Curriculum vitae

PERSONAL INFORMATION

Family name, First name: Rettenwander, Daniel

ORCID: 0000-0002-2074-941X

Date of birth: May 13th, 1981

Nationality: Austria

URL for web site: https://www.tugraz.at/institute/ictm/research/rettenwander-group/

MAIN RESEARCH AREAS

Synthesis and characterization of structure-property relationships in single crystal, ceramics, and composite ceramic/polymer materials for energy applications, including solid-state batteries ▪ Electrochemical analysis, including micro-contact impedance spectroscopy, of material inhomogeneity effects on battery performance ▪ Electrochemical and structural analysis of material degradation and failure mechanisms of energy materials under various environmental, thermal, and electrochemical conditions

EDUCATION

2014/07 Dr. techn. (PhD) in Materials Science, University of Salzburg, Salzburg, Austria.
Thesis title: "*A study to get a crystal chemical insight in $Li_7La_3Zr_2O_{12}$ doped with Fe^{3+}, Al^{3+} and Ga^{3+}*", Supervisior: Prof. Georg Amthauer

2011/10 Mag. rer. nat. (MSc) in Chemistry, Karl-Franzens University of Graz, Austria, Diploma Thesis title: *Computational Characterization of Methionine,* Supervisor: Prof. Georg Gescheidt.

CURRENT & PREVIOUS POSITIONS

Since 2017/05 **Habilitand** at the Institute of Chemistry and Technology of Materials (ICTM), Graz University of Technology (TUG), Graz, Austria.
Main achievements: Approved stand-alone project grant from the Austrian Science agency (€400,000). Receipt of the Habilitation Award of the Austrian Chemical Society, 2018.

2016 – 2017 **Postdoctoral Associate** at the Department of Materials Science & Engineering at the Massachusetts Institute of Technology (MIT), Cambridge, USA, Prof. Yet-Ming Chiang
Main achievements: Design and construction of in-situ X-ray diffraction devices enabling electrochemical measurement at temperatures up to 800 °C in reactive atmospheres to investigate electrochemically driven phase transitions in hydrogen-loaded metal thin films.

2014 – 2015 **Postdoctoral Associate** at the Department of Chemistry and Physics of Materials at the University of Salzburg, Austria, Prof. Georg Amthauer
Main achievements: First micro-contact impedance spectroscopy measurements of single crystals in the µm-scale. Observation of a not-before-considered space group for Ga-stabilized $Li_7La_3Zr_2O_{12}$ (LLZO) explaining its high Li-ion conductivity. Discovery of new supervalent cations to stabilize the cubic LLZO garnet modification. Receipt of the Christian Doppler Award for materials science.

AWARDS & FELLOWSHIPS

2018 Habilitation Award of the Austrian Chemical Society (GÖCH) - € 2,000.-

2018 Recipient of the Initial funding program of the TUG 2018, 10th call - € 6,000.-

2017 Recipient of the Initial funding program of the TUG 2017, 10th call - € 10,000.-

2016 Christian-Doppler Award for Natural Science of the Austrian Government - € 3,000.-

2016 Recipient of the research-funding scheme "International Communication" of the Austrian Research Association (ÖFG)

2014 Recipient of the research-funding scheme "International Communication" of the Austrian Research Association (ÖFG)

2012 Visiting Research Fellowships HPC-Europa 2 Transnational Access program at the Department of Chemistry at the University of Helsinki, Finland

KEYNOTE LECTURES AT CONFERENCES

2018 International Meeting on Energy Storage Devices, Roorkee, India, 2018.

INVITED TALKS TO CONFERENCES

2019 2nd World Conference on Solid Electrolytes for Advanced Applications: Garnets And Competitors, Shizuoka, Japan, 2019, will be announced.

2018 National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, 2018, Solid electrolytes: From single crystalline materials to application.

2018 Journal of Electroceramics Board Workshop on Advance Electronic Materials, 2018, "The interplay of ionic conductivity and crystal chemistry in ceramic electrolytes for all solid-state batteries"

2017 21st International Conference on Solid State Ionics, I-3 All Solid-State Batteries in Padua, Italy, 2017, "Structure-property relationships of single crystalline Li/Na-ion conducting solid electrolytes"

2016 IUMRS-ICEM, Symposium G, Advances in Smart Energy Storage for a Sustainable Energy Future – Electrochemistry, Mechanics and Applications in Singapore, 2016 "Crystal structure of garnet-related Li-ion conductor $Li_{7-3x}Ga_xLa_3Zr_2O_{12}$: Fast Li-ion conduction caused by a different cubic modification?"

