

PUBLIKATIONEN, KONFERENZBEITRÄGE, VORTRÄGE  
UND PREISE (1997-2022)

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**Published Articles**

**2022**

- *Cooperative Light-Induced Breathing of Soft Porous Crystals via Azobenzene Buckling*, S. Krause, J.D. Evans, V. Bon, S. Crespi, W. Danowski, W.R. Browne, S. Ehrling, F. Walenzus, D. Wallacher, N. Grimm, D.M. Töbrens, M.S. Weiss, S. Kaskel, B.L. Feringa, *Nature Communications* 13, 1951 (2022)
- *Temperature-Dependent EXAFS Measurements of the Pb L3-Edge Allow Quantification of the Anharmonicity of the Lead–Halide Bond of Chlorine-Substituted Methylammonium (MA) Lead Triiodide*, G. Schuck, D. Töbrens, D. Wallacher, N. Grimm, S. Schorr, *J. Phys. Chem. C* 126, 5388 (2022)

**2021**

- *Facilitated crystal handling using a simple device for evaporation reduction in microtiter plates*, T. Barthel, F. Huschmann, D. Wallacher, C.G. Feiler, G. Klebe, M.S. Weiss, J. Wollenhaupt, *J. Appl. Cryst.* 54, 376 (2021)
- *Effects of Cr Doping and Water Content on the Crystal Structure Transitions of Ba<sub>2</sub>In<sub>2</sub>O<sub>5</sub>*, R. Finger, M. Widenmeyer, T.C. Hansen, D. Wallacher, S. Savvin, M. Bertmer, A. Weidenkaff and H. Kohlmann, *crystals* 11, 1548 (2021)
- *CO<sub>2</sub> Adsorption Enhanced by Tuning the Layer Charge in a Clay Mineral*, W.B. Hunvik, P. Loch, D. Wallacher, A. Kirch, L. Cavalcanti, M. Riess, M. Daab, V. Josvanger, S. Grätz, F. Yokaichiya, K. Knudsen, C. Rodrigues Miranda, J. Breu, J.O. Fossum, *Langmuir* 37, 14491 (2021)
- *Workflow and Tools for Crystallographic Fragment Screening at the Helmholtz-Zentrum Berlin*, J. Wollenhaupt, T. Barthel, G.M.A. Lima, A. Metz, D. Wallacher, E. Jagudin, F.U. Huschmann, T. Hauß, C.G. Feiler, M. Gerlach, M. Hellmig, R. Förster, M. Steffien, A. Heine, G. Klebe, U. Müller, M.S. Weiss, *J. Vis. Exp.* 169, e62208 (2021)
- *Massive pressure amplification by stimulated contraction of mesoporous frameworks*, V. Bon, S. Krause, I. Senkovska, N. Grimm, D. Wallacher, D.M. Töbrens, S. Kaskel, *Angew. Chem. Int. Ed.* 60, 11735 (2021)

- *Direct Observation of the Xenon Physisorption Process in Mesopores by Combining In Situ Anomalous Small-Angle X-ray Scattering and X-ray Absorption Spectroscopy*, E. Gericke, D. Wallacher, R. Wendt, G. Greco, M. Krumrey, S. Raoux, A. Hoell, S. Mascotto, *J. Phys. Chem. Lett.* 12, 4018 (2021)
- *The Role of Temperature and Adsorbate on Negative Gas Adsorption in the Mesoporous Metal-Organic Framework DUT-49*, S. Krause, J. Evans, V. Bon, I. Senkovska, D. Töbrens, D. Wallacher, N. Grimm, S. Kaskel, *Faraday Discussions* 225, 168 (2021)
- *Influence of Surface Wettability on Methane Hydrate Formation in Hydrophilic and Hydrophobic Mesoporous Silicas*, M.E. Casco, S. Grätz, D. Wallacher, N. Grimm, D. Töbrens, M. Bilo, N. Speil, M. Fröba, L. Borchardt, *Chemical Engineering Journal* 405, 126955 (2021)
- *Phonons in single-crystalline mesoporous silicon: the absence of phonon-softening upon structuring silicon on sub-10 nanometer length scales*, T. Hofmann, D. Kojda, H. Haseeb, D. Wallacher, O. Sobolevc, K. Habicht, *Microporous and Mesoporous Materials* 312, 110814 (2021)

