

# 1st ELSICS workshop

13. – 14. September 2021

Energy Landscapes and Structure in Ion Conducting Solids (ELSICS)

Monday, 13. September 2021

Before noon: Arrival of participants

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Time	Name	Title
12.30	<b>Welcome remarks</b> Chairman Prof. Dr. Weitzel	
	<b>Transport 1</b>	
13:00 - 13:45	Prof. Dr. Manfred Martin (Aachen) (Invited)	<i>Ion Transport in Oxide Electrolytes for Energy Conversion</i>
13:45 - 14:05	Dr. Jan Wiemer (Marburg)	Li <sup>+</sup> Ion Site Energy Distribution in Lithium Aluminum Germanium Phosphate
14:05 - 14:25	Dr. Martin Schäfer (Marburg)	Li <sup>+</sup> Ion Site Energy Distribution in Lithiumborate
	<b>Transport 2</b>	
14:30 - 15:15	Dr. Rotraut Merkle (Stuttgart) (Invited)	<i>Oxygen vacancies and protons in perovskites</i>
15:15 - 15:35	Daniel Uxa (Clausthal-Zellerfeld)	Activation Enthalpies of Lithium Tracer Diffusion in Lithium-Metal- Oxide Compounds for Lithium-Ion Batteries
15:35 - 15:55	Hongchu Du (Aachen)	Imaging and spectroscopy of oxygen vacancies and Ti valence states in SrTiO <sub>3</sub>
16.00 – 16.30	<b>Coffee break</b>	
	<b>Atom Probe Tomography</b>	
	Prof. Dr. Dr. h.c. Guido Schmitz (Stuttgart, Invited)	<i>Atom probe tomography: A useful tool for solid state ionics?</i>
	Jan Erik Rybak (Göttingen)	Atom Probe Analysis of a Lithium Borate Glass
	Dr. David Diercks (Golden, CO, USA)	Correlative Microscopy for Preparation and Analysis of

		Ceramics by Atom Probe Tomography
19:00 - 21:00	<b>Dinner</b>	

## Tuesday, 14. September 2021

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Time	Name	Title
	<b>Theory 1</b>	
9.00 - 9:45	Prof. Dr. Jürgen Horbach (Düsseldorf, Invited)	<i>Elucidating the ion transport in amorphous solids via computer simulation of simple model systems</i>
9:45 - 10:05	Marco Bosi (Osnabrück)	Predicting conductivities based on site energy distributions in ion conducting network glasses
10:05 - 10:25	Prof. Sergei Baranovski (Marburg)	On the conduction mechanism in ionic glasses
	<b>Theory 2</b>	
10:30 - 11:15	Prof. Dr. Eckhard Spohr (Duisberg-Essen, Invited)	<i>Computer Simulations of Electrolyte Solutions near Interfaces: From Liquids to Confined Solids</i>
11:15 - 11:25	Carmen Fuchs (Ulm)	Theoretical Studies on the Ion Migration through crystalline materials
11:25 - 11:55	Dr. Steffen Grieshammer (Aachen)	Kinetic Monte Carlo simulations of ionic conductivity in crystals
12:00 - 13:30	<b>Lunch</b>	
	<b>Nuclear Magnetic Resonance</b>	
13:30 - 14:15	Prof. Dr. Paul Heitjans (Hannover) (Invited)	<i>Ion Dynamics and Transport in Solids as Seen by Solid State Nuclear Magnetic Resonance Techniques</i>
14:15 - 14:35	Frau Edda Winter (Darmstadt)	<sup>7</sup> Li Field-Cycling and Field-Gradient NMR Studies of Ion Transport in Solids

14:35 - 14:55	Dr. Katharina Hogrefe (Graz)	With a Little Help from $^{31}\text{P}$ NMR: From Localized Hopping to Long-Range $\text{Li}^+$ Transport in Argyrodite-Type $\text{Li}_6\text{PS}_5\text{I}$
	<b>Electron Microscopy</b>	
15:00 - 15:45	Prof. Dr. Christina Scheu (Düsseldorf) Invited,	<i>Unraveling structure and imperfections of functional oxides</i>
15:45 - 16:05	Prof. Christian Jooss (Göttingen)	On the relation between grain boundary segregation and built in electric fields
16:05 - 16:25	Dr. Xian Kui Wei (Aachen)	In-situ TEM study of structural transition pathway in energy-storage $\text{PbZrO}_3$ at atomic resolution
16.30 – 17.00	<b>Coffee break</b>	
17.00 – 18.00	<b>Round table discussion</b>	
18.00	<b>Closing remarks</b>	