2015 Workshop on Solid Lithium Ion Conductors in Vienna, Austria, 2015, "High Performance Li-Ion Conducting Ceramics for All- Solid-State-Li-Ion Batteries: The SoLiK Project"

COMMISSIONS OF TRUST

2018 Member of the International Advisory Board, International Conference on Electroceramics (ICE-2019)

Since 2017 Member of editorial board - Journal of Electroceramics.

2017 Co-Editor - Special Issue: All Solid-State Batteries in the Journal of Electroceramics

Since 2013 Regular reviewer for: Advanced Materials, Advanced Energy Materials, Journal of Material Chemistry A, Journal of Physical Chemistry Letters, Journal of Physical Chemistry C, Solid State Ionics, Journal of Electroceramics, Journal of the American Ceramic Society

ORGANISATION OF SCIENTIFIC MEETINGS

2017 Session Chair: 21st International Conference on Solid State Ionics in Padua, Italy

2016 Session Chair: IUMRS-ICEM in Singapore

MEMBERSHIPS OF SCIENTIFIC SOCIETIES

Austrian Chemical Society, Material Research Society, Austrian Ceramic Society

SUPERVISION OF GRADUATE STUDENTS

Ongoing 5 PhD (Caroline Hiebl, Patrick Posch, Isabel Hanghofer, Martin Philipp, Lukas Ladenstein, / 2 Master Students (Isabel Diem, Astrid Kiesl, Sarah Eisbacher), Graz University of Technology, Austria.

2017 – 2018 2 Master Student (Lukas Ladenstein (now PhD), 5 Bachelor Students, Graz University of Technology, Austria.

2013 – 2016 2 PhD students (Reinhard Wagner, Maria Maier) 1 Master Students (Christian Arrer), 2 Bachelor Students, University of Salzburg, Austria.

TEACHING ACTIVITIES

2018 Class – Lecture about "Batteries and Supercapacitors" @TUG, 3h/week.

2018 Lab course – Basics of Chemistry

2017/2018 Lab course – Technical Chemistry

2017/2018 Lab course – Technical Chemistry II

MAJOR COLLABORATIONS

Prof. J. Fleig (Vienna University of Technology, Vienna, Austria): Collaboration in a FWF project on the "Nature of Interface in All Solid-State Batteries" Within the project the collaborator is depositing electrode materials on ceramic electrolytes by pulse laser deposition and RF magnetron sputtering.

Prof. Y.-M. Chiang, Prof. J. Rupp, Prof. B. Yildiz (MIT, Cambridge, MA, USA): Chiang: Collaboration in the investigation of Li dendrite formation in single crystalline electrolytes. Yildiz: Collaboration in the study of interfaces between solid electrolyte and cathodes by high energy X-ray photoelectron spectroscopy. Rupp: Close collaboration on garnets and the preparation of ceramic thin-film for energy applications.

Prof. Martin Wilkening (Graz University of Technology, 8010 Graz, Austria): He strongly supports my work by providing me with access to equipment and existing know-how in NMR spectroscopy, which is highly valuable and important for the proposed work.

Dr. L. Miara (Samsung, Boston, MA, USA): Collaborator for theoretical calculations in order to interpret experimental observations on a fundamental level

Dr. M.M. Doeff (LBNL, Berkeley, CA, USA): Collaboration on composite electrolytes and electrodes.

Prof. Günther Redhammer (University of Salzburg, Austria): Collaboration on structure property relationships in solid electrolytes (e.g., garnets, NASICON, anti-perovskites) using diffraction techniques.

