

# CURRICULUM VITAE

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## Employment

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- since 2019      **Distinguished R&D Staff** at Oak Ridge National Laboratory, USA.
- since 2017      **Science Initiative Lead High Performance Computing and Data Analytics** at Oak Ridge National Laboratory, USA.
- 2012 - 2017      **Director Neutron Data Analysis and Visualization Division** at Oak Ridge National Laboratory, USA.
- 2011 - 2012      **Distinguished R&D Staff and Diffraction Group Leader** at Oak Ridge National Laboratory, USA.
- 2001 - 2011      **Technical Staff Member** at Lujan Neutron Scattering Center, Los Alamos National Laboratory, USA.
- 1998 - 2001      **Research Associate** with Prof. S.J.L Billinge at the Department of Physics and Astronomy, Michigan State University, USA.
- 1995 - 1998      **Postdoctoral Fellow** with Dr. T.R. Welberry at the Research School of Chemistry, The Australian National University, Australia.
- 1992 - 1995      **Doctoral Fellow** with Prof. F. Frey at the Neutron Scattering Group, Department of Mineralogy and Crystallography, Ludwig Maximilians Universität (LMU), Munich, Germany.

## Education

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- 28 Jun 1995      **PhD (Dr. rer. nat.)** "Disorder and diffuse neutron and X-ray scattering from zirconia at temperatures up to 1500 K using newly designed experimental X-ray techniques" at Ludwig Maximilians Universität, Munich, Germany
- 04 Feb 1992      **Diploma (Physics)** "Disorder in CaO stabilized zirconia studied using diffuse neutron scattering from RT to 1750 K", at Ludwig Maximilians Universität, Munich, Germany
- 25 May 1983      **Abitur (High School Graduation)** at Helene-Lange Gymnasium, Rendsburg, Germany

## Awards

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2018	Tennessee Governor's Volunteer Star Award for work with Oak Ridge Computer Science Girls.
2014	UT-Battelle Awards Night - Community Outreach.
2009	Selected for the Leadership Development Initiative program of the Los Alamos National Laboratory's Experimental Science's Directorate.
2006	Los Alamos National Laboratory Women's Career Development Outstanding Mentoring Award.
2006	Los Alamos LAAP Award (for achievements as local chair of the American Conference on Neutron Scattering).
2005	Los Alamos LAAP Award (for achievements related to preparation for Lujan Center review by the Department of Energy).
2002	Los Alamos National Laboratory Individual Distinguished Performance Award.

## Official functions

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since 2021	American Association for the Advancement of Science
since 2020	Fellow of the Neutron Scattering Society of America
since 2020	IUCr Journals Commissioning Editor for Methods, Instrumentation and Materials
2019-2020	Member of the International Program Committee for the 25th Congress and General Assembly of the International Union of Crystallography
since 2018	Member of the ORNL Artificial Intelligence Steering Committee
since 2018	Fellow of the American Crystallographic Association
2018	Member of the TMS Data Infrastructure Task Force
since 2017	Member of the IUCr Commission on Crystallographic Computing
2016	Member of the ORNL-UT Task Force to establish a joined Data Science and Engineering PhD Program
since 2016	Co-Chair of the Research Data Alliance Interest Group on Research data needs of the Photon and Neutron Science community
since 2015	Member of the IUCr Commission on Neutron Scattering
since 2016	Chair of the Experimental Facilities Computing Group
2014-2020	Co-Editor of <i>Journal of Applied Crystallography</i>
since 2004	Editor Board member of <i>Zeitschrift für Kristallographie</i> .
2012-2018	Member of the <i>Mantid</i> project management board.
2011-2017	Member of executive cabinet of the Neutron Sciences Directorate at Oak Ridge National Laboratory.
2012-2015	Co-chair of the scientific and technical advisory panel for powder diffraction at the European Spallation Source.

