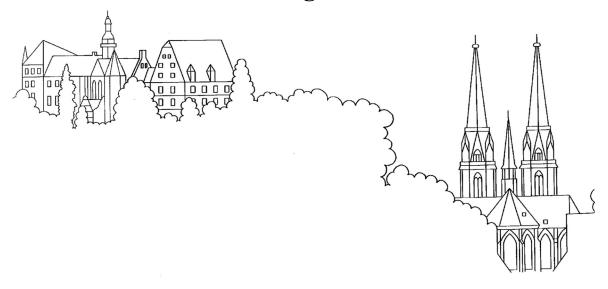
### Program



# 4<sup>th</sup> ELSICS Conference and International Bunsen-Discussion Meeting on

## **Energy Landscapes and Structure in Ion Conducting Solids (ELSICS)**

## September 30 – October 2, 2024

Conference location TTZ Conference Center, Marburg, Germany Software-Center 3, 35037 Marburg

#### **Contact:**

Prof. Dr. Karl-Michael Weitzel Philipps-Universität Marburg, Department of Chemistry Phone: +49 6421-282-2360 (weitzel@chemie.uni-marburg.de) <u>www.uni-marburg.de/fb15/ag-weitzel/</u> <u>www.uni-marburg.de/en/fb15/for5065</u>

## Program: 4th ELSICS Conference 2024 in Marburg Energy Landscapes and Structure in Ion Conducting Solids (ELSICS) September 30<sup>th</sup> – October 2<sup>nd</sup>, 2024

Monday, 30<sup>th</sup> September

Time	Name	Title	Nr
12:00	Welcome remarks	Chairman: Karl-Michael Weitzel	
12:30 – 13:15	Invited # 1 Hellmut Eckert	Crystallization Mechanisms of NASICON-type Glass-Ceramic Electrolytes and Related Systems Studied by Solid-State NMR	01
13:15 – 13:45	Michael Vogel	Distribution of Activation Energies for Lithium Ion Jumps in Various Types of Solids Revealed by NMR Field- Cycling Relaxometry	02
13:45 – 14:30	Invited # 2 Leo van Wüllen	Local Cation Coordination and Dynamics in Solid Electrolytes or NMR is Wunderbar	O3
14:30 – 15:00	Martin Wilkening	NMR at cryogenic Temperatures to Study Lithium-ion Dynamics in Electrolytes with Ultrafast Charge Carriers	04
15:00 – 15:30	Coffee break		
15:30 – 16:15	Invited # 3 Katsuyo Thornton	Examining the Role of Mechanics in Electrochemical Systems	O5
16:15 – 16:45	Philipp Maass	Modeling Charge Attachment Induced ion Transport in Glasses	O6
16:45 – 17:15	Marco Bertani	ECOSISTER. Computational Study of Mixed Oxy-Sulfide Glassy Solid Electrolytes for Sodium-Based Batteries	07
18:00	Dinner (on your own)		

## Tuesday, October 1st

Time	Name	Title	Nr.
8:30 – 9:15	Invited # 4 Yue Qi	Interface Potentials inside Solid- State Batteries: Origins and Implications	08
9:15 – 9:45	Jacob group: Carmen Fuchs	Modeling Cationic Diffusion in Crystalline SrTiO <sub>3</sub> : a DFT+U Study on Transport	O9
9:45 – 10:30	Invited # 5 Payam Kaghazchi	Configurational Space Sampling and Multiscale Structure Calculation of Complex Ionic Crystals	O10
10:30 – 11:00	Coffee break		
11:00 – 11:45	Invited # 6 Dina Fattakhova- Rohlfing	How Grain Boundaries Affect the Performance of Garnet Solid-State Batteries	011
11:45 – 12:15	Joos group: Qian Ma	Study on the Diffusion of Cobalt lons in Strontium Titanate	012
12:15 – 12:45	Ben Zion	Effect of Hydration on Electrical and Electromechanical Properties of Lanthanum-Cerium Oxides	O13
12:45 – 13:45	Lunch		
13:45 – 14:30	Invited # 7 Takahisa Omata	Mixed Protonic and Electronic Conduction in n-type Oxide Semiconductors	014
14:30 – 15:00	Weitzel group: Kevin Rein	Alkali deuteron substitution in a S53P4 bioglass	O15
15:00 – 15:30	Weitzel group: Timo Kassubek	Lithium Diffusion in Doped and Undoped Crystalline Silicon	O16
16:00 – 16:30	Coffee break		
16:30 – 19:00	Free Time for Discussion and Sightseeing		
19:00 - 22:00	Conference Dinner	Restaurant Bückingsgarten	

## Wednesday, October 2<sup>nd</sup>

Time	Name	Title	Nr.
9:00 – 9:45	Invited # 8 Manfred Martin	Kinetics of Unmixing Caused by Electrochemical Potential Gradients	017
9.45 – 10:15	Reona Miayazaki	Ion Dynamics in Li+/Na+ Mixed Halide Solid Electrolytes and the Charge-Discharge Performances of the Solid-State Battery using Nal- NaBH <sub>4</sub> -Lil Electrolyte	O18
10:15 – 11:00	Invited # 9 Rotraut Merkle	Effects of Acceptors in Triple- Conducting Perovskites	O19
11:00 – 11:30	Coffee Break		
11:30 – 12:15	Invited # 10 Jincheng Du	Elucidating the Effect of Anion Doping on Lithium Ion Transport in LLZO-based Solid Electrolytes from Atomistic Computer Simulations	O20
12:15 – 12:45	Andreas Heuer	Impact of Interfaces on the Lithium Dynamics in Electrolytes	O21
12:45 – 13:00	Rotraut Merkle	Introduction to space charge zones	O22a
13:00 – 13:15	Jooss group: Iniyan Sivakumar	Investigation of Atomic, Chemical and Electric Field Structure of Low-Angle Grain Boundary in SrTiO <sub>3</sub>	O22b
13:15 – 14:15	Lunch		
14:15 – 15:00	Invited #11 Yug Joshi	Multiscale Investigations of Lithium Diffusion and Phase Transformation: APT to optical microscopy	O23
15:00 – 15:45	Volkert group: Jan-Erik Rybka	Unlocking SrTiO <sub>3</sub> for APT: A Correlative Atomic-Scale Investi- gation of a SrTiO <sub>3</sub> Grain Boundary	O24a
	Annika Korn	Nanoindentation of Surface Ion- Exchanged Borosilicate Glass	O24b
15:45 – 16:15	Weitzel group: Victor Gunawan Martin Schäfer	Alkali Ion Transport in Lithium Borate Glass: New Insights from Double- CAIT experiments	O25
16:15	Closing remarks	Chairman: Karl-Michael Weitzel	
16:30	Coffee to go		
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