-Pressure Science
Russell J. Hemley, Carnegie Institution of Washington

11:30

Phonon Thermodynamics in Materials under Extreme Conditions
Brent Fultz, Caltech

11:45

Interfaces at High Pressure
Dana D. Dlott, University of Illinois at Urbana-Champaign

12:00

Optical Spectroscopy under Extreme Conditions
Alexander Goncharov, Carnegie Institution of Washington

12:15

Magnetism and Superconductivity at High Pressures
Viktor V. Struzhkin, Carnegie Institution of Washington

14:00 – 15:45

Session 3: Dense Condensed-Matter Physics-II

<i>APS Auditorium</i>		<i>Chair: Russell J. Hemley, Carnegie Institution of Washington</i>
14:00	Understanding Condensed Matter at Extreme Conditions: How to Integrate Dynamic and Static Compression Methods <i>Yogendra Gupta, Washington State University</i>	
14:30	Grand Challenges in f-Electron Metals Research at High Pressures and Low Temperatures Using Designer Diamond Anvils <i>Yogesh Vohra, University of Alabama</i>	
14:45	On Some Not-So-Sharp Phase Transitions <i>Malcolm F. Nicol, University of Nevada at Las Vegas</i>	
15:00	Spectroscopies to Aid in the BP/T Exploration of Condensed Matter Physics <i>Stan Tozer, National Magnetic Laboratory</i>	
15:15	Inelastic X-Ray and Nuclear Resonant Scattering <i>Wolfgang Sturhahn, Argonne National Laboratory</i>	
15:30	Metallization of Structural Distortion under High Pressure <i>Ji Feng, Cornell University</i>	
16:00 – 18:00		Session 4: Chemical Bonding under Compression
<i>APS Auditorium</i>		<i>Chair: Ross Angel, Virginia Tech</i>
16:00	Gigabar Pressures and Kilovolt Chemistry <i>Raymond Jeanloz, UC - Berkeley</i>	
16:30	Electronic Structure of Materials under High Pressure <i>Choong-Shik Yoo, Lawrence Livermore National Laboratory</i>	
16:45	Electron Density of Materials at High Pressure <i>Nancy Ross, Virginia Tech</i>	
17:00	Structural Transformations in Liquids and Glasses under Extreme Conditions <i>Jeff L. Yarger, Arizona State University</i>	
17:15	Neutron's Prospects on the Future Hydrogen Economy <i>Yusheng Zhao, Los Alamos National Laboratory</i>	
17:30	Experimental Opportunities at the High-Pressure Beamline 12.2.2 of the ALS <i>Martin Kunz, Advanced Light Source</i>	
20:30 – 21:30	Facility Tour at APS	

April 30 Sunday

8:30 – 10:15		Session 5: High Pressure Seismology and Elasticity
<i>APS Auditorium</i>		<i>Chair: Jay Bass, University of Illinois at Urbana-Champaign</i>
8:30	Seismic Tomography and Mineral Physics: Questions to Be Answered <i>Adam M. Dziewonski, Harvard University</i>	
9:00	Review of Lower Mantle Seismic Complexity <i>Donald V. Helmberger, CalTech</i>	
9:30	Towards Direct Seismic Waveform Inversion for Thermal and Compositional 3D Structure of the Mantle: What We Need From Mineral Physics <i>Barbara Romanowicz, UC - Berkeley</i>	
10:00	The Role of High Pressure Mineral Physics in Geodynamics <i>David A. Yuen, University of Minnesota</i>	
10:15	Measuring Stress at High Pressure <i>Donald Weidner, Stony Brook University</i>	
10:45 – 12:15		Session 6: Mission to the Earth's Core
<i>APS Auditorium</i>		<i>Chair: J. Michael Brown, University of Washington</i>
10:45	Evolution and Dynamics of the Earth's Core: Current Questions and New Opportunities <i>Bruce A. Buffett, University of Chicago</i>	
11:15	Elasticity of Fe-rich Silicate Post-Perovskite <i>Wendy Mao, Los Alamos National Laboratory</i>	
11:30	Thermal Expansion of Iron-Rich Alloys and the Light Element Composition of the Core <i>Jie Li, University of Illinois at Urbana-Champaign</i>	
11:45	Experimental Studies of Core Materials at Core Conditions <i>Dion L. Heinz, University of Chicago</i>	

