

Prof. Dr. Oliver Oeckler

Peer-reviewed Publications

- [241] **Incommensurately modulated $\text{Cu}_{0.9}\text{Pb}_{1.2}\text{Sb}_{2.9}\text{Se}_6$**
M. Grauer, L. Staab, K. Ueltzen, C. Benndorf, C. Paulmann, O. Oeckler
Inorg. Chem. **2023**, *62*, 20874 – 20877.
- [240] **Tetra-Face-Capped Octahedra in a Tetrahedra Network – Structure Determination and Scanning Transmission Electron Microscopy of $\text{SrAl}_5\text{P}_4\text{N}_{10}\text{O}_2\text{F}_3$**
M. M. Pointner, O. Oeckler, W. Schnick
Chem. Eur. J. **2023**, *29*, e202301960.
- [239] **Combining MN_6 Octahedra and PN_5 Trigonal Bipyramids in the Mica-like Nitridophosphates MP_6N_{11} ($M = \text{Al, In}$)**
S. J. Ambach, M. Pointner, S. Falkai, C. Paulmann, O. Oeckler, W. Schnick
Angew. Chem. **2023**, *135*, e202303580; *Angew. Chem. Int. Ed. Engl.* **2023**, *62*, e202303580.
- [238] **Modular Principle for Complex Disordered Tetrahedral Frameworks in Quenched High-Pressure Phases of Phosphorus Oxide Nitrides**
D. Günther, D. Baumann, W. Schnick, O. Oeckler
Chem. Eur. J. **2023**, *29*, e202203892 and e202300736 (cover profile).
- [237] **Decomposition behavior and thermoelectric properties of copper selenide - graphite composites**
L. Staab, T. Kötzsch, T. J. Noack, O. Oeckler
Appl. Phys. Lett. **2023**, *122*, 083901.
- [236] **Layered GaGe_2Te : structure and chemical bonding**
T. Juhlke, S. Steinberg, L. Staab, E. Lawrence Bright, O. Oeckler
Z. Anorg. Allg. Chem. **2023**, *640*, e202300107.
- [235] **Tracing the pathway toward decomposition: Crystal structure of $\text{Ag}_3(\text{PO}_2\text{NH})_3$ and $\text{K}_3(\text{PO}_2\text{NH})_3$ as a function of temperature**
D. Günther, C. Paulmann, O. Oeckler
J. Solid State Chem. **2023**, *323*, 124009.
- [234] **Oxonium diimidotriphosphate from the hydrolysis of trimetaphosphimic acid**
D. Günther, C. Paulmann, O. Oeckler
Monatsh. Chem. **2023**, *154*, 325 – 330.
- [233] **Monoammonium Trimetaphosphimate $(\text{NH}_4)\text{H}_2(\text{PO}_2\text{NH})_3$**
D. Günther, C. Paulmann, O. Oeckler
Crystals **2023**, *13*, 111.
- [232] **Comprehensive Investigation of Anion Species in Crystalline Li^+ ion Conductor $\text{Li}_{27-x}[\text{P}_4\text{O}_{7+x}\text{N}_{9-x}]\text{O}_3$ ($x \approx 1.9(3)$)**
S. Schneider, E.-M. Wendinger, V. Baran, A.-K. Hatz, B. V. Lotsch, M. Nentwig, O. Oeckler, T. Bräuniger, W. Schnick
Chem. Eur. J. **2023**, *29*, e202300174.

- [231] **Cu_{1.5}Se_yTe_{1-y} (y = 0.2 – 0.7): A Series of Narrow Band Gap Semiconductors with Low Thermal Conductivity at Ambient Temperature**
A. Rabenbauer, A. Vogel, J. Venturini, M. Moslemi, O. Oeckler, D. Daisenberger, T. Nilges
Inorg. Chem. **2023**, *62*, 12600 – 12610.
