Publications in international peer-reviewed scientific journals
Publikationen in internationalen, referierten Journalen

1. Y. Deng, H. B. L. Nguyen, C. Eames, O. Pecher, M. Courty, B. Fleu-tot, J.-N. Chotard, C. P. Grey, C. Masquelier, M. S. Islam. Scandium substituted NASICON solid electrolyte: structural and mechanistic insights. *J. Am. Chem. Soc.* **2017**, *submitted*.

2. Joshua M. Stratford, Martin Mayo, Phoebe K. Allan, Oliver Pecher, Olaf J. Borkiewicz, Kamila M. Wiaderek, Chris J. Pickard, Andrew J. Morris, Clare P. Grey. Investigating Sodium Storage Mechanisms in Tin Anodes: A Combined Pair Distribution Function Analysis, Density Functional Theory and Solid-State NMR Approach. *J. Am. Chem. Soc.* **2017**, *submitted*.

3. Wei Meng, Roberta Pigliapochi, Paul M. Bayley, Oliver Pecher, Michael W. Gaultois, Ieuan D. Seymour, Hanpu Liang, Wenqian Xu, Kamila M. Wiaderek, Karena W. Chapman, Clare P. Grey. Unravelling the Complex Delithiation and Lithiation mechanisms of the high capacity cathode material V_6O_{13}. *Chem. Mater.* **2017**, *submitted*.

4. O. Pecher, D. M. Halat, J. Lee, Z. Liu, K. J. Griffith, M. Braun, C. P. Grey. Enhanced efficiency of solid-state NMR investigations of energy materials via the external Automatic Tuning/Matching (eATM) robot. *J. Magn. Reson.* **2017**, *275*, 127-136. (http://dx.doi.org/10.1016/j.jmr.2016.12.008).

5. O. Pecher, J. Carretero-González, K. J. Griffith, C. P. Grey. Materials' Methods: NMR in Battery Research. *Chem. Mater.* **2017**, *29*, 213-242. (http://pubs.acs.org/doi/abs/10.1021/acs.chemmater.6b03183)

   Ranked Chem. Mater. "Most Read Articles (Top 20)" of Jan and Feb 2017 with 1,545 article views by 15 March 2017.

6. O. Pecher, B. Mausolf, V. Peters, A. Korthaus, F. Haarmann. Unravelling local atomic order of the anionic sublattice in $M(Al_{1-x}Ga_x)_4$ with M = Sr and Ba by NMR spectroscopy and quantum mechanical modelling. *Chem. Eur. J.* **2016**, *22*, 17833-17842. (10.1002/chem.201602475)

7. J. M. Stratford, P. K. Allan, O. Pecher, P. A. Chater, C. P. Grey. Mechanistic insights into sodium storage in hard carbon anodes using local structure probes. *Chem. Comm.* **2016**, 52, 12430-12433. (10.1039/C6CC06990H)

8. L. M. Scherf, O. Pecher, K. J. Griffith, F. Haarmann, C. P. Grey, T. F. Fässler. The Ternary Zintl Phases $K_{4-x}Na_xSi_4$ ($1 \leq x \leq 2.2$) and K_7NaSi_8 – Synthesis, Crystal Structure, and Solid State NMR Spectroscopic Investigations. *Eur. J. Inorg. Chem.* **2016,** *2016(28)*, 4674-4682. (10.1002/ejic.201600735)

9. G. Oyama, O. Pecher, K. J. Griffith, S. Nishimura, R. Pigliapochi, C. P. Grey, A. Yamada. Sodium Intercalation Mechanism of 3.8 V Class Alluaudite Sodium Iron Sulfate. *Chem. Mater.* **2016**, *18(15)*, 5321-5328. (10.1021/acs.chemmater.6b01091)

10. O. Pecher, P. M. Bayley, H. Liu , Z. Liu, N. M. Trease, C. P. Grey. Automatic Tuning Matching Cycler (ATMC) *in situ* NMR spectroscopy as a novel approach for real-time investigations of Li- and Na-ion batteries*. J. Magn. Reson.* **2016**, *265*, 200-209*.* (10.1016/j.jmr.2016.02.008)

