

Beyond Imperfections: New Structure-Property Relationships in Ceramics and Glasses

788. WE-Heraeus-Seminar

22 – 24 May 2023

at the Physikzentrum Bad Honnef/Germany

**WILHELM UND ELSE
HERAEUS-STIFTUNG**



Program (CEST)

Sunday, 21 May 2023

17:00 – 21:00 ARRIVAL and REGISTRATION

18:30 *BUFFET SUPPER*

Monday, 22 May 2023

08:00 *BREAKFAST*

09:00 – 09:15 **Welcome / Opening**

Ferroics 1
Chair: D. Meier

09:15 – 09:55 Beatriz Noheda **Ferroelastic Domain Walls as Memristive Networks**

09:55 – 10:35 Hiroko Yokota **The Investigations of Polar Domain Boundary in Ferroics**

10:35 – 11:00 *COFFEE BREAK*

Structure and Properties 1
Chair: P. Zubko

11:00 – 11:40 Jürgen Rödel **Dislocation-tuned Functionality in Ceramics**

11:40 – 12:10 Donald Evans **Nanoengineering Material Properties without Changing the Bulk Symmetry or Composition**

12:10 – 12:20 **Conference Photo (outside at the main entrance)**

12:20 – 13:30 *LUNCH BREAK*

Program (CEST)

Glasses 1

Chair: S. Kohara

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|---------------|------------------------|--|
| 13:30 – 14:10 | László Pusztai | Understanding Disordered Structures by Combining Diffraction Experiments and Computer Simulations via Reverse Monte Carlo Modelling |
| 14:10 – 14:50 | Wolf-Christian Pilgrim | Structure Determination of an Amorphous Molecular Solid with Strong Nonlinear Optical Properties |
| 14:50 – 15:20 | <i>COFFEE BREAK</i> | |

Glasses 2

Chair: A. Zeidler

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|---------------|--------------------|---|
| 15:20 – 16:00 | Matthieu Micoulaut | Properties of Network Glasses in Relationship with Elastic Phase Transitions |
| 16:00 – 16:30 | Benjamin D. Klee | Reverse Monte-Carlo Modeling in Molecular Amorphous Systems |

Forest Award Talks 1

Chair: K. Hayashi

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|---------------|-------------------------|--|
| 16:30 – 16:45 | Taro Kuwano | Insulation of Aliovalent-doped Rutile-type TiO₂ |
| 16:45 – 17:00 | Hiromi Murashige | Observation of the Length Selective Alkane Absorption in P4MP1 Films in the Small-angle Scattering Region |
| 17:00 – 17:30 | <i>BREAK</i> | |
| 17:30 – 19:00 | Poster Session 1 | |
| 19:00 | <i>DINNER</i> | |

Program (CEST)

Tuesday, 23 May 2023

08:00 *BREAKFAST*

Ferroics 2

Chair: H. Yokota

09:00 – 09:40 Dennis Meier **Structure-property Relations at Charged Interfaces in Ferroelectric and Multiferroic Oxides**

09:40 – 10:20 Pavlo Zubko **Functional Properties of Ferroelectric Superlattices with Inhomogeneous Polarisation**

10:20 – 10:50 *COFFEE BREAK*

Structure and Properties 2

Chair: D. Evans

10:50 – 11:30 Ayako Nakata **Large-scale DFT Calculations of Materials with Complex Structures**

11:30 – 12:00 Benedict Paulus **XANES Simulations of Amorphous RMC Models**

12:00 – 13:30 *LUNCH BREAK*

Structure and Properties 3

Chair: W.-C. Pilgrim

13:30 – 14:10 Kouichi Hayashi **Elucidation of Lattice Distortion in Mn-doped ZnSnAs₂ by X-ray Fluorescence Holography**

14:10 – 14:50 Tomohiro Matsushita **Photoelectron Holography of Dopants in Crystal and Defect at the Interface**

14:50 – 15:20 *COFFEE BREAK*

15:20 – 16:00 Matthias Muntwiler **Measuring True Corrugation of a h-BN Nanomesh Layer**

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Forest Award Talks 2

Chair: T. Kuwano

16:00 – 16:15	Shunta Sasaki	Local Structure Analysis of Rare-earth Rich Borate Glasses
16:15 – 16:30	Yuta Shuseki	Structural Properties of MgO–SiO₂ Liquids and Glasses
16:30 – 16:45	Tomoki Nakayoshi	Computational Study of the Effect of Active Center Reduction on the Structure of Plant-type Ferredoxin
16:45 – 17:30	<i>BREAK</i>	
17:30 – 19:00	Poster Session 2	
19:00	<i>HERAEUS DINNER at the Physikzentrum (cold & warm buffet, with complimentary drinks)</i>	

Program (CEST)

Wednesday, 24 May 2023

08:00 *BREAKFAST*

Glasses 3

Chair: B. Klee

09:00 – 09:40 Anita Zeidler **What Can and Can't We Learn from the FSDP**

09:40 – 10:20 Ying Shi **Medium-range Structure
Characterization of Silicate Glass and
its Correlation with Liquid Fragility**

10:20 – 10:50 *COFFEE BREAK*

Glasses 4

Chair: L. Pusztai

10:50 – 11:30 Milos Krbal **Formation of Oriented Layered
Transition-metal Dichalcogenides from
Amorphous Thin Films**

11:30 – 12:10 Shinji Kohara **Order within Disorder in Glasses and
Liquids**

12:10 – 12:30 **Poster Prize Awards and Closing**

12:30 *LUNCH*

End of Seminar / Departure