12:00	Experimental Studies of Phase Diagram of Iron <i>Guoyin Shen, Carnegie Institution of Washington</i>
14:00 – 15:45	Session 7: High Pressure Mineral Sciences - I
<i>APS Auditorium</i>	<i>Chair: Hans-Rudolf Wenk, UC - Berkeley</i>
14:00	Orogenic UHP Garnet Peridotite: A New Window for Mantle Petrochemical Processes <i>Juhn G. Liou, Stanford University</i>
14:30	Hydrothermal Diamond Anvil Cell, the Value of Visual Observations <i>William A. Bassett and Kenji Mibe, Cornell University</i>
14:45	Determining Intersite Cation Partitioning at High Pressure <i>Ross Angel, Virginia Tech</i>
15:00	Whither Mineral Physics? <i>J. Michael Brown, University of Washington</i>
15:15	Challenges in Studying the Chemistry of Deep Interior of the Earth <i>Yingwei Fei, Carnegie Institution of Washington</i>
15:30	Elastic Properties of Hydrous Minerals and Implications for Seismic Studies of the Upper Mantle <i>Thomas S. Duffy, Princeton University</i>
16:00 – 17:30	Session 8: High Pressure Mineral Sciences - II
<i>APS Auditorium</i>	<i>Chair: Thomas S. Duffy, Princeton University</i>
16:00	Some Recent Advances in Velocity Measurements at High Pressures and Implications for the Earth <i>Jay Bass, University of Illinois at Urbana-Champaign</i>
16:15	Characteristics of Thermal and Chemical Heterogeneities in the Lower Mantle <i>Baosheng Li, Stony Brook University</i>
16:30	Deformation Experiments at Ultrahigh Pressure: Where We Are and Where We Should Be Going <i>Hans-Rudolf Wenk, UC - Berkeley</i>
16:45	Ultrasonic Measurements of Sound Velocities in Minerals under Mantle P & T Conditions in Conjunction with Synchrotron X-Radiation <i>Robert C. Liebermann, Stony Brook University</i>
17:00	High P - T Structural Refinement of CaSiO ₃ (\pm Al ₂ O ₃) Perovskite <i>Yanbin Wang, University of Chicago</i>
17:15	Physical Properties of Minerals and Melts under High-Pressure <i>Jennifer M. Jackson, Carnegie Institution of Washington</i>
17:30 – 18:00	Session 9: Biological and Organic Systems under Pressures
<i>APS Auditorium</i>	<i>Chair: Thomas S. Duffy, Princeton University</i>
17:30	Opportunities at Ultra Low High Pressures <i>Keith Brister, Northwestern University</i>
17:45	Organic Synthesis and Biology at High Pressures <i>Anurag Sharma, Rensselaer Polytechnic Institute</i>
May 1 Monday	
8:30 – 10:15	Session 10: Deep Earth Geochemistry, Petrology and Mineralogy-I
<i>Room A1100</i>	<i>Chair: Robert C. Liebermann, Stony Brook University</i>
8:30	Theory of Iron at High Pressure and Temperature <i>Ronald E. Cohen, Carnegie Institution of Washington</i>
8:45	Dissociation of MgSiO ₃ in the Cores of the Giants and in Terrestrial Exoplanets <i>Renata M.M. Wentzcovitch, University of Minnesota</i>
9:00	The Way Frameworks Respond to Pressure <i>John B. Parise, Stony Brook University</i>
9:15	High Pressure Thermal Conductivity <i>Anne M. Hofmeister, Washington University</i>
9:30	Effects of Hydration on Physical Properties of Mantle Minerals <i>Joseph Smyth, University of Colorado</i>
9:45	Phase Transition in the Earth's Mantle <i>Sang-Heon (Dan) Shim, MIT</i>
10:00	Experimental High Pressure Mineral Physics in 3-Di