11. L. M. Scherf, A. J. Karttunen, O. Pecher, P. Magusin, C. P. Grey, T. F. Fässler. $[Ge_2]^{4-}$ Dumbbells with Very Short Ge—Ge Distances in the Zintl Phase Li_3NaGe_2 – a

Solid State Equivalent to Molecular O_2. *Angew Chem. Int. Ed.* **2015**, *55*, 1075-1079 (10.1002/anie.201508044); *Angew. Chem.* **2015**, *128*, 1087-1091. (10.1002/ange.201508044)

Ranked as VIP paper; highlight article on this publication: U. Ruschewitz. $[Ge=Ge]^{4-}$ Dumbbells in the Zintl Phase Li_3NaGe_2. *Angew. Chem. Int. Ed.* **2016**, *55*, 3264. (10.1002/anie.201600424); *Angew. Chem.* **2016**, *128*, 3320. (10.1002/ange.201600424).

12. O. Pecher, B. Mausolf, K. Lamberts, D. Oligschläger, C. Niewieszol (née Merkens), U. Englert, F. Haarmann. The Solid Solution $Sr_{1-x}Ba_xGa_2$: Substitutional Disorder and Chemical Bonding Visited by NMR Spectroscopy and Quantum Mechanical Calculations. *Chem. Eur. J.* **2015**, *21*, 13971-13982. (10.1002/chem.201501910)

    Ranked as "hot paper", inside-cover.

13. Y. Deng, C. Eames, J.-N. Chotard, F. Lalère, V. Seznec, S. Emge, O. Pecher, C. P. Grey, M. S. Islam, C. Masquelier. Structural and mechanistic insights into fast lithium-ion conduction in Li_4SiO_4—Li_3PO_4 solid electrolytes. *J. Am. Chem. Soc.* **2015**, *137*, 9136-9145. (10.1021/jacs.5b04444)

14. O. Pecher, M. Esters, A. Görne, B. Mausolf, A. Ormeci, F. Haarmann. The Zintl Phase Cs_7NaSi_8 – From NMR Signal Line Shape Analysis and Quantum Mechanical Calculations to Chemical Bonding. *Z. anorg. allg. Chem.* **2014**, *640(11)*, 2169-2176. (10.1002/zaac.201400194)

15. M. Waibel, O. Pecher, B. Mausolf, F. Haarmann, T. F. Fässler. $NaRb_7(Si_{4-x}Ge_x)_2$ – Soluble Zintl Phases Containing Heteroatomic Tetrahedral $[Si_{4-x}Ge_x]^{4-}$ Clusters. *Eur. J. Inorg. Chem.* **2013**, *32*, 5541-5546. (10.1002/ejic.201300943)

16. O. Pecher, F. Haarmann. Looking Into Intermetallic Phases. *Nachr. Chem.* **2013**, *61*, 1018-1021. (10.1002/nadc.201390315)

17. C. Merkens, O. Pecher, F. Steuber, S. Eisenhut, A. Görne, F. Haarmann, U. Englert. Crystal-to-Crystal Transformations in a Seven-Coordinated Sc Complex. *Z. anorg. allg. Chem.* **2013**, *639(2)*, 340-346. (10.1002/zaac.201200386)

18. T. Goebel, A. Ormeci, O. Pecher, F. Haarmann. The Silicides M_4Si_4 with M = Na, K, Rb, Cs and Ba_2Si_4 – NMR Spectroscopy and Quantum Mechanical Calculations. *Z. anorg. allg. Chem.* **2012**, *638(10)*, 1437-1445. (10.1002/zaac.201200198)

19. Y. Liang, B. Böhme, A. Ormeci, H. Borrmann, O. Pecher, F. Haarmann, W. Schnelle, M. Baitinger, Yu. Grin. A Clathrate-I Phase with Li-Ge Framework. *Chem. Eur. J.* **2012**, *18(32)*, 9818-9822. (10.1002/chem.201202069)