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- *A Novel Electrochemical Anodization Cell for the Synthesis of Mesoporous Silicon*, N. Gostkowska-Lekner, D. Wallacher, N. Grimm, K. Habicht, T. Hofmann, *Rev. Sci. Instr.* 91, 105113 (2020)
- *CO<sub>2</sub> Capture by Nickel Hydroxide Interstratified in the Nanolayered Space of a Synthetic Clay Mineral*, K.W.B. Hunvik, P. Loch, D. Wallacher, L. Cavalcanti, K. Seljelid, P. Røren, S. Rudic, D. Wallacher, A. Kirch, K. Knudsen, C. Miranda Rodrigues, J. Breu, H. Bordallo, J. Fossum, accepted in *J. Phys. Chem.* (2020)
- *Evolution of distance between  $\omega$  particles in metastable  $\beta$ -Ti alloy determined from in-situ small angle neutron scattering*, P. Zháňal, V. Ryukhtin, G. Farkas, P. Kadletz, U. Keiderling, D. Wallacher, P. Harcuba, *MATEC Web. Conf.* 321, 12027 (2020)
- *Pore size gradient effect in monolithic silica mesopore networks revealed by in-situ-SAXS-physorption*, S.A. Kube, K. Turke, R. Ellinghaus, D. Wallacher, M. Thommes, B. Smarsly, *Langmuir* 36, 11996 (2020)
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- *An advanced structural characterization of templated meso-macroporous carbon monoliths by small- and wide-angle scattering techniques*, F. Badaczewski, M. Loeh, T. Pfaff, D. Wallacher, D. Clemens, B. Smarsly, Beilstein J. Nanotechnol. 11, 310 (2020); *Correction: An advanced structural characterization of templated meso-macroporous carbon monoliths by small- and wide-angle scattering techniques*, F. Badaczewski, M. Loeh, T. Pfaff, D. Wallacher, D. Clemens, B. Smarsly, Beilstein J. Nanotechnol. 11, 678 (2020)

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- *Exploiting Dynamic Opening of Apertures in Partially Fluorinated MOF for Enhancing H<sub>2</sub> Desorption Temperature and Isotope Separation*, L. Zhang, S. Jee, J. Park, M. Jung, D. Wallacher, A. Franz, W. Lee, M. Yoon, K.M. Choi, M. Hirscher, H. Oh, J. Am. Chem. Soc. 141, 19850 (2019)
- *Experimental Evidence of Confined Methane Hydrate in Hydrophilic and Hydrophobic Model Carbons*, M.E. Casco, E. Zhang, S. Grätz, S. Krause, V. Bon, D. Wallacher, N. Grimm, D. Többens, T. Hauss, and L. Borchardt, J. Phys. Chem. C 123, 24071 (2019)
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- *BerILL: The ultimate humidity chamber for neutron scattering*, J. Gonthier, M.A. Barrett, O. Aguetaz, S. Baudoin, E. Bourgeat-Lami, B. Demé, N. Grimm, T. Hauß, K. Kiefer E. Lelièvre-Berna, A. Perkins, D. Wallacher, J. Neutron Research 21, 65 (2019)
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- *Peering into the structural evolution of glass-like carbons derived from phenolic resin by combining small-angle neutron scattering with an advanced evaluation method for wide-angle X-ray scattering*, F. Badaczewski, M.O. Loeh, T. Pfaff, S. Dobrotka, D. Wallacher, D. Clemens, J. Metz, B.M. Smarsly, Carbon 141, 169 (2019)

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- Dissertation: „Porenkondensierte Materie in der Nähe des Fest-Flüssig-Dampf-Tripelpunktes - Thermodynamische Untersuchungen an Adsorