
“Advances in Static and Dynamic High-Pressure Crystallography”

2013 Workshop of the IUCr Commission on High Pressure

September 8th – 11th
DESY, Hamburg

Final Schedule

Sunday September 8 th		
18:00 – 20:00	Registration and Reception	Lobby of Auditorium
Monday September 9 th		
7:45 – 8:15	Registration and Breakfast	Lobby of Auditorium
8:15 – 8:20	Welcome IUCr Commission on High-Pressures	I. Loa (Secretary of Commission on High Pressure)
8:20 – 8:25	Welcome from DESY	E. Weckert (DESY)
8:25 – 8:30	Greetings from the DKG	U. Schwarz (DGK)
<i>Session A</i> <i>Rising Stars</i> <i>Chairs: Yoshinori Katayama and Francesca Fabbiani</i>		
8:30 – 9:05 (invited talk)	Experimental constraints on thermal conductivity of the core mantle boundary region	K. Ohta (Osaka U.)
9:05 – 9:40 (invited talk)	Gas Hydrates – when water meets gas under pressure	A. Falenty (U. Göttingen)
9:40 – 10:10	Coffee Break	Lobby of Auditorium

Session B Electronic and magnetic phenomena Chairs: B. Winkler and K. Kamenev		
10:10 – 10:45 (invited talk)	Pressure-induced interrelated structural and electronic transitions in α -FeOOH and Fe_2O_3	E. Greenberg (Tel-Aviv U.)
10:45 – 11:20 (invited talk)	Pressure-induced magnetic phase transition in Cr_2O_3 determined by second harmonic generation measurements	L. Bayarjargal (U. Frankfurt)
11:20 – 11:40	High pressure studies of structural and electronic properties of lead selenide	P. Bhambhani (Banasthali U.)
11:40 – 12:00	High Pressure and Low Temperature Studies on Raman Spectra and Resistivity on Bi_2Se_3 Single Crystals	V. Bhatt Sandip (Sardar Patel U.)
12:00 – 13:30	Lunch Break	Lobby of Auditorium
Session C Polymorphism and crystal chemistry Chairs: Kamil Dziubek and Przemyslaw Dera		
13:30 – 14:05 (invited talk)	Zeolite host-guest systems under pressure: towards the high pressure synthesis of zeolite/polymer nanocomposites	J. Haines (CNRS-Université Montpellier)
14:05 – 14:40 (invited talk)	Copious in Polymorphs Dabco Monosalts	A. Olejniczak (Adam Mickiewicz U.)
14:40 – 15:00	Advancing from static to dynamic diffraction studies on the high pressure melting of materials	R. Briggs (Edinburgh U.)
15:00 – 15:20	High-Pressure Mixing in the Water-Ammonia System	J. S. Loveday (Edinburgh U.)
15:20 – 15:40	Order-Disorder and Intra-phase Transitions in Incommensurate Host-Guest Potassium	E.E. McBride (Edinburgh U.)
15:40 – 16:10	Coffee Break	Lobby of Auditorium

Session D <i>Amorphous, liquid, non-crystalline and crypto-crystalline solids</i> <i>Chairs: Andrew Goodwin and Vadim Brazhkin</i>		
16:10 – 16:45 (invited talk)	Networks under Pressure	P. Salmon (U. Bath)
16:45 – 17:00	Structural Behaviour of Metallic Glasses under High Pressure	N. Mattern (IFW Dresden)
17:00 – 17:15	In-situ high-pressure XRD studies of Co-Zr metallic glass	J. Bednarcik (DESY)
17:15 – 17:30	Pressure-induced structural change in molten basalt	P. Dalladay-Simpson (U. Edinburgh)
17:30 – 18:30	Tour of Flash and PETRA III Meeting of the IUCr Commission on High-Pressure	
18:30 – 21:00	Poster Session and BBQ	DESY Cantina

Tuesday September 10 th		
Session E <i>Crystallographic controls on rheology and elasticity</i> <i>Chairs: Simon Redfern and Nori Nishiyama</i>		
8:00 – 8:30	Registration and Breakfast	Lobby of Auditorium
8:30 – 9:05 (invited talk)	Defect chemistry and Si-diffusion in forsterite	T. Katsura (BGI)
9:05 – 9:40 (invited talk)	Advances in high-pressure materials rheology: from single-crystal to aggregate plasticity	P. Raterron (CNRS / Université Lille 1)
9:40 – 10:10	Coffee Break	Lobby of Auditorium
10:10– 10:30	In-situ observation of crystallographic preferred orientation of olivine deformed in simple shear	T. Ohuchi (GRC, Ehime Univ.)
10:30– 10:50	In Situ Stress-Strain Measurements on Ringwoodite at 18 GPa and 1700 K Using a Deformation-DIA Apparatus Combined with Synchrotron Radiation	T. Kawazoe (BGI)
10:50 – 11:10	Brillouin Scattering and X-ray Diffraction of Solid Argon to 65 GPa and 700 K: Shear Strength of Argon	H. Marquardt (GFZ)
Session F <i>New Frontiers in Extreme Conditions Crystallography</i> <i>Chairs: H.-P. Liermann and Ingo Loa</i>		
11:10 – 11:45 (invited talk)	Equations of state of metals from X-ray diffraction data at static pressures above 5 Mbar	L. Dubrovinsky (BGI)
11:45 – 12:20 (invited talk)	Time-resolved studies of phase transition dynamics in Bismuth and Krypton	W. Evans (LLNL)
12:20 – 13:30	Lunch Break	Lobby of Auditorium
13:30 – 13:50	Melting Studies of iron from in-situ XRD at megabar pressures with short laser pulses	Z. Konôpková (DESY)
13:50 – 14:10	Novel high-pressure Fe ₂ O ₃ polymorph	E. Bykova (BGI)