20. F. Haarmann, K. Koch, P. Jeglič, O. Pecher, H. Rosner, Yu. Grin. NMR Spectroscopy of Intermetallic Compounds: An Experimental and Theoretical Approach to Local Atomic Arrangements in Binary Gallides. *Chem. Eur. J.* **2011**, *17(27)*, 7560-7568. (10.1002/chem.201003486)

21. T. Goebel, Yu. Prots, A. Ormeci, O. Pecher, F. Haarmann. Synthesis, Crystal Structure and Chemical Bonding of the Zintl Phase Rb_7NaSi_8. *Z. anorg. allg. Chem.* **2011**, *637*, 1982-1991. (10.1002/zaac.201100349)

22. D. Bräunling, O. Pecher, D. M. Trots, A. Senyshyn, D. A. Zherebtsov, F. Haarmann, R. Niewa. Synthesis, Crystal Structure and Li Motion of Li_8SeN_2 and Li_8TeN_2. *Z. anorg. allg. Chem.* **2010**, *636*, 936-946. (10.1002/zaac.201000002)

23. O. Pecher, S.-T. Kong, T. Goebel, V. Nickel, K. Weichert, C. Reiner, H. J. Deiseroth, J. Maier, F. Haarmann, D. Zahn. Atomistic Characterisation of Li^+ Mobility and Conductivity in $Li_{7-x}PS_{6-x}I_x$ Argyrodites from Molecular Dynamics Simulations, Solid-State NMR and Impedance Spectroscopy. *Chem. Eur. J.* **2010**, *16*, 8347-8354. (10.1002/chem.201000501)

24. F. Haarmann, K. Koch, D. Grüner, W. Schnelle, O. Pecher, R. Cardoso-Gil, H. Borrmann, H. Rosner, Yu. Grin. Electronic Structure, Chemical Bonding, and Solid-State NMR Spectroscopy of the Digallides of Ca, Sr, and Ba. *Chem. Eur. J.* **2009**, *15*, 1673-1684. (10.1002/chem.200801131)

Book chapters
Buchkapitel

1. Pieter C. M. M. Magusin, Ieuan Seymour, Oliver Pecher, Clare P. Grey. NMR on Electrochemical Storage Materials. In *Modern Methods in Solid-State NMR* (Editor Paul Hodkinson) **2017**, *submitted.*

Publications from conference proceedings
Publikationen aus Konferenzbeiträgen

1. O. Pecher, A. Vyalikh, C. P. Grey. Challenges and new opportunities of *in situ* NMR characterization of electrochemical processes. *AIP Conference Proceedings* **2016**, *1765*, 020011. (10.1063/1.4961903)
2. O. Pecher, S. Emge, Y. Deng, S. Islam, C. Masquelier, C. P. Grey. Crystal structures and Li ion dynamics of Li_3PO_4—Li_4SiO_4 revisited by NMR. *Z. Kristallogr.* **2015**,*Suppl. 35*, 39-40.
3. O. Pecher, H. Liu, C. P. Grey. Next level real-time studies of $LiFePO_4$ electrodes by ^{7}Li *in situ* NMR. *Z. anorg. allg. Chem.* **2014**, *640(11)*, 2339. (10.1002/zaac.201404005)
4. V. Peters, O. Pecher, B. Mausolf, F. Haarmann. $Ba_{21}Al_{40}$ investigated by NMR and quantum mechanical calculations. *Z. anorg. allg. Chem.* **2014**, *640(11)*, 2362. (10.1002/zaac.201404053)
5. O. Pecher, F. Haarmann. Substitutional Disorder in Intermetallic Phases: Investigations of Chemical Bonding by XRD—NMR—QM. *Z. Kristallogr.* **2013**, *Suppl. 33*, 30.
6. F. Haarmann, O. Pecher. Local order in intermetallic compounds investigated by SMARTER NMR spectroscopy. *Z. Kristallogr.* **2013**, *Suppl. 33*, 28-29.
7. O. Pecher, F. Haarmann. Ga Bonding Variability in $Ca_{1-x}Ga_{2+3x}$ Visited by Solid-State NMR Spectroscopy. *Z. anorg. allg. Chem.* **2012**, *638(10)*, 1622.
8. O. Pecher, F. Haarmann. The Automatic Tuning Matching Goniometer (ATMG) Probe System: Mapping Chemical Questions Using Orientation Dependent NMR Experiments. *Z. Kristallogr.* **2012**, *Suppl. 32*, 24.
9. O. Pecher, F. Haarmann. $Sr_{1-x}Ba_xGa_2$: NMR Spectroscopy. *Z. anorg. allg. Chem.* **2010**, *636(11)*, 2089.
10. O. Pecher, H. Borrmann, Yu. Prots, F. Haarmann. The Ga-Rich Part of the Phase Diagram Ca–Ga. *Z. Kristallogr.* **2009**, *Suppl. 29*, 32.
11. O. Pecher, F. Haarmann. Solid-State NMR of $Ca_{1-x}Ga_{2+3x}$. *Z. anorg. allg. Chem.* **2008**, *634(11)*, 2069.