ON-GOING GRANTS

Project Title	*Funding source*	*Amount (Euros)*	*Period*	*Role of the PI*	*Relation to current ERC proposal*
The nature of interfaces in all solid-state batteries	Austrian Science Fund (FWF)	405k	2018/09 - 2021/08	PI	none

FINISHED GRANTS

Project Title	*Funding source*	*Amount (Euros)*	*Period*	*Role of the PI*	*Relation to current ERC proposal*
"SoLiK" - High Li-ion conducting ceramics for all solid state batteries	Austrian Research Promotion Agency (FFG)	780k	2014/5 – 2017/4	Co-applicant	none
NDA	Toyota Europe	80k		Co-applicant	none
NDA	Toyota Europe	80k		Co-applicant	none
NDA	Toyota Europe	80k		Co-applicant	none

ACCESS TO CENTRAL FACILITIES[a]

Project Title	*Facility /Device*	*Project ID*	*Date*	*Measure time (d)*	*Role of the PI*	*Relation to ERC proposal*
Neutron Powder Diffraction Study on Al and Ga in Mixed Doped $Li_{5.8}Ga_{0.4-x}Al_xLa_3Zr_2O_{12}$ Garnet Solid Solutions with x = 0.0—0.4	ILL/ D20	5-22-735	2015/06/07 - 2015/07/07	1	PI	none
Neutron Powder Diffraction Study on Bi Doped $Li_{7-x}La_3Zr_{2-x}Bi_xO_{12}$ Garnet Solid Solutions with *x* = 0.1-1.0	ILL/ D2b	5-26-216	2015/11/30 - 2015/12/02	2	Co-PI	none
Neutron Powder Diffraction Study on Mo Site Preference in $Li_{6.25}La_3Zr_{1.75}Mo_{0.25}O_{12}$ Garnet	ILL/ D2b	EASY-258	2014/12/19 - 2014/12/20	2	PI	none
Neutron Powder Diffraction Study on garnet-type Li-ion conductor $Li_{7-3x}Fe_xLa_3Zr_2O_{12}$ (x = 0.16, 0.24)	HZB/ E9	161037 45-ST-1.-N	2016/01/25 - 2016/01/27	3	Co-PI	none
Neutron Powder Diffraction Study on "garnet-similar" Li-ion conductor $Li_{7-3x}Ga_xLa_3Zr_2O_{12}$: Fast Li-ion conduction caused by a new cubic modification?	MLZ/ SPODI	11307	2016/08/09 - 2016/08/11	3	Co-PI	none
A Neutron Diffraction study of $Li_{6.28}Al_{0.24}La_3Zr_2O_{12}$ and $Li_6La_3ZrTaO_{12}$ Single Crystals[b]	MLZ/ Heidi	11478	2016/11/14 - 2016/12/04	21	PI	none
Probing the Li-ion transport in Lithium-Rich $Li_3OCl_{1-x}Br_x$ Anti-Perovskite Superionic Conductors	MLZ/ SPODI	14092	2018/02/23-2018/02/24	2	PI	none
A high temperature neutron Diffraction study of $Li_7La_3Zr_2O_{12}$ and $Li_6La_3ZrTaO_{12}$ single crystals	MLZ/ HEIDI	13984	2018/04/24 - 2018/05/08	15	Co-PI	none
Li-position and temperature dependent Li-diffusion in NASICON – type $Li_{1+x}Ti_{2-x}Fe_x(PO_4)_3$ solid solution compounds (x = 0.6, 0.8, 1.5)	MLZ/ SPODI	14363	NN	1	Co-PI	none
The impact of Li-ion insertion on the diffusion mechanism in $Li_{3+x}V_{(3-x)_2}(PO_4)_3$ anodes	MLZ/ SPODI	14739	NN	4	PI	none
Li-position and temperature dependent Li-diffusion in NASICON – type $Li_{1+x}Ti_{2-x}Fe_x(PO_4)_3$ solid solution compounds (x = 0.5, 0.75, 1.5)	MLZ/ SPODI	14329	NN	4	Co-PI	none

[a] MLZ: Maier Leibnitz Zentrum, FRM-2 Garching; HZB: Helmholz-Zentrum Berlin, BER-1; ILL: Institute Laue , Grenoble (F). [b]highlight proposal of the proposal round N. 23 at the MLZ

FIVE MOST IMPORTANT PUBLICATIONS [Citations]

Rettenwander, D.; Preishuber-Pflügl, F.; Cheng, L.; Wagner, R.; Welzl, A.; Suard, E.; Redhammer, G.; Doeff, M. M.; Wilkening, M.; Fleig. J.; Amthauer, G. *Structural and Electrochemical Consequences of Al and Ga Cosubstitution in $Li_7La_3Zr_2O_{12}$ Solid Electrolytes: Chem. Mater.*, **2016**, 28, 2384-2392, DOI: 10.1021/acs.chemmater.6b00579.