2009-2012	Communications Officer on the Executive Committee of the Neutron Scattering Society of America.
2009-2010	Member of the Communications Standing Committee of the American Crystallographic Association.
2008-2010	Member of the Los Alamos National Laboratory's Experimental Science's Directorate Promotion Committee.
2009	Organizer of the symposium "Quantitative Characterization of Nanostructured Materials" at the MRS spring meeting.
2007	Organizer of the transaction symposium at the Annual Meeting of the American Crystallographic Association.
2007	Local chair and member of the Program Committee of the American Conference on Neutron Scattering in Santa Fe.
2006-2010	Member of the Los Alamos National Laboratory Postdoc Committee (Chair of committee in 2009).
2005	Member of the Program Committee for the European Powder Diffraction Conference.
2004	Guest Editor of Zeitschrift für Kristallographie Special Issue: <i>Structure of Complex Materials</i> .
2003-2008	Member of the Instrument Advisory Team (IAT) for the disordered materials diffractometer (NOMAD) for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory.
2003-2010	Member of the NeXus International Advisory Committee.
2002-2003	President of the Neutron Scattering Special Interest Group of the American Crystallographic Association.
2002-2006	Member of the executive committee for the single crystal diffractometer (SCD) for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory.
2001-2006	Member of the Instrument Advisory Team (IAT) for the high-resolution powder diffractometer (POWGEN) for the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory.
2001-2003	Member of the LANSCE Materials Program Advisory Committee (PAC).
1998-2005	Responsible for development of difCIF, an extension of the Crystallographic Information File format to include diffuse scattering.

## Other Activities

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- Frequent reviewer of papers for major scientific journals including Science, Physical Review Letters and Journal of the American Chemical Society.
- Reviewer of funding proposals of major funding agencies including the Office of Science of the Department of Energy and the European Commission's CORDIS program.
- Member of experimental proposal review committees of national user facilities including ISIS, NIST, LANSCE and SNS.
- Organizer of ~ 30 workshops on total scattering analysis.
- Participant in the 2012 Anderson County Leadership Program and 2015 Oak Ridge Leadership Program.

## Outreach

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- Founder and Director of non-profit Oak Ridge Computer Science Girls - [www.orcsgirls.org](http://www.orcsgirls.org).
- Frequent judge at local science fair and First Lego League robotics competition.
- Collaboration with Katharine Page and Daniel Olds on development of outreach materials funded by ACA grant.
- Lead for the the Neutron Science trailer as part of the ORNL Traveling Science Fair.

## Mentorship

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- Mentor in the Oak Ridge National Laboratory mentoring program.
- Member of the thesis committee of Katharine Page (University of California Santa Barbara).
- Mentor of four postdocs and 20 graduate and undergraduate students.
- Supervision of ~ 80 students and postdocs visiting as users of the NPDF instrument.
- Served on the Rosen Thesis Award Committee.

## Memberships

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American Association for the Advancement of Science

American Crystallographic Association

Neutron Scattering Society of America

Association for Computing Machinery

Minerals, Metals & Materials Society

## Publications (H index: 48)

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### Books and book chapters

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- [1] **TH. PROFFEN** AND G. GRANROTH. Cross-Cutting Software Solutions in Support of Experimental Analysis Challenges at National Scattering Facilities. In KERSTIN KLEESE, STUART CAMPBELL, KEVIN YAGER, RICHARD FARNSWORTH, AND MAARTJE VAN DAM, editors, *Handbook on Big Data and Machine Learning in the Physical Sciences, Vol 2: Advanced Analysis Solutions for Leading Experimental Techniques*. World Scientific, 2020.
- [2] K. PAGE, **TH. PROFFEN**, AND R.B. NEDER. Structure of Nanoparticles from Total Scattering. In E.J. MITTERMEIJER, editor, *Modern Diffraction Methods*. Wiley Verlag GmbH, Weinheim, 2013. doi:[10.1002/9783527649884.ch3](https://doi.org/10.1002/9783527649884.ch3).
- [3] B. PALOSZ, E. GRZANKA, S. GIERLOTKA, M. WOJDYR, W. PALOSZ, **TH. PROFFEN**, R. RICH, AND S. STELMAKH. Looking beyond Limitations of Diffraction Methods of Structural Analysis of Nanocrystalline Materials. In R. PYRZ AND J.C. RAUHE, editors, *IUTAM Symposium on Modelling Nanomaterials and Nanosystems. IUTAM Bookseries, 13*, pages 75–88. Springer, Dordrecht, 2009. doi:[10.1007/978-1-4020-9557-3\\_9](https://doi.org/10.1007/978-1-4020-9557-3_9).
- [4] R. UBIC, G. SUBODH, M. SEBASTIAN, D. GOUT, AND **TH. PROFFEN**. Effective Size of Vacancies In The  $\text{Sr}_{1-3x}/2\text{Ce}_x\text{TiO}_3$  Superstructure. In K.M. NAIR, R.W. SUVOROV, AND R. GUO, editors, *Advances in Electroceramic Materials: Ceramic Transactions, 204*, pages 177–185. The American Ceramic Society, 2009. doi:[10.1002/9780470528990.ch20](https://doi.org/10.1002/9780470528990.ch20).
- [5] R.B. NEDER AND **TH. PROFFEN**. *Diffuse Scattering and Defect Structure Simulations: A cook book using the program DISCUS*. IUCr Texts on Crystallography. Oxford University Press, Oxford, 2008. doi:[10.1093/acprof:oso/9780199233694.001.0001](https://doi.org/10.1093/acprof:oso/9780199233694.001.0001).
- [6] **TH. PROFFEN**. Analysis of Disordered Materials using Total Scattering and the Atomic Pair Distribution Function. In H.-R. WENK, editor, *Reviews in Mineralogy and Geochemistry: Neutron Scattering in Earth Sciences, 63*, pages 255–274. Mineralogical Society of America, 2006. doi:[10.2138/rmg.2006.63.11](https://doi.org/10.2138/rmg.2006.63.11).

### Peer reviewed papers

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- [1] FREDERICK P. MARLTON, ZHAOMING ZHANG, YUANPENG ZHANG, **TH. PROFFEN**, CHRIS D. LING, AND BRENDAN J. KENNEDY. Lattice disorder and oxygen migration pathways in pyrochlore and defect-fluorite oxides. *Chemistry of Materials*, **33**(4), 1407–1415, 2021. doi:[10.1021/acs.chemmater.0c04515](https://doi.org/10.1021/acs.chemmater.0c04515).
- [2] MATHIEU DOUCET, ANJANA M SAMARAKOON, CHANGWOO DO, WILLIAM T. HELLER, RICHARD ARCHIBALD, D. ALAN TENNANT, THOMAS PROFFEN, AND GARRETT E. GRANROTH. Machine learning for neutron scattering at ORNL. *Mach. Learn.: Sci. Technol.*, **2**(2), 023001, Dec 2020. doi:[10.1088/2632-2153/abcf88](https://doi.org/10.1088/2632-2153/abcf88).
- [3] K. KUPWADE-PATIL, P.J. BOUL, D.K. RASNER, S.M. EVERETT, **TH. PROFFEN**, K.L. PAGE, D. MA, D. OLDS, THAEMLITZ C.J., AND O. BÜYÜKÖZTÜRK. Retarder Effect on Hydrating Oil Well Cements Investigated using in situ Neutron/X-ray Pair Distribution Function Analysis. *Cement and Concrete Research*, **126**, 105920, 2019. doi:[10.1016/j.cemconres.2019.105920](https://doi.org/10.1016/j.cemconres.2019.105920).
- [4] D. OLDS, C.N. SAUNDERS, M. PETERS, **TH. PROFFEN**, J. NEUEFEIND, AND K. PAGE. Precise Implications for Real-Space Pair Distribution Function Modeling of Effects Intrinsic to Modern Time-of-Flight Neutron Diffractometers. *Acta Cryst. A*, **74**, 293–307, 2018. doi:[10.1107/S2053273318003224](https://doi.org/10.1107/S2053273318003224).
- [5] E. DEELMAN, C. CAROTHERS, A. MANDAL, B. TIERNEY, J.S. VETTER, I. BALDIN, C. CASTILLO, G. JUVE, D. KROL, V. LYNCH, B. MAYER, J. MEREDITH, **TH. PROFFEN**, P. RUTH, AND R.F. DA SILVA. PANORAMA: An approach to performance modeling and diagnosis of extreme-scale workflows. *International Journal of High Performance Computing Applications*, **31**(1), 4–18, 2017. doi:[10.1177/1094342015594515](https://doi.org/10.1177/1094342015594515).
- [6] V.E. LYNCH, J.M. BORREGUERO, D. BHOWMIK, P. GANESH, B.G. SUMPTER, **TH. PROFFEN**, AND M. GOSWAMI. An Automated Analysis Workflow for Optimization of Force-Field Parameters using Neutron Scattering Data. *J. Comput. Phys.*, **340**, 128–137, 2017. doi:[10.1016/j.jcp.2017.03.045](https://doi.org/10.1016/j.jcp.2017.03.045).
- [7] P.M.M. THYGESEN, C.A. YOUNG, E.O.R. BEAKE, F.D. ROMERO, L.D. CONNOR, **TH. PROFFEN**, A.E. PHILLIPS, M.G. TUCKER, M.A. HAYWARD, D.A. KEEN, AND A.L. GOODWIN. Local Structure Study of the Orbital Order/Disorder Transition in  $\text{LaMnO}_3$ . *Phys. Rev. B*, **95**(17), 2017. doi:[10.1103/PhysRevB.95.174107](https://doi.org/10.1103/PhysRevB.95.174107).
- [8] M.P. ATTFIELD, M. FEYGENSON, J.C. NEUEFEIND, **TH. PROFFEN**, T.C.A. LUCAS, AND J.A. HRILJAC. Reprobing the Mechanism of Negative Thermal Expansion in Siliceous Faujasite. *RSC Advances*, **6**(24), 19903–19909, 2016. doi:[10.1039/c5ra23827g](https://doi.org/10.1039/c5ra23827g).
- [9] D. LEE, D.J. WILLIAMS, S.C. VOGEL, **TH. PROFFEN**, J.D. THOMPSON, L.L. DAEMEN, AND S. PARK. Tailoring Structure and Magnetic Properties of  $\text{Ni}_x\text{Co}_{1-x}(\text{N}(\text{CN})_2)_2$  Molecular Magnets. *Current Applied Physics*, **16**(9), 1100–1104, 2016. doi:[10.1016/j.cap.2016.06.015](https://doi.org/10.1016/j.cap.2016.06.015).
- [10] A. BOEHNLEIN, B. MATTHEWS, **TH. PROFFEN**, AND F. SCHLUENZEN. The Research Data Alliance Photon and Neutron Science Interest Group. *Synchrotron Radiation News*, **28**(2), 43–47, 2015. doi:[10.1080/08940886.2015.1013421](https://doi.org/10.1080/08940886.2015.1013421).
- [11] N.W. MCNUTT, O. RIOS, M. FEYGENSON, **TH. PROFFEN**, AND D.J. KEFFER. Structural Analysis of Lignin-Derived Carbon Composite Anodes. *J. Appl. Cryst.*, **47**, 1577–1584, 2014. doi:[10.1107/S1600576714014666](https://doi.org/10.1107/S1600576714014666).