Talks
Vorträge

1. *Forthcoming:* 5th Annual Meeting of the STFC Batteries Network (Abingdon, UK) 31 March – 1 June **2017**. Oliver Pecher and Wei Meng. In situ *solid-state NMR and HT XRD investigations on energy storage materials – challenges and recent developments.*

2. 58th Experimental Nuclear Magnetic Resonance Conference (ENC; Asilomar Conference Grounds, Pacific Grove, California) 26 – 31 March **2017**. Oliver Pecher, Joshua M. Stratford, Phoebe K. Allan, David M. Halat, Alexander C. Forse, Ieuan D. Seymour, and Clare P. Grey. *Recent Developments in the use of NMR, MRI and PFG Methods to Study Batteries and Supercapacitors.*
3. Lancaster University, Materials Chemistry (Lancaster, UK) 1 Feb **2017**. In situ… *everything? New approaches on* in situ *NMR and automation in solid state NMR spectroscopy.*
4. WMG Battery School 2016 (Warwick, UK) October **2016** (invited).
   NMR in battery research
5. Cambridge Enterprise Ltd. – Physical Sciences Commercialisation Workshop (Cambridge, UK) 5 October **2016**. *When it matters: GREY MATTER Enterprise.*
6. 2nd Meeting of the DGK's Young Crystallographers (Berlin, DE) 21 – 23 Sept **2016**.
   In situ NMR on Li- and Na-ion battery materials. (Lightning Talk)
7. Technical University Dresden (DE), Inorganic Chemistry II Meeting, 8 July **2016**.
   Operando NMR investigations on Li- and Na-ion battery materials
8. HäKo (Karlsruhe, DE) 17 – 19 March **2016**.
   "BATTASS" – Exploring $LiFePO_4$/Li_4SiO_4—Li_3PO_4 all-solid-state batteries
9. 24th DGK's Annual Meeting (Stuttgart, DE) 14 – 17 March **2016**.
   In situ solid-state NMR on Li- and Na-ion battery materials
10. Leipzig University (DE), Inorganic Chemistry / Crystallography, 20 Jan **2016** (invited).
    In situ NMR on Li- and Na-ion battery materials
11. The DGK's Young Crystallographers Lab Meeting @ STOE (Darmstadt, DE) 8-9 Sept **2016**. *In situ NMR on Li- and Na-ion battery materials.* (Lightning Talk)
12. "White Nights Science" Meeting and Summer School on New Concepts in Energy Storage (Tallinn, EST) 13 – 20 June **2015** (invited).
    Real-time studies of Li- and Na-ion battery materials
13. 2nd International Freiberg Conference on Electrochemical Storage Materials, ESTORM (Freiberg, DE) 11 – 12 June **2015** (invited).
    In situ solid-state NMR investigations of Li- and Na-ion battery materials.
14. 23rd DGK's Annual Meeting (Göttingen, DE) 16 – 19 March **2015**.
    The solid solution Li_3PO_4—Li_4SiO_4: Crystal structures and Li ion dynamics revisited by diffraction, MD, and NMR.
15. HäKo (Munich, DE) 26 – 28 Feb **2015**.
    "Feuertaufe" – in situ solid state NMR spectroscopy on $LiFePO_4$.
16. 1st Meeting of the DGK's Young Crystallographers (Bremen, DE) 28 – 30 Sept **2014**.
    Atomic Disorder in Intermetallic Phases Locally Resolved. (Lightning Talk)
17. SMARTER 4 Conference (Durham, UK) 01 – 04 Sep **2014**.
    Atomic disorder in intermetallics visited by the combined application of XRD-NMR-QM.
18. Johnson Matthey Technology Centre (Sonning Common, UK) 03 July **2014** (invited).
    ATMC in situ NMR on LIBs and NIBs.
19. Hirschegg (AT) Seminar on Solid-State Chemistry, 20 May – 02 June **2013**.
    Atomic Disorder Locally Resolved.
20. 21st DGK's Annual Meeting (Freiberg, DE) 19 – 22 March **2013**.