This paper shows for the first time that a phase transition from garnet to a "non-garnet-like" space group is responsible for the order of magnitude higher Li-ion conductivity observed in Ga-stabilized Li-oxide garnet compared to its Al analogue. A wide spectrum of methods was applied to show that the improvement is due to higher Li-ion diffusivity caused by a change in the Li-ion diffusion mechanism in the altered Li-ion sub-lattice. The paper is prepared based on my ideas, and studies are performed either by myself or by others under my supervision as PI. Based on this publication, I was recently awarded the Habilitation Award of the Austrian Chemical Society. [42]

Rettenwander, D.; Welzl, A.; Pristat, S.; Tietz, F.; Redhammer, G.; Fleig. J. *A microcontact impedance study on NASICON-type $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ ($0 < x < 0.5$ single crystals* ***2015****, J. Mater. Chem. A* 2016,**4**, 1506-1513, DOI: 10.1039/C5TA08545D.

In this publication, I developed a method to study the Li-ion conductivity of small single crystals (< 100 µm) by micro-contact impedance spectroscopy using small circular Pt electrodes (30 µm). Finite element calculations were used to validate the quality and accuracy of this method and its results. The impedance data were correlated to single crystals diffraction data to understand the underlying structure-property relationships. Based on this study we were able to provide an explanation for a huge jump in the Li-ion conductivity of $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ after the first incorporation of Al into the NASICON structure. The paper has been cited 26 times and is the basis of several follow up studies as well as an FWF grant application, which is currently under evaluation. [22]

Porz, L.; Swamy, T.; Sheldon, B. W.; **Rettenwander, D.**; Frömling, T.; Thama, H. L.; Berendts, S.; Uecker, R.; Carter, W. C.; Chiang, Y.-M. *Mechanism of Lithium Metal Penetration through Inorganic Solid Electrolytes: Adv. Energy Mater.* **2017**, 1701003, DOI: 10.1002/aenm.201701003.

This paper is an example of a successful collaboration among groups from MIT, Brown University, and Graz University of Technology. We demonstrated and provided a model for the first time that Li dendrites can penetrate even through single crystals garnets using a mechanism that is governed by a combination of surface defects, crack formation, and the current density applied. Studying the limitations of these materials in the presence of Li is a very important contribution to the field of batteries, since solid electrolytes, such as these garnets, have been widely considered as a replacement for traditional liquid electrolytes in creating a stable barrier against Li metal dendrites. [29]

Rettenwander, D.; Welzl, A.; Fleig, J.; Musso, M.; Amthauer, G. *Synthesis, Crystal Chemistry, and Electrochemical Properties of Cubic Phase $Li_7La_3Zr_2O_{12}$ Garnet – The substitution of Zr^{4+} by Mo^{6+}: Inorg. Chem.* **2015**, 54, 10440-10449, DOI: 10.1021/acs.inorgchem.5b01895.

This paper shows my ability to synthesize new compositions of Li-oxide garnets, which crystallize in highly conductive cubic crystal structures. (In previous papers, I have also shown that other transition metals such as Fe can be used, Rettenwander, D.; et al. Inorg. Chem. 2013, 52, 8005-8009). These results are, in particular, important for the proposed work within the START award application, since similar strategies to boost Li-ion conductivity are used. Furthermore, in this publication we demonstrate exemplary methodology for how Li-oxide garnets should be analyzed by impedance spectroscopy to differentiate between various electrical contributions to the total conductivity and how they should be related to structural features. The work was performed either by myself or by others under my supervision and is fully based on my ideas. [23]

Hanghofer, I.; Redhammer, G. J.; Rohde, S.; Hanzu, I.; Senyshyn, A.; Wilkening, H. M.. R.; **Rettenwander, D.** *Untangling Structure and Dynamics of Lithium-Rich Anti-Perovskites Envisaged as Solid Electrolytes for Batteries: Chem. Mater.*, **2018**, accepted.

To untangle the various stories about Li-rich anti-perovskites (LiRAPs) presented in literature we used in situ powder X-ray diffraction (XRD), neutron diffraction, nuclear magnetic resonance (NMR) spectroscopy, and impedance spectroscopy to correlate atomic structure with dynamic properties. In this contribution we present the first structural models for the cubic and orthorhombic polymorphs of $Li_{3-x}(OH_x)Cl$, including structural details for hydrogen atoms present. Moreover, we utilized in situ XRD to unambiguously reveal the extreme air-sensitivity of LiRAPs when exposed to air, a fact that drastically weakens arguments for the stability of glassy LiRAPs that were claimed to have record-breaking ionic conductivities in earlier studies. Since these materials are consider to be the Holy Grail to realize next generation Li-ion batteries, a strong impact on the field is expected. This contribution is my first paper as a PI at the TUG and an example of the successful supervision of PhD students.

FULL LIST OF PUBLICATIONS

[40] Hanghofer, I.; Eisbacher, S. L.; Uitz, M.; Henning, V.; Bitschnau, B.; Rettenwander, D.; Wilkening, H. M. R., *Structure and ion dynamics of agryodite materials*, **2018**, under review.

[39] Swamy, T.; Park, R.; Sheldon, B.; Rettenwander, D.; Porz, L.; Berendts, S.; Uecker, R.; Carter, C.; Chiang, Y.-M. *Lithium Metal Penetration Induced by Electrodeposition through Solid Electrolytes: Example in Single-Crystal $Li_6La_3ZrTaO_{12}$ Garnet*, **2018**, under review.

[38] Benck, J. D.; Jackson, A.; Young, D.; Rettenwander, D.; Chiang, Y.-M., *Apparatus for Operando X-ray Diffraction of Fuel Electrodes in High Temperature Solid State Electrochemical Cells*, **2018**, under review.

[37] Young, D.; Jackson, A., Fork, D.; Sadat, S.; Rettenwander, D.; Benck, J.; Chiang, Y.-M., *An operando calorimeter for high temperature electrochemical cells*, **2018**, under review.

[36] Benck, J. D.; Jackson, A.; Young, D.; Rettenwander, D.; Chiang, Y.-M., *Producing High Concentrations of Hydrogen in Palladium via Electrochemical Insertion from Aqueous and Solid Electrolytes*, **2018**, under review.

[35] Di Stefano, D.; Miglio, A.; Robeyns, K.; Filinchuck, Y.; Lechartier, M.; Senyshyn, A.; Ishida, H.; Spannenberger, S.; Prutsch, D.; Lunghammer, S.; Rettenwander, D.; Wilkening, M.; Roling, B.; Kato, Y.; Hautier, G., *Superionic diffusion through frustrated energy landscape*, **2018**, under review.

[34] Schoiber, J.; Fischer, P.; Berger, R. J.; Redhammer, G. J.; Mariano, M.; Tippelt, G.; Rettenwander, D.; Senyshiyn, A.; Fleig, J.; Wohlfahrt-Mehrens, M.; Hüsing, N., *$MgMPO_4F$ (M = Mn, Fe, Co) as an Insertion Material?*, **2018**, under review.

[33] Wachter-Welzl, A.; Smetaczek, S.; Brunauer, G. C.; Bonta, M.; Rettenwander, D.; Taibl, S.; Limbeck, A.; Amthauer, G.; Fleig, J., *Li-ion conductivity fluctuations within $Li_7La_3Zr_2O_{12}$ solid electrolytes and their relation to local stoichiometric changes*, **2018**, under review.

[32] Prutsch, D.; Gadermaier, B.; Brandstätter, H.; Pregartner, V.; Stanje, B.; Wohlmuth, D.; Epp, V.; Rettenwander, D.; Wilkening, H. M. R., *Anomalous spin relaxation in nanocrystalline β-Li_3PS_4 reveals snake-like Li diffusion in an isotropic matrix, Chem. Mater.*, **2018**, accepted.

[31] Hanghofer, I.; Redhammer, G. J.; Rohde, S.; Hanzu, I.; Senyshyn, A.; Wilkening, M.; Rettenwander, D., *Untangling Structure and Dynamics of Lithium-Rich Anti-Perovskites Envisaged as Solid Electrolytes for Batteries, Chem. Mater*, **2018**, accepted.

[30] Rettenwander, D.; Wilkening, M. Lithium-Festelektrolyte für Energiespeicher, Nachrichten aus der Chemie, **2018**, 499-504. DOI: 10.1002/nadc.20184066404

[29] Lunghammer, S.; Prutsch, D.; Breuer, S.; Rettenwander, D.; Hanzu, I.; Ma, Q.; Tietz, F.; Wilkening, M., ^{23}Na NMR spin-lattice relaxation reveals ultrafast Na ion dynamics in the solid electrolyte $Na_{3.4}Sc_{0.4}Zr_{1.6}(SiO_4)_2PO_4$, *Scientific Reports*, **2018**, 8, 11970, DOI: 10.1038/s41598-018-30478-7.

[28] Lunghammer, S.; Ma, Q.; Rettenwander, D.; Tietz, F.; Wilkening, M., Bulk and grain-boundary ionic conductivity in sodium zirconophosphosilicate $Na_3Zr_2(SiO_4)_2PO_4$ (NASICON), Phys. Chem. Lett. **2018**, 701, 147-150, DOI: 10.1016/j.cplett.2018.04.037.

[27] Rettenwander, D.; Redhammer, G.; Guin, M.; Pristat, S.; Tietz, F.; Fleig. J., *Arrhenius behaviour of the bulk Na-ion conductivity in $Na_3Sc_2(PO_4)_3$ single crystals observed by microcontact impedance spectroscopy, Chem. Mater.*, **2018**, 30, 1776-1781, DOI: 10.1021/acs.chemmater.8b00179.

[26] Rettenwander, D.; Wagner, R.; Reyer, A.; Bonta, M.; Cheng, L.; Doeff, M. M.; Limbeck, A.; Wilkening, M.; Amthauer, G. *Interface instability of Fe-stabilized $Li_7La_3Zr_2O_{12}$ versus Li metal*, **2018**, 122, 3780-3785, DOI: 10.1021/acs.jpcc.7b12387.

[25] Rupp, J.; Rettenwander, D.; Kilner, J.; Doeff, M. M. *Editorial for the JECR special issue on all solid-state batteries: J. Electroceramics*, **2017**, DOI: 10.1007/s10832-017-0102-1.

[24] Kubicek, M.; Wachter-Welzl, A.; Rettenwander, D.; Wagner, R.; Amthauer, G.; Hutter, H.; Fleig, J. *Oxygen Vacancies in Fast Lithium-Ion Conducting Garnets: Chem. Mater.*, **2017**, 7189-7196, DOI: 10.1021/acs.chemmater.7b01281.

[23] Porz, L.; Swamy, T.; Sheldon, B.; Rettenwander, D.; Thaman, H.; Frömling, T.; Berendts, S.; Uecker, R.; Chiang, Y.-M. *Lithium Plating Mechanism in Li-ion Conducting Solid electrolytes: Adv. Energy Mater.*, **2017**, 1701003, DOI: 10.1002/aenm.201701003.

[22] Wachter-Welzl, A.; Kirowitz, J.; Wagner, R.; Smetaczek, S.; Brunauer, G. C.; Bonta, M.; Rettenwander, D.; Taibl, S.; Limbeck, A.; Amthauer, G.; Fleig, J. *The origin of conductivity variation in Al-stabalized $Li_7La_3Zr_2O_{12}$*, Solid State Ionics, **2018**, 319, 203-208, DOI: 10.1016/j.ssi.2018.01.036.

[21] Stanje, B.; Rettenwander, D.; Breuer, S.; Uitz, M.; Berendts, S.; Lerch, M.; Uecker, R.M Redhammer, G.; Hanzu, I.; Wilkening, M. *Solid Electrolytes: Extremely Fast Charge Carriers in Garnet-Type $Li_6La_3ZrTaO_{12}$*: *Annal. Phys.*, **2017**, 529, 1700140, DOI: 10.1002/andp.201700140.

[20] Giarola, M.; Sanson, A., Tietz, F.; Pristat, S.; Dashjav, Rettenwander, D.; Redhammer, G. J.; Mariotto, G. *Structure and vibrational dynamics of NASICON-type $LiTi_2(PO_4)_3$*: *J. Phys. Chem. C*, **2017**, 121, 3697-3706, DOI: 10.1021/acs.jpcc.6b11067.