14:10 – 14:30	Newly Developed Micro X-ray Focusing Optics for High-pressure X-ray Diffraction at SPring-8	Y. Ohishi (Spring-8)
14:30 – 14:50	New perspectives for dynamic high-pressure research: the high-energy density instrument at the European XFEL	K. Appel (Euro. XFEL)
14:50 – 15:20	Coffee Break	Lobby of Auditorium
<p style="text-align: center;">Session G</p> <p style="text-align: center;">Studies of Organic and Biological Systems</p> <p style="text-align: center;">Chairs: Andrzej Katrusiak and Elena Boldyreva</p>		
15:20 – 15:55 (invited talk)	Proton dynamics in <i>Shewanella oneidensis</i> at high pressure	P. McMillan (UCL)
15:55 – 16:30 (invited talk)	Crystallographic structure of neuroglobin under high hydrostatic pressure. A tribute to Roger Fourme	N. Colloc'h (U. Caen)
16:30 – 16:50	The Effect of Water on an Imidazolium Based Ionic Liquid	S. Saouane (U. Göttingen)
16:50 – 17:10	Pressure effect on D,L-mandelic acid racemate crystallization	M. Andrzejewski (Adam Mickiewicz U.)
17:10 – 17:30	Conformationally Assisted Compression in Methyl Benzoate	W. Cai (Adam Mickiewicz U.)
18:00	Leave for Banquet with Bus	
19:00 – 22:00	Banquet on the Alster River	
ca. 22:00	Return to DESY	

Wednesday September 11th

Session J

Computational approaches

Chairs: Nandini Garg and Rajeev Ahuja

8:00 – 8:50	Registration and Breakfast	Lobby of Auditorium
8:50 – 9:25 (invited talk)	Density Functional Theory: Applications to High-Pressure Crystallography	M. Mattesini (U. Computense Madrid)
9:25 – 10:00 (invited talk)	Melting Curve and Atomic Diffusion in Solid Molecular Hydrogen at Extreme Pressures	M. Ramzan (Uppsala U.)
10:00 – 10:30	Coffee Break	Lobby of Auditorium

Session H

Materials Science

Chairs: Wilson Crichton and Vladimir Turkevich

10:30 – 11:05 (invited talk)	Creation of bulk nanostructured ultra-hard materials by extreme conditions	Y. Le Godec (U. P&M Curie, Paris)
11:05 – 11:40 (invited talk)	The local view of materials under pressure @ ISIS and Diamond	M. Tucker (ISIS/RAL)
11:40 – 12:00	High-pressure behavior of unconventional spin-Peierls compounds TiOCl and TiPO ₄	M. Bykov
12:00 – 13:30	Lunch Break	Lobby of Auditorium
13:30– 13:50	Pressure-Temperature Phase Diagram of LuFe ₂ O ₄	J. Rouquette
13:50 – 14:10	Pressure induced water insertion in synthetic clays	A. V. Talyzin

Session I Chemistry <i>Chairs: Vladimir Solozhenko and Alexandr Talyzin</i>		
14:10 – 14:45 (invited talk)	High-Pressure Chemistry of Light Elements: New Compounds and Crystal Structures	O.O. Kurakevych (U. Paris 6)
14:45 – 15:20 (invited talk)	Recent Advances in the High-Pressure Chemistry of Alkali Metal Borates	H. Huppertz (U. Innsbruck)
15:20 – 15:50	Coffee Break	Lobby of Auditorium
15:50 – 16:25 (invited talk)	Metal Hydrides at Extreme Conditions	E. Gregoryanz (Uni. Edinburgh)
16:25– 16:45	Chemical reactions at extreme conditions – polymerization of CO and decomposition of SF ₆ in the diamond anvil cell	N. Rademacher (U. Frankfurt)
16:45 – 17:05	High-(p,T) synthesis and stability of tantalum and rhenium nitrides and their characterization	A. Friedrich (U. Frankfurt)
17:05 – 17:25	Calcium – Hydrogen System under High Pressures	S. Besedin (MPI Mainz)
17:25 – 17:45	The high-pressure behavior of the H ₂ O-CO ₂ system	D.M. Amos (U. Edinburgh)
17:45 – 18:00	Concluding Remarks	I. Loa (Secretary of Commission on High Pressure)