- [230] **Experimental and computational study on dimers of 5-halo-1*H*-indole-2-carboxylic acids and their microbiological activity**
M. Balcerak, K. Szmigiel-Bakalarz, M. Lewanska, D. Günther, O. Oeckler, M. Malik, B. Morzyk-Ociepa
J. Mol. Struct. **2023**, *1274*, 134492.
- [229] **Endotaxial Intergrowth of Copper Telluride in GeTe-Rich Germanium Antimony Tellurides Leads to High Thermoelectric Performance**
S. Schwarzmüller, D. Souchay, G. Wagner, P. Kemmesies, D. Günther, M. Bittner, G. Zhang, Z. Ren, A. Feldhoff, G. J. Snyder, O. Oeckler
Chem. Mater. **2022**, *34*, 10025 – 10039.
- [228] **Temperature-dependent Cu and Ag ion mobility and associated changes of transport properties in pavonite-type Cu_{1.4}Ag_{0.4}Bi_{5.4}Se₉**
C. Fraunhofer, T. Paul, O. Oeckler
Dalton Trans. **2022**, *51*, 14581 – 14589.
- [227] **Sodalite-type Ga_{16/3}[P₁₂N₂₄]O₂: Synthesis, Electron Crystallography and Powder X-ray Diffraction**
D. Günther, L. Eisenburger, W. Schnick, O. Oeckler
Z. Anorg. Allg. Chem. **2022**, *648*, e202200280.
- [226] **A new modification of oxonium trimetaphosphimate monohydrate**
D. Günther, C. Kalischer, O. Oeckler
Z. Anorg. Allg. Chem. **2022**, *648*, e202200259.
- [225] **Discovery of Two Polymorphs of TiP₄N₈ Synthesized from Binary Nitrides**
L. Eisenburger, V. Weippert, C. Paulmann, D. Johrendt, O. Oeckler, W. Schnick
Angew. Chem. **2022**, *134*, e202202014; *Angew. Chem. Int. Ed. Engl.* **2022**, *61*, e202202014.
- [224] **Nitridic Analogs of Micas AESi₃P₄N₁₀(NH)₂ (AE = Mg, Mg_{0.94}Ca_{0.06}, Ca, Sr)**
L. Eisenburger, P. Strobel, P. J. Schmidt, T. Bräuninger, J. P. Wright, E. Lawrence Bright, C. Giacobbe, O. Oeckler, W. Schnick
Angew. Chem. **2022**, *134*, e202114902; *Angew. Chem. Int. Ed. Engl.* **2022**, *61*, e202114902.
- [223] **Pnictide-Capped Butterfly Cluster in the Crystal Structure of Nb₄PnX₁₁ (Pn = N, P; X = Cl, Br, I)**
M. Ströbele, O. Oeckler, M. Thelen, R. F. Fink, A. Krishnamurthy, S. Kroeker, H.-J. Meyer
Inorg. Chem. **2022**, *61*, 17599 – 17608.
- [222] **Large Exchange Bias, High Dielectric Constant, and Outstanding Ionic Conductivity in a Single-Phase Spin Glass**
M. R. Ghazanfari, A. Santhosh, K. Siemensmeyer, F. Fuß, L. Staab, J. C. Vrijmoed, B. Peters, M. Liesegang, S. Dehnen, O. Oeckler, P. Jerabek, G. Thiele
Adv. Electron. Mater. **2022**, *8*, 2200483.
- [221] **NMR Study of AgInTe₂ at Normal and High Pressures**
R. Guehne, C. Kattinger, M. Bertmer, S. Welzmler, O. Oeckler, J. Haase
J. Phys. Chem. C **2022**, *126*, 8461 – 8466.

- [220] **^{125}Te NMR study of the bulk of topological insulators Bi_2Te_3 and Sb_2Te_3**
J. Nachtigal, S. V. Chong, G. V. M. Williams, A. Isaeva, O. Oeckler, J. Haase, R. Guehne
Z. Anorg. Allg. Chem. **2022**, *648*, e202200208.
- [219] **Structure Elucidation of Complex Endotaxially Intergrown Lanthanum Barium Oxonitridosilicate Oxides by Combination of Microfocused Synchrotron Radiation and Transmission Electron Microscopy**
L. Gamperl, L. Neudert, P. Schultz, D. Durach, W. Schnick, O. Oeckler
Chem. Eur. J. **2021**, *27*, 12835 – 12844.