[19] Welzl, A.; Wagner, R.; Rettenwander, D., Taibl, S.; Amthauer, G. *Microelectrodes for local conductivity and degradation measurements on Al doped $Li_7La_3Zr_2O_{12}$ garnets: J. Electroceramics*, **2016**, 37, 1-6, DOI: 10.1007/s10832-016-0058-6.

[18] Wagner, R.; Rettenwander, D.; Schmidt, W.; Tippelt, G.; Redhammer, G.; Wilkening, M.; Amthauer, G. *The influence of the unit-cell parameter a_0 on structure and Li-ion dynamic studied on cubic $Li_{7-x}La_3Zr_{2-x}Bi_xO_{12}$ garnet: Inorg. Chem*, **2016**, 55, 12211-12219, DOI: 10.1021/acs.inorgchem.6b01825.

[17] Rettenwander, D.; Wagner, R.; Langer, J.; Maier, M. E.; Wilkening, M.; Amthauer, G.; *Crystal chemistry of "Li_7 La_3 Zr_2 O_{12}" garnet doped with Al, Ga, and Fe: a short review on local structures as revealed by NMR and Mößbauer spectroscopy studies: Eur. J.. Mineral.* **2016**, 28, 619, DOI: 10.1127/ejm/2016/0028-2543-629,

[16] Redhammer, G. J.; Rettenwander, D.; Pristat, S.; Dashjav, E.; Kumar, C. M. N.; Topa, D.; Tietz, F. *A single crystal X-ray and powder neutron diffraction study on NASICON-type $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ ($0 \leq x \leq 0.5$) crystals: Implications on ionic conductivity*: *Solid State Sci.* **2016**, 60, 99-107, DOI: 10.1016/j.solidstatesciences.2016.08.011.

[15] Wagner, R.; Redhammer, G. Rettenwander, D.; Tippelt, G.; Welzl, A.; Taibl, S.; Franz, A.; Lottermoser, W.; Amthauer, G. *Fast Li-ion conducting garnet related $Li_{7-3x}Fe_xLa_3Zr_2O_{12}$ with uncommon I-43d structure*: *Chem. Mater.* **2016**, 28, 5943-5951, DOI: 10.1021/acs.chemmater.6b02516.

[14] John, M.; Heuss-Aßbichler, S.; Ullrich, A.; Rettenwander, D. Purification of heavy metal loaded wastewater from electroplating industry under synthesis of delafossite (ABO_2) by "Lt-delafossite process: Water Res. **2016**, 100, 98-104, DOI: 10.1016/j.watres.2016.04.071.

[13] Rettenwander, D.; Preishuber-Pflügl, F.; Cheng, L.; Wagner, R.; Welzl, A.; Suard, E.; Redhammer, G.; Doeff, M. M.; Wilkening, M.; Fleig. J.; Amthauer, G. *Structural and Electrochemical Consequences of Al and Ga Cosubstitution in $Li_7La_3Zr_2O_{12}$ Solid Electrolytes: Chem. Mater.*, **2016**, 28, 2384-2392, DOI: 10.1021/acs.chemmater.6b00579.

[12] Wagner, R.; Redhammer, G. Rettenwander, D.; Senyshyn, A.; Schmid, W.; Wilkening, M.; Amthauer, G. *Crystal structure of garnet-related Li-ion conductor $Li_{7-3x}Ga_xLa_3Zr_2O_{12}$: Fast Li-ion conduction caused by a different cubic modification*: *Chem. Mater.* **2016**, 28, 1861-1871, DOI**:** 10.1021/acs.chemmater.6b00038.

[11] Rettenwander, D.; Welzl, A.; Pristat, S.; Tietz, F.; Redhammer, G.; Fleig. J. *A micro-contact impedance study on NASICON-type $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ ($0 < x < 0.5$ single crystals **2015**, J. Mater. Chem. A* **2016**,4, 1506-1513, DOI: 10.1039/C5TA08545D.

[10] John, M.; Heuss-Aßbichler, S.; Park, S.-H.; Benka, G.; Petersen, N.; Rettenwander, D.; Horn, S. *Low-temperature synthesis of $CuFeO_2$ crystals (Delafossite) at 70 °C: A new process solely by precipitation and ageing: J. Solid. State. Chem.* **2015**, 233, 390-396, DOI: 10.1016/j.jssc.2015.11.011.