10:15	<i>Abby Kavner, UC – Los Angeles</i> Identifying Hydration in the Mantle Transition Zone: Emerging Constraints from Mineral Physics and Seismology <i>Steven D. Jacobsen, Northwestern University</i>
10:45 – 11:45 <i>Room A1100</i>	Session 11: Deep Earth Geochemistry, Petrology and Mineralogy-II <i>Chair: Anne M. Hofmeister, Washington University</i>
10:45	Shearing Instabilities at High Pressure, Application to Deep Earthquakes, and Progress Toward Experiments <i>In-Situ</i> <i>Harry W. Green, UC - Riverside</i>
11:00	Deep Mantle Melting and Geochemical Tests of the Transition-Zone Water-Filter Model <i>Shun-ichiro Karato, Yale University</i>
11:15	Melts Density Study at High Pressures Using X-Ray Absorption and Diffraction Enhanced Imaging <i>Jiuhua Chen, Stony Brook University</i>
11:30	A Look Inside of Diamond-Growing Fluid: Observations From Natural Samples and Experiments <i>Larrisa Dobrzhinetskaya, UC - Riverside</i>
11:45	High-Pressure Rheology: Challenges and Opportunities <i>William B. Durham, Lawrence Livermore National Laboratory</i>
12:00 – 12:15	Closing Remarks
13:30 – 16:00	Facility Tours at APS

III. List of participants (Total of 112)

Last Name	First Name	Institution
Acatrinei	Alice I.	Los Alamos National Laboratory
Aksoy	Resul	Texas Tech University
Alatas	Ahmet	Argonne National Laboratory
Alp	E. Ercan	Argonne National Laboratory
Angel	Ross	Virginia Tech
Bass	Jay D.	University of Illinois
Bassett	William A..	Cornell University
Balasubramanian	Mali	Argonne National Laboratory
Bommannavar	Arun S.	Carnegie Institution of Washington
Brister	Keith E.	Northwestern University
Brown	J. Michael	University of Washington
Buffet	Bruce	University of Chicago
Cai	Yong Q.	Synchrotron Radiation Research Center
Cauble	Robert	Lawrence Livermore National Laboratory
Cavell	Ronald G.	University of Alberta
Chapman	Karena W.	Argonne National Laboratory
Chen	Jiuhua	Stony Brook University
Chupas	Peter J.	Argonne National Laboratory
Cohen	Ronald E.	Carnegie Institution of Washington
Cooper	Rusty	University of Illinois at Urbana Champaign
Ding	Yang	Carnegie Institution of Washington
Dlott	Dana D.	University of Illinois at Urbana Champaign
Dobrzhinetskaya	Larissa	University of California at Riverside
Dolan	Daniel H.	Sandia National Labs
Duffy	Thomas S.	Princeton University
Durham	Bill	Lawrence Livermore National Laboratory
Dziewonski	Adam M.	Harvard University
Fei	Yingwei	Carnegie Institution of Washington
Feng	Ji	Cornell University
Feng	Yejun	The University of Chicago
Fultz	Brent	Caltech
Gibson	Murray	Argonne National Laboratory
Goncharov	Alexander F.	Carnegie Institution of Washington
Green	Harry W.	University of California, Riverside
Guo	Quanzhong	Carnegie Institution of Washington
Gupta	Yogendra M.	Washington State University
Halevy	Itzhak	California Institute of Technology
Haskel	Daniel	Argonne National Laboratory
Heinz	Dion L.	The University of Chicago
Helmberger	Don V.	Caltech
Hemley	Russell J.	Carnegie Institution of Washington
Hoffmann	Roald	Cornell University
Hofmeister	Anne	Washington University
Hong	Xinguo	The University of Chicago
Hu	Jingzhu	Carnegie Institution of Washington
Hu	Yu (Michael)	Carnegie Institution of Washington