Substitutional Disorder in Intermetallic Phases: Investigations of Chemical Bonding by XRD—NMR—QM.

21. HäKo (Freiburg i.Br., DE) 07 – 09 March **2013**.
    Locally: 4 times Ga.
22. University of Bayreuth (DE), Inorganic Chemistry III, 20 – 21 Feb **2013** (invited).
    Complex Disorder in Intermetallic Phases Resolved by Orientation Dependent NMR Experiments.
23. University of Cambridge (UK), Department of Chemistry, 12 – 14 Feb **2013** (invited).
    Complex Disorder in Intermetallic Compounds Resolved by Orientation Dependent NMR Experiments.
24. Laue Day and 20th DGK's Annual Meeting (Munich, DE) 12 – 15 March **2012**.
    The Automatic Tuning Matching Goniometer (ATMG) Probe System: Mapping Chemical Questions Using Orientation Dependent NMR Experiments.
25. HäKo (Oldenburg, DE) 08 – 10 March 2012.
    The Solid Solution $Sr_{1-x}Ba_xGa_2$: Characterisation and NMR Spectroscopy.
26. Hirschegg (AT) Seminar on Solid-State Chemistry, 23 – 26 June **2011**.
    News in the Ga-Rich Part of the Phase Diagram Ca–Ga.
27. Hirschegg (AT) Seminar on Solid-State Chemistry, 03 – 06 June **2010**.
    $Sr_{1-x}Ba_xGa_2$: NMR Spectroscopy.
28. NMR Workshop Understanding Inorganic Materials with the Help of NMR Spectroscopy and Electronic Calculations (Dresden, DE) 24 – 15 March **2009**.
    Complex Disorder and Solid-State NMR Spectroscopy of Intermetallics: $Ca_{1-x}Ga_{2+3x}$ with $0.056 \leq x \leq 0.115$.

Poster presentations
Posterbeiträge

1. SMARTER 5 Conference (Bayreuth, DE) 4 – 8 September **2016**.
   Na-ion battery materials studied by ATMC in situ NMR spectroscopy
2. IMLB (Chicago, USA) 19 – 24 June **2016**.
   O. Pecher, Z. Liu, P. M. Bayley, H. Liu, N. M. Trease, C. P. Grey. *Electrode Materials for Na-Ion Batteries Studied by ATMC in situ NMR Spectroscopy (poster no.1176);*
   W. Meng, P. M. Bayley, O. Pecher, M. W. Gaultois, C. P. Grey. *Toward a High Temperature V_6O_{13} Based Li-Ion Battery (poster no. 614).*
3. EUROMAR (Prague, CZ) 5 – 10 July **2015**.
   Real-time investigations of Li- and Na-ion batteries by Automatic Tuning Matching Cycler (ATMC) in situ NMR spectroscopy.
4. UK Energy Storage Conference (UKES 2014, Warwick, UK) 25 – 27 Nov **2014**.
   Initial attempts on next level real-time studies of battery materials by ATMC in situ NMR spectroscopy.
5. 17th GDCh Solid-State Chemistry Conference (Dresden, DE) 15 – 18 Sep **2014**.
   Next Level Real-Time Studies of LFP Electrodes by ^{7}Li in situ NMR @ Initial attempts on next level real-time studies of battery materials by ATMC in situ NMR spectroscopy.
6. SMARTER 4 Conference (Durham, UK) 01 – 04 Sep **2014**.
   Initial attempts on next level real-time studies of battery materials by ATMC in situ NMR spectroscopy.
7. 16th GDCh Solid-State Chemistry Conference (Darmstadt, DE) 17 – 19 Sep **2012**.
   Ga Bonding Variability in $Ca_{1-x}Ga_{2+3x}$ Visited by Solid-State NMR Spectroscopy.