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- [13] K.M.O. JENSEN, M. CHRISTENSEN, H.P. GUNNLAUGSSON, N. LOCK, E.D. BOJESEN, **TH. PROFFEN**, AND B.B. IVERSEN. Defects in Hydrothermally Synthesized  $\text{LiFePO}_4$  and  $\text{LiFe}_{1-x}\text{Mn}_x\text{PO}_4$  Cathode Materials. *Chem. Mater.*, **25**(11), 2282–2290, 2013. doi:[10.1021/cm4008393](https://doi.org/10.1021/cm4008393).
- [14] H. KIM, K. SAKAKI, H. OGAWA, Y. NAKAMURA, J. NAKAMURA, E. AKIBA, A. MACHIDA, T. WATANUKI, AND **TH. PROFFEN**. Origin of Degradation in the Reversible Hydrogen Storage Capacity of  $\text{V}_{1-x}\text{Ti}_x$  Alloys from the Atomic Pair Distribution Function Analysis. *J. Phys. Chem. C*, **117**(50), 26543–26550, 2013. doi:[10.1021/jp408766r](https://doi.org/10.1021/jp408766r).
- [15] J. PETERSON, J. TENCADE, **TH. PROFFEN**, T. DARLING, H. NAKOTTE, AND K. PAGE. Quantifying Amorphous and Crystalline Phase Content with The Atomic Pair Distribution Function. *J. Appl. Cryst.*, **46**, 332–336, 2013. doi:[10.1107/S0021889812050595](https://doi.org/10.1107/S0021889812050595).
- [16] J.L. PROVIS, A. HAJIMOHAMMADI, C.E. WHITE, S.A. BERNAL, R.J. MYERS, R.P. WINARSKI, V. ROSE, **TH. PROFFEN**, A. LLOBET, AND J.S.J. VAN DEVENTER. Nanostructural Characterization of Geopolymers by Advanced Beamline Techniques. *Cement Concrete Comp.*, **36**, 56–64, 2013. doi:[10.1016/j.cemconcomp.2012.07.003](https://doi.org/10.1016/j.cemconcomp.2012.07.003).
- [17] K. SAKAKI, N. TERASHITA, H. KIM, **TH. PROFFEN**, E.H. MAJZOUB, S. TSUNOKAKE, Y. NAKAMURA, AND E. AKIBA. Crystal Structure and Local Structure of  $\text{Mg}_{2-x}\text{Pr}_x\text{Ni}_4$  ( $x=0.6$  and  $1.0$ ) Deuteride Using in Situ Neutron Total Scattering. *Inorganic Chem.*, **52**(12), 7010–7019, 2013. doi:[10.1021/ic400528u](https://doi.org/10.1021/ic400528u).
- [18] H.-W. WANG, D.J. WESOŁOWSKI, **TH. PROFFEN**, L. VLCEK, W. WANG, L.F. ALLARD, A.I. KOLESNIKOV, M. FEYGENSON, L.M. ANOVITZ, AND R.L. PAUL. Structure and Stability of  $\text{SnO}_2$  Nanocrystals and Surface-Bound Water Species. *J. Am. Chem. Soc.*, **135**(18), 6885–6895, 2013. doi:[10.1021/ja312030e](https://doi.org/10.1021/ja312030e).
- [19] H. KIM, J. NAKAMURA, H. SHAO, Y. NAKAMURA, E. AKIBA, K.W. CHAPMAN, P.J. CHUPAS, AND **TH. PROFFEN**. Variation in the Ratio of  $\text{Mg}_2\text{Co}$  and  $\text{MgCo}_2$  in Amorphous-Like Mechanically Alloyed  $\text{Mg}_x\text{Co}_{100-x}$  using Atomic Pair Distribution Function Analysis. *Z. Krist.*, **227**(5), 299–303, 2012. doi:[10.1524/zkri.2012.1496](https://doi.org/10.1524/zkri.2012.1496).