Jackson	Jennifer M.	Carnegie Institution of Washington
Jacobsen	Steve	Carnegie Institution of Washington
Japel	Stefanie L.	New Mexico State University
Jaramillo	Rafael	The University of Chicago
Jeanloz	Raymond	University of California, Berkeley
Kao	Chi-chang	Brookhaven National Laboratory
Karato	Shun-ichiro	Yale University
Kavner	Abby	University of California, Los Angeles
Kerch	Helen	U.S. Department of Energy
Kharlamova	Svetlana A.	Argonne National Laboratory
Kunz	Martin	Lawrence Berkeley Laboratory
Kuznetsov	Alexei	The University of Chicago
Lang	Jonathan	Argonne National Laboratory
Lerche	Michael	University of Illinois at Urbana-Champaign
Li	Baosheng	Stony Brook University
Li	Jie	University of Illinois at Urbana-Champaign
Liebermann	Robert C.	COMPRES
Liermann	Hanns-Peter	Carnegie Institution of Washington
Liou	Juhn G.	Stanford University
Liu	Haozhe	Carnegie Institution of Washington
Liu	Zhenxian	Carnegie Institution of Washington
Long	Gabrielle G.	Argonne National Laboratory
Long	Hongbo	Stony Brook University
Lozano	Aaron	University of Illinois at Urbana Champaign
Manghnani	Murli H.	University of Hawaii
Mao	Agnes L.	Carnegie Institution of Washington
Mao	Ho-Kwang (David)	Carnegie Institution of Washington
Mao	Wendy L.	Los Alamos National Laboratory
Meng	Yue	Carnegie Institution of Washington
Nicol	Malcolm F.	University of Nevada, Las Vegas
O'Connor	Veronica	Carnegie Institution of Washington
Parise	John B.	State University of New York, Stony Brook
Prakapenka	Vitali B.	The University of Chicago
Prewitt	Charles T.	University of Arizona
Ricolleau	Angele	Carnegie Institution of Washington
Rivers	Mark L.	The University of Chicago
Rod	Eric A.	Carnegie Institution of Washington
Romanowicz	Barbara A.	University of California at Berkeley
Ross	Nancy	Virginia Tech
Rushmer	Tracy	University of Vermont
Said	Ayman H.	Argonne National Laboratory
Seagle	Christopher T.	The University of Chicago
Selvi	Emre	Texas Tech University
Sharma	Anurag	Rensselaer Polytechnic Institute
Shen	Guoyin	Carnegie Institution of Washington
Shim	Sang-Heon (Dan)	Massachusetts Institute of Technology
Sinogeikin	Stanislav V.	Carnegie Institution of Washington
Smyth	Joseph	Colorado University
Song	Yang	The University of Western Ontario
Stevenson	David J.	California Institute of Technology

Struzhkin	Viktor V.	Carnegie Institution of Washington
Sturhahn	Wolfgang	Argonne National Laboratory
Surber	Eric	University of Illinois Urbana-Champaign
Tozer	Stan	The National High Magnetic Field Laboratory
Tseng	Yuan-Chieh	Northwestern University
Vohra	Yogesh K.	University of Alabama at Birmingham
Wang	Yanbin	The University of Chicago
Wenk	Rudy	University of California, Berkeley
Wentzcovitch	Renata M. M.	University of Minnesota
Wiedner	Don	Stony Brook University
Yang	Wenge	Carnegie Institution of Washington
Yarger	Jeff L.	Arizona State University
Yoo	Choong-Shik	Lawrence Livermore National Laboratory
Yuen	Dave A.	University of Minnesota
Zhao	Yusheng	Los Alamos National Laboratory
Zhuravlev	Kirill K.	Los Alamos National Laboratory