8. SMARTER 3 Conference (Versailles, FR) 10 – 13 Sep **2014**.
   Substitutional Disorder in Intermetallic Phases: Investigations of Chemical Bonding by XRD—NMR—QM.
9. 15th GDCh Solid-State Chemistry Conference (Berlin, DE) 20 – 22 Sep **2012**.
   $Sr_{1-x}Ba_xGa_2$: NMR Spectroscopy.
10. 3rd International Symposium on Structure-Property-Relationships in Solid-State Materials (Stuttgart, DE) 27 June – 02 July **2010**.
    $Sr_{1-x}Ba_xGa_2$: NMR Spectroscopy and Chemical Bonding of the Ga Atoms.
11. DFT Meets Solid-State Chemistry / FPLO Workshop (Dresden, DE) 25 – 29 Oct **2009**.
    The Solid Solution $Sr_{1-x}Ba_xGa_2$: Investigations of the EFG by Solid-State NMR.
12. 12th EU Conference on Solid-State Chemistry (Münster, DE) 20 – 23 Sep **2009**.
    The Solid Solution $Sr_{1-x}Ba_xGa_2$: Substitutional Disorder and Chemical Bonding, a Solid-State NMR Approach.
13. ChemKrist Workshop 2009 (Freiburg i.Br., DE) 14 – 17 Sep **2009**.
    Crystallographic Disorder and Superstructure in $Ca_{1-x}Ga_{2+3x}$.
14. 17th DGK's Annual Meeting (Hannover, DE) 09 – 12 March **2009**.
    The Ga-Rich Part of the Phase Diagram Ca–Ga.
15. 14th GDCh Solid-State Chemistry Conference (Bayreuth, DE) 24 – 26 Sep **2008**.
    Solid-State NMR of $Ca_{1-x}Ga_{2+3x}$.

Outreach activities, features, and press releases
Outreach-Aktivitäten und Pressemitteilungen

1. University of Cambridge, Department of Chemistry's news "Chem@Chem" (editor Carmen Pryce) – leaving article (04/2017)
2. BBC Radio 4 (Howard Mustoe) Comment on the use of Lithium and Lithium ion technologies (01/2017) with Dr. Elizabeth Castillo Martinez.
3. University of Cambridge ➜🗋 Instagram feature (09/2016) used in Department of Chemistry (@ChemCambridge) ➜🗋 Tweets (09/2016)
4. Cambridge Science Festival: ➜🗋 *Chemistry in Action* (University of Cambridge, Department of Chemistry, 03/2016)
5. Cambridge News ➜🗋 "Ask an Academic" Interview (02/03/2016); also featured on the webpage of the University of Cambridge, Department of Chemistry
6. Cambridge Science Festival Roadshows: *Experimenting with Electricity* ('Hardwick and Cambourne Primary School' and 'St Alban's Catholic Primary School', 03/2016)
7. Scientific Lunch Break: *Materials of the Future* (Highgate School London, 09/2015)
8. duz Magazine (Deutsche Universitätszeitung); Volume October 2008 (24/10/2008). ➜🗋 *Sächsische Brückenschläge.*