[9] Rettenwander, D.; Welzl, A.; Fleig, J.; Musso, M.; Amthauer, G. *Synthesis, Crystal Chemistry, and Electrochemical Properties of cubic Phase $Li_7La_3Zr_2O_{12}$ Garnet – The substitution of Zr^{4+} by Mo^{6+}: Inorg. Chem.* **2015**, 54, 10440-10449, DOI: 10.1021/acs.inorgchem.5b01895.

[8] Bottke, P.; Rettenwander, D.; Schmidt, W. Amthauer, G. Wilkening, M. *Ion Dynamics in Solid Electrolytes: NMR Reveals the Elementary Steps of Li^+ Hopping in the Garnet $Li_{6.5}La_3Zr_{1.75}Mo_{0.25}O_{12}$: Chem. Mater.* **2015**, 27, 6571-6582, DOI: 10.1021/acs.chemmater.5b02231.

[7] Rettenwander, D.; Langer, J.; Schmidt, W.; Arrer, C.; Harris, K.; Terskikh, V.; Goward, G.; Wilkening, M.; Amthauer, G. *Site Occupation of Ga and Al in Stabilized Cubic $Li_{7-3(x+y)}Ga_xAl_yLa_3Zr_2O_{12}$ Garnets As Deduced from ^{27}Al and ^{71}Ga MAS NMR at Ultrahigh Magnetic Fields: Chem. Mater.* **2015**, *27*, 3135–3142, DOI: 10.1021/acs.chemmater.5b00684.

[6] Rettenwander, D.; Geiger, C. A.; Tribus, M.; Tropper, P.; Wagner, R.; Tippelt, G.; Lottermoser, W.; Amthauer, G. *The Solubility and Site Preference of Fe^{3+} in $Li_{7-3x}Fe_xLa_3Zr_2O_{12}$ Garnets: Solid State Chem.* **2015**, 266–271, DOI: 10.1016/j.jssc.2015.01.016.

[5] Meister, P.; Chapligin, B.; Picard, A.; Meyer, H.; Fischer, C.; Rettenwander, D.; Amthauer, G.; Vogt, C.; Aiello, I. W. *Early diagenetic quartz formation at a deep iron oxidation front in the Eastern Equatorial Pacific - a modern analogue for banded iron/chert formations?: Geochim. Cosmochim. Acta*, **2014**, 137, 188-207, DOI: 10.1016/j.gca.2014.03.035.

[4] Rettenwander, D.; Geiger, C. A.; Tribus, M.; Tropper, P; Amthauer, G. *A Synthesis and Crystal Chemical Study of the Fast Ion Conductor $Li_{7-3x}Ga_xLa_3Zr_2O_{12}$ with x = 0.08 to 0.84: Inorg. Chem.* **2014**, 53, 6264-6269, DOI: 10.1021/ic500803h.

[3] Rettenwander, D.; Blaha, P.; Laskowski, R.; Schwarz, K.; Bottke, P.; Wilkening, M.; Amthauer, G. *DFT Study of the Role of Al^{3+} in the Fast Ion-Conductor $Li_{7-3x}Al^{3+}{}_xLa_3Zr_2O_{12}$ Garnet: Chem. Mater.* **2014**, 26, 2617-2623, DOI: 10.1021/cm5000999.

[2] Rettenwander, D.; Geiger, C. A.; Amthauer, G. *Synthesis and Crystal Chemistry of the Fast Li-Ion Conductor $Li_7La_3Zr_2O_{12}$ Doped with Fe: Inorg. Chem.* **2013**, 52, 8005-8009, DOI: 10.1021/ic400589u.

[1] Berger, R. J. F., Rettenwander, D., Spirk, S., Wolf, C. Patzschke, M.; Ertl, M.; Monkowius, U. Mitzel, N. W., *Relativistic effects in triphenylbismuth and their influence on molecular structure and spectroscopic properties: Phys. Chem. Chem. Phys.* 14 (2012) 15520-15524.

BOOK CHAPTERS

[B1] Wagner, R.; Rettenwander, D.; Amthauer, G. (**2017**) *Li-ion conducting oxide garnets.* In: Heuss-Aßbichler, S.; Amthauer, G.; John, M. (eds): Highlights in Applied Mineralogy. DeGruyter.