- [20] **TH. PROFFEN**. Neutron Total Scattering Analysis of Nanoparticles. *Jom*, **64**(1), 112–116, 2012. doi:[10.1007/s11837-011-0216-x](https://doi.org/10.1007/s11837-011-0216-x).
- [21] N. RADEMACHER, L.L. DAEMEN, E.L. CHRONISTER, AND **TH. PROFFEN**. Pair Distribution Function Analysis of Molecular Compounds: Significance and Modeling Approach Discussed Using the Example of p-Terphenyl. *J. Appl. Cryst.*, **45**, 482–488, 2012. doi:[10.1107/S0021889812016159](https://doi.org/10.1107/S0021889812016159).
- [22] K.A. ROSS, **TH. PROFFEN**, H.A. DABKOWSKA, J.A. QUILLIAM, L.R. YARASKAVITCH, J.B. KYCIA, AND B.D. GAULIN. Lightly Stuffed Pyrochlore Structure of Single-Crystalline  $\text{Yb}_2\text{Ti}_2\text{O}_7$  Grown by the Optical Floating Zone Technique. *Phys. Rev. B*, **86**(17), 2012. doi:[10.1103/PhysRevB.86.174424](https://doi.org/10.1103/PhysRevB.86.174424).
- [23] C.E. WHITE, J.L. PROVIS, **TH. PROFFEN**, AND J.S.J. VAN DEVENTER. Molecular Mechanisms Responsible for the Structural Changes Occurring During Geopolymerization: Multiscale Simulation. *Aiche Journal*, **58**(7), 2241–2253, 2012. doi:[10.1002/aic.12743](https://doi.org/10.1002/aic.12743).
- [24] J. GREEDAN, S. DERAKHSHAN, F. RAMEZANIPOUR, J. SIEWENIE, AND **TH. PROFFEN**. A Search for Disorder in the Spin Glass Double Perovskites  $\text{Sr}_2\text{CaReO}_6$  and  $\text{Sr}_2\text{MgReO}_6$  Using Neutron Diffraction and Neutron Pair Distribution Function Analysis. *J. Condens. Matter Phys.*, **23**(16), 2011. doi:[10.1088/0953-8984/23/16/164213](https://doi.org/10.1088/0953-8984/23/16/164213).
- [25] H. KIM, J. NAKAMURA, H. SHAO, Y. NAKAMURA, E. AKIBA, K. CHAPMAN, P. CHUPAS, AND **TH. PROFFEN**. Local Structural Evolution of Mechanically Alloyed  $\text{Mg}_{50}\text{Co}_{50}$  Using Atomic Pair Distribution Function Analysis. *J. Phys. Chem. C*, **115**(15), 7723–7728, 2011. doi:[10.1021/jp111711c](https://doi.org/10.1021/jp111711c).
- [26] H. KIM, J. NAKAMURA, H. SHAO, Y. NAKAMURA, E. AKIBA, K.W. CHAPMAN, P.J. CHUPAS, AND **TH. PROFFEN**. Insight into the Hydrogenation Properties of Mechanically Alloyed  $\text{Mg}(50)\text{Co}(50)$  from the Local Structure. *J. Phys. Chem. C*, **115**(41), 20335–20341, 2011. doi:[10.1021/jp207197k](https://doi.org/10.1021/jp207197k).
