Past, Present and Future of Reverse Monte Carlo Modeling: Recent Challenges in Determining Structure- Property Relationship in Materials

861. WE-Heraeus-Seminar

27. – 31. July 2026

at the Physikzentrum Bad Honnef, Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Program

Monday, 27 July 2026

17:00 – 20:00	Registration	
18:00	*BUFFET SUPPER and informal get-together*	
19:30 – 20:30	Robert McGreevy	**The first 10 years of RMC and the next 10 years of ML' or 'The power of images'**

Tuesday, 28 July 2026

07:30	*BREAKFAST*	
08:45 - 09:00	Scientific organizers	**Welcome words**
09:00 – 09:40	Matt Tucker	**38 years of Reverse Monte Carlo Modelling**
09:40 – 10:20	Martin Dove	**Data quality and RMC**
10:20 – 10:50	*COFFEE BREAK*	
10:50 – 11:30	Mirijam Zobel	**Modulation Excitation Pair Distribution Function Experiments to Increase Phase Sensitivity**
11:30 – 11:45	Roman Holomb	**Laser-induced structural transformations in chalcogenides: finite-cluster approach to local structural rearrangements**
11:45 – 12:00	Adam Edward Stones	**Inverting PDFs to measure effective interactions decodes complexity in amorphous calcium carbonate**
12:00	*LUNCH*	

Program

Tuesday, 28 July 2026

14:00 – 14:40	Thibault Charpentier	**Designing structural disorder in oxide glasses from NMR: A Reverse Monte Carlo approach**
14:40 – 15:20	Dora Zalka	**RMC-XANES builder: A flexible workflow for XANES calculations**
15:20 – 15:50	*COFFEE BREAK / Flash poster test*	
15:50 – 17:00	**Flash poster session**	
17:00 – 18:00	**Poster session**	
18:00	*DINNER*	
19:30 – 20:30	**Poster session** (continued)	

Program

Wednesday, 29 July 2026

07:30	*BREAKFAST*	
08:45 – 09:25	Alexei Kuzmin	**From atomic structure to color switching**
09:25 – 10:05	Markus Winterer	**Combining Reverse Monte Carlo analysis of X-ray scattering and extended X-ray absorption spectroscopy**
10:05 – 10:35	*COFFEE BREAK*	
10:35 – 11:15	Ildiko Pethes	**Using EXAFS in RMC++ for amorphous materials: Features and advantages**
11:15 – 11:30	Hanna M. Wenzel	**Molecular RMC on tetrel-chalcogenid clusters with extreme nonlinear optical properties**
11:30 – 11:45	Thomas Nicholas	**The structure and topology of an amorphous metal–organic framework**
11:45 – 12:00	Valeri Petkov	**Resonant total scattering and differential PDFs in Reverse Monte Carlo modeling**
12:00	*LUNCH*	
13:30 – 18:00	**Excursion**	
18:30	*HERAEUS DINNER* *(social event with cold & warm buffet with complimentary drinks)*	

Program

Thursday, 30 July 2026

07:30	*BREAKFAST*	
08:45 – 09:25	David Keen	**Measuring total scattering data faster than the timescales of dynamical processes: implications for structural modelling**
09:25 – 10:05	Karen Appel	**Application of single shot pair distribution function techniques during shock compression at EuXFEL to study melt structure in-situ**
10:05 – 10:35	*COFFEE BREAK*	
10:35 – 11:15	Andrew Goodwin	**Understanding amorphous networks with HRMC**
11:15 – 11:30	Wojciech Slawinski	**RMC reveals hidden complexity in D_2O Ice VII**
11:30 – 11:45	Ida Nielsen	**Local structure of hydrated and dehydrated prussian white cathode materials**
11:45 – 12:00	Ying-Lung Steve Tse	**Flexible polarizable water model parameterized via gaussian process regression**
12:00	*LUNCH*	

Program

Thursday, 30 July 2026

14:00 – 14:40	Andrea Fantin	**Chemical short-range order in high-entropy alloys: Experimental limitations and implications for Reverse Monte Carlo modeling**
14:40 – 14:55	Lewis Owen	**Exploring local structure in metallic systems - challenges and opportunities**
14:55 – 15:10	Niels Schreiner	**Characterization of short range order in Ni_4Mo and its disorder-order transition through total scattering and Reverse Monte Carlo modelling.**
15:10 – 15:40	*COFFEE BRREAK*	
15:40 – 15:55	Lei Tan	**RMC Study of local structure and disorder in inorganic halide lead perovskite quantum dots**
15:55 – 16:10	Long Yang	**3D Probing of hidden nanoscale states in functional materials**
16:10 – 16:25	Akihisa Koga	**Stealthy hyperuniform bond disorder in the honeycomb Hubbard model**
16:25 – 18:00	**Poster** session	
18:00	*DINNER*	

Program

Friday, 31 July 2026

07:30	*BREAKFAST*	
08:45 – 09:25	Yohei Onodera	**Density-driven interplay of pentahedral pyramids and octahedra for high dielectric permittivity in bulk amorphous alumina**
09:25 – 09:40	Pál Jóvári	**Short-range order in $GeSb_2S_5$-Ag glasses**
09:40 – 10:20	Ayako Nakata	**Efficient analysis of local properties in complex systems by large-scale DFT and statistical methods**
10:20 – 10:50	*COFFEE BREAK*	
10:50 – 11:30	Albert Bartok-Partay	**Structure elucidation using machine learning based property predictions and interatomic potentials**
11:30 – 11:45	Yuanpeng Zhang	**Combining exhaustive symmetry and attention based learning for phase transition studies**
11:45 – 12:00	Scientific organizers	**Closing words**
12:00	*LUNCH*	

End of the seminar and departure

NO DINNER for participants leaving on Saturday; however, a self-service breakfast will be provided on Saturday morning