- [218] **Anomalous Raman modes in tellurides**
F. J. Manjón, S. Gallego-Parra, P. Rodríguez-Hernández, A. Muñoz, C. Drasar, V. Muñoz-Sanjosé, O. Oeckler
J. Mater. Chem. C **2021**, *9*, 6277 – 6289.
- [217] **High-Pressure Synthesis of $\text{Sc}_5\text{P}_{12}\text{N}_{23}\text{O}_3$ and $\text{Ti}_5\text{P}_{12}\text{N}_{24}\text{O}_2$ by Activation of the Binary Nitrides ScN and TiN with NH_4F**
L. Eisenburger, V. Weippert, O. Oeckler, W. Schnick
Chem. Eur. J. **2021**, *27*, 14184 – 14188.
- [216] **High-Pressure High-Temperature Synthesis of Mixed Nitridosilicatephosphates and Luminescence of $\text{AESiP}_3\text{N}_7\text{Eu}^{2+}$ ($\text{AE} = \text{Sr}, \text{Ba}$)**
L. Eisenburger, O. Oeckler, W. Schnick
Chem. Eur. J. **2021**, *27*, 4461 – 4465.
- [215] **Liquid Exfoliated SnP_3 Nanosheets for Very High Areal Capacity Lithium-Ion Batteries**
R. Tian, A. Griffin, M. McCrystal, M. Breshears, A. Harvey, C. Gabbett, D. V. Horváth, C. Backes, Y. Jing, T. Heine, S.-H. Park, J. Coelho, V. Nicolosi, M. Nentwig, C. Benndorf, O. Oeckler, J. N. Coleman
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- [214] **Ceramic composites based on $\text{Ca}_3\text{Co}_{4-x}\text{O}_{9+\delta}$ and $\text{La}_2\text{NiO}_{4+\delta}$ with enhanced Δ thermoelectric properties**
R. Hinterding, Z. Zhao, M. Wolf, M. Jakob, O. Oeckler, A. Feldhoff
Open Ceramics **2021**, *6*, 100103.
- [213] **Improved thermoelectric properties in ceramic composites based on $\text{Ca}_3\text{Co}_4\text{O}_9$ and $\text{Na}_2\text{Ca}_2\text{Nb}_4\text{O}_{13}$**
R. Hinterding, M. Wolf, M. Jakob, O. Oeckler, A. Feldhoff
Open Ceramics **2021**, *8*, 100198.
- [212] **Linarite from Cap Garonne**
C. Paulsen, C. Benndorf, D. Günther, O. Oeckler, H. Osthues, N. L. Doltsinis, V. Galéa-Clolus, P. Clolus, R. Pöttgen
Z. Naturforsch. B **2021**, *76*, 577 – 538.
- [211] **Structural (X-ray), spectroscopic (FT-IR, FT-Raman) and computational (DFT) analysis of intermolecular interactions in 1*H*-indazole-3-carbaldehyde**
B. Morzyk-Ociepa, K. Szmigiel-Bakalarz, M. Nentwig, O. Oeckler, M. Malik
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- [210] **A layered tin bismuth selenide with three different building blocks that account for an extremely large lattice parameter of 283 Å**
M. Nentwig, L. Eisenburger, F. Heinke, O. Oeckler
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- [209] **Decomposition Phenomena of $Zn_{13-8}Sb_{10}$ under Working Conditions of Thermo electric Generators and Minimum Current Densities for Electromigration**
M. Jakob, M. Grauer, P. Ziolkowski, O. Oeckler
ACS Appl. Energy Mater. **2020**, *3*, 2103 – 2109.
- [208] **Lithium atom mobility in lithium germanium antimony tellurides elucidated by neutron diffraction and quasielastic neutron scattering**
S. Schwarzmüller, M. Hölzel, K. Fritsch, Z. Evenson, K. Habicht, O. Oeckler
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- [207] **Hall-effect Measurements and Transport Properties of Heterostructures in the Model System $NiTe_2-Sn_{12}Sb_2Te_{15}$**
C. Fraunhofer, S. Schwarzmüller, J. L. Gardiner, G. J. Snyder, O. Oeckler
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- [206] **Characterization and Decomposition of the Natural van der Waals $SnSb_2Te_4$ under Compression**
J. A. Sans, R. Vilaplana, E. L. da Silva, C. Popescu, V. P. Cuenca-Gotor, A. Andrada-Chacón, J. Sánchez-Benitez, O. Gomis, A. L. J. Pereira, P. Rodríguez-Hernández, A. Muñoz, D. Daisenberger, B. García-Domene, A. Segura, D. Errandonea, R. S. Kumar, O. Oeckler, P. Urban, J. Contreras-García, F. J. Manjón
Inorg. Chem. **2020**, *59*, 9900 – 9918.
- [205] **Nitridophosphate-Based Ultra-Narrow-Band Blue-Emitters: Luminescence Properties of $AEP_8N_{14}:Eu^{2+}$ ($AE = Ca, Sr, Ba$)**
S. Wendl, L. Eisenburger, P. Strobel, D. Günther, J. P. Wright, P. J. Schmidt, O. Oeckler, W. Schnick
Chem. Eur. J. **2020**, *26*, 7292 – 7298.
- [204] **$BaP_6N_{10}NH:Eu^{2+}$ as a Case Study – An Imidonitridophosphate Showing Luminescence**
S. Wendl, L. Eisenburger, M. Zipkat, D. Günther, J. P. Wright, P. J. Schmidt, O. Oeckler, W. Schnick
Chem. Eur. J. **2020**, *26*, 5010 – 5016.
- [203] **Squares of gold atoms and linear infinite chains of Cd atoms as building units in the intermetallic phases $REAu_4Cd_2$ ($RE = La-Nd, Sm$) with $YbAl_4Mo_2$ -type structure**
C. Paulsen, T. Block, C. Benndorf, O. Oeckler, J. Bönnighausen, O. Janka, R. Pöttgen
Z. Naturforsch. B. **2020**, *75*, 73 – 82.
- [202] **New Zn(II) coordination polymer of indole-3-acetic acid, a plant-growth promoting hormone: Crystal structure, spectroscopic characterization, DFT calculations and microbiological activity**
K. Szmigiel-Bakalarz, A. Skoczynska, M. Lewanska, D. Günther, O. Oeckler, M. Malik-Gajewska, D. Michalska, B. Morzyk-Ociepa
Polyhedron **2020**, *185*, 114582.
- [201] **7-Azaindole-3-carboxylic acid and its Pt(II) and Pd(II) complexes: Crystal structure of the ligand, vibrational spectra, DFT calculations and *in vitro* antiproliferative activity**
K. Szmigiel-Bakalarz, M. Nentwig, O. Oeckler, M. Malik-Gajewska, B. Filip-Psurska, B. Morzyk-Ociepa
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- [200] **Sodium and lithium one-dimensional coordination polymers with 1H-indazole-3-carboxylic acid: Crystal structures, vibrational spectra and DFT calculations**
K. Szmigielski-Bakalarz, M. Nentwig, D. Günther, O. Oeckler, M. Malik-Gajewska, D. Michalska, B. Morzyk-Ociepa
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- [199] **Effect of phosphonium ionic liquid/Pd ratio on the catalytic activity of palladium nanoparticles in Suzuki cross-coupling reaction**
D. Arkhipova, V. Ermolaev, V. Miluykov, G. Gaynanova, L. Zakharova, G. Wagner, O. Oeckler, E. Hey-Hawkins
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- [198] **The Long-Periodic Loop-Branched Chain Structure of the Oxonitridophosphate $\text{La}_{21}\text{P}_{40}\text{O}_{46}\text{N}_{57}$, Elucidated by a Combination of TEM and Microfocused Synchrotron Radiation**
M. Nentwig, S. D. Kloß, L. Neudert, L. Eisenburger, W. Schnick, O. Oeckler
Chem. Eur. J. **2019**, *25*, 14382 – 14387.