- [27] L. MALAVASI, G. ARTIOLI, H. KIM, B. MARONI, B. JOSEPH, Y. REN, **TH. PROFFEN**, AND S. BILLINGE. Local structural investigation of  $\text{SmFeAsO}_{1-x}\text{F}_x$  High Temperature Superconductors. *J. Condens. Matter Phys.*, **23**(27), 2011. doi:[10.1088/0953-8984/23/27/272201](https://doi.org/10.1088/0953-8984/23/27/272201).
- [28] K. PAGE, T. HOOD, **TH. PROFFEN**, AND R. NEDER. Building and Refining Complete Nanoparticle Structures with Total Scattering Data. *J. Appl. Cryst.*, **44**, 327–336, 2011. doi:[10.1107/S0021889811001968](https://doi.org/10.1107/S0021889811001968).
- [29] K. PAGE, C. WHITE, E. ESTELL, R. NEDER, A. LLOBET, AND **TH. PROFFEN**. Treatment of Hydrogen Background in Bulk and Nanocrystalline Neutron Total Scattering Experiments. *J. Appl. Cryst.*, **44**, 532–539, 2011. doi:[10.1107/S0021889811001609](https://doi.org/10.1107/S0021889811001609).
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- [31] F. RAMEZANIPOUR, J.E. GREEDAN, J. SIEWENIE, **TH. PROFFEN**, D.H. RYAN, A.P. GROSVENOR, AND R.L. DONABERGER. Local and Average Structures and Magnetic Properties of  $\text{Sr}_2\text{FeMnO}_{5+y}$ ,  $y=0.0, 0.5$ . Comparisons With  $\text{Ca}_2\text{FeMnO}_5$  And The Effect of the A-Site Cation. *Inorganic Chem.*, **50**(16), 7779–7791, 2011. doi:[10.1021/ic200919m](https://doi.org/10.1021/ic200919m).
- [32] Y. REN, J.-Q. YAN, J.-S. ZHOU, J.B. GOODENOUGH, J.D. JØRGENSEN, S. SHORT, H. KIM, **TH. PROFFEN**, S. CHANG, AND R.J. MCQUEENEY. Spin-state Transitions in  $\text{PrCoO}_3$  Studied with Neutron Powder Diffraction. *Phys. Rev. B*, **84**(21), 2011. doi:[10.1103/PhysRevB.84.214409](https://doi.org/10.1103/PhysRevB.84.214409).



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- [34] P. TONG, D. LOUCA, X. GU, S. POON, G. SHIFLET, AND **TH. PROFFEN**. Fluctuations of the Local Atomic Environment with Chemical Alloying in Fe Bulk Metallic Glasses. *Metall. Mater. Trans. A*, **42A**(6), 1481–1485, 2011. doi:[10.1007/s11661-011-0695-y](https://doi.org/10.1007/s11661-011-0695-y).
- [35] C. WHITE, J. PROVIS, L. GORDON, D. RILEY, **TH. PROFFEN**, AND J. VAN DEVENTER. Effect of Temperature on the Local Structure of Kaolinite Intercalated with Potassium Acetate. *Chem. Mater.*, **23**(2), 188–199, 2011. doi:[10.1021/cm102648n](https://doi.org/10.1021/cm102648n).
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