- [197] **Cobalt germanide precipitates indirectly improve the properties of thermoelectric germanium antimony tellurides**
D. Souchay, S. Schwarzmüller, H. Becker, S. Kante, G. J. Snyder, A. Leineweber, O. Oeckler
J. Mater. Chem. C **2019**, *7*, 11419 – 11430.
- [196] **Layered manganese bismuth tellurides with GeBi_4Te_7 - and $\text{GeBi}_6\text{Te}_{10}$ -type structures: towards multifunctional materials**
D. Souchay, M. Nentwig, D. Günther, S. Keilholz, J. de Boor, A. Zeugner, A. Isaeva, M. Ruck, A. U. B. Wolter, B. Büchner, O. Oeckler
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- [195] **Structures and transport properties of metastable solid solutions $(\text{NaSbTe}_2)_{1-x}(\text{GeTe})_x$**
S. Schwarzmüller, F. Yang, O. Oeckler
J. Alloys Compd. **2019**, *806*, 774 – 779.
- [194] **The Sodium Antimony Telluridogermanate(III) $\text{Na}_9\text{Sb}[\text{Ge}_2\text{Te}_6]_2$**
S. Schwarzmüller, V. H.-T. Tran, F. Yang, O. Oeckler
Z. Anorg. Allg. Chem. **2019**, *645*, 1037 – 1024.
- [193] **Cationic Pb_2 Dumbbells Stabilized in the Highly Covalent Lead Nitridosilicate $\text{Pb}_2\text{Si}_5\text{N}_8$**
P. Bielec, R. Nelson, R. P. Stoffel, L. Eisenburger, D. Günther, A.-K. Henß, J. P. Wright, O. Oeckler, R. Dronskowski, W. Schnick
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- [192] **Targeting Vacancies in Nitridosilicates: Aliovalent Substitution of M^{2+} (M = Ca, Sr) by Sc^{3+} and U^{3+}**
P. Bielec, L. Eisenburger, H. L. Deubner, D. Günther, F. Kraus, O. Oeckler, W. Schnick
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- [191] **Reduced Local Symmetry in Lithium Compound $\text{Li}_2\text{SrSiO}_4$ Distinguished by an Eu^{3+} Spectroscopy Probe**
L. Chen, P. Cheng, Z. Zhang, L. He, Y. Jiang, G. Li, X. Jing, Y. Qin, M. Yin, T.-S. Chan, B. Hong, S. Tao, W. Chu, Z. Zhao, H. Ni, H. Kohlmann, O. Oeckler
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- [189] **Structure Elucidation of a Melam–Melem Adduct by a Combined Approach of Synchrotron X-ray Diffraction and DFT Calculations**
F. K. Kessler, A. M. Burow, G. Savasci, T. Rosenthal, P. Schultz, E. Wirthner, O. Oeckler, C. Ochsenfeld, W. Schnick
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- [188] **A High-Pressure Praseodymium Fluoride Borate Linking Multiple Structural Features of Apatite-Type Compounds**
M. Glätzle, A. Pitscheider, O. Oeckler, K. Wurst, H. Huppertz
Chem. Eur. J. **2019**, *25*, 1767 – 1772.
- [187] **$\text{K}_2\text{Hg}_2\text{Te}_3$: Straightforward and Large-Scale Mercury-Flux Synthesis of a Small-Band-Gap Photoconducting Material**
G. Thiele, P. Bron, S. Lippert, F. Nietschke, O. Oeckler, M. Koch, B. Roling, S. Dehnen
Inorg. Chem. **2019**, *58*, 4052 – 4054.
- [186] **$\text{Cu}_{9.1}\text{Te}_4\text{Cl}_3$: A Thermoelectric Compound with Low Thermal and High Electrical Conductivity**
A. Vogel, T. Miller, C. Hoch, M. Jakob, O. Oeckler, T. Nilges
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- [185] **Ammonothermal Synthesis of the Mixed-Valence Nitrogen-Rich Europium Tantalum Ruddlesden-Popper Phase $\text{Eu}^{\text{II}}\text{Eu}^{\text{III}}_2\text{Ta}_2\text{N}_4\text{O}_3$**
N. Cordes, M. Nentwig, L. Eisenburger, O. Oeckler, W. Schnick
Eur. J. Inorg. Chem. **2019**, *25*, 2304 – 2311.
- [184] **Low Thermal Conductivity in Thermoelectric Oxide-Based Multiphase Composites**
M. Wolf, K. Menekse, A. Mundstock, R. Hinterding, F. Nietschke, O. Oeckler, A. Feldhoff
J. Electron. Mater. **2019**, *48*, 7551 – 7561.
- [183] **$\text{Y}_{23}\text{Sr}_{17}[\text{Si}_{38}\text{O}_{18}\text{N}_{67}]\text{O}_9$ – An Oxonitridosilicate Oxide with a Unique Layered Structure**
C. Maak, R. Niklaus, O. Oeckler, W. Schnick
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- [182] **Hydrogenation Properties of LnAl_2 ($\text{Ln} = \text{La}, \text{Eu}, \text{Yb}$), LaGa_2 , LaSi_2 and the Crystal Structure of $\text{LaGa}_2\text{H}_{0.71(2)}$**
A. Werwein, C. Benndorf, M. Bertmer, A. Franz, O. Oeckler, H. Kohlmann
Crystals **2019**, *9*, 193.
- [181] **Platinum(II) and copper(II) complexes of 7-azaindole-3-carboxaldehyde: crystal structures, IR and Raman spectra, DFT calculations and *in vitro* antiproliferative activity of the platinum(II) complex**
B. Morzyk-Ociepa, K. Szmigiel-Bakalarz, M. Nentwig, O. Oeckler, M. Malik-Gajewska, E. Turlej, J. Wietrzyk, D. Michalska
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K. Dysz, K. Szmigiel-Bakalarz, M. Nentwig, O. Oeckler, M. Malik-Gajewska, E. Turlej, D. Michalska, B. Morzyk-Ociepa
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- [179] **Tuning the Vacancy Concentration in Lithium Germanium Antimony Tellurides – Influence on Phase Transitions, Lithium Mobility, and Thermoelectric Properties**
S. Schwarzmüller, M. Jakob, M. Nentwig, T. Schröder, A. Kuhn, A. Düvel, P. Heitjans, O. Oeckler
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- [177] **Structure and thermoelectric properties of the silver lead bismuth selenides Ag₅Pb₉Bi₁₉Se₄₀ and AgPb₃Bi₇Se₁₄**
F. Heinke, F. Nietschke, C. Fraunhofer, I. Dovgaliuk, J. Schiller, O. Oeckler
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- [176] **Phase transitions to superionic Li₂Te and Li₂Se – A high-temperature neutron powder diffraction study, atom displacements, probability density functions and atom potentials**
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- [175] **Structural variations in indium tin tellurides and their thermoelectric properties**
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- [174] **Argyrodite-Type Cu₈GeSe_{6-x}Te_x (0 ≤ x ≤ 2): Temperature- Dependent Crystal Structure and Thermoelectric Properties**
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- [173] **RE₄Ba₂[Si₁₂O₂N₁₆C₃]:Eu²⁺ (RE = Lu, Y): Green-Yellow Emitting Oxonitridocarbido silicates with a Highly Condensed Network Structure Unraveled through Synchrotron Microdiffraction**
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- [172] **Ammonothermal Synthesis and Crystal Structure of the Nitridoalumogermanate Ca_{1-x}Li_xAl_{1-x}Ge_{1+x}N₃ (x ≈ 0.2)**
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- [171] **The Effect of Scandium Ternary Intergrain Precipitates in Al-Containing High-Entropy Alloys**
S. Riva, S. Mehraban, N. P. Lavery, S. Schwarzmüller, O. Oeckler, S. G. R. Brown, K. V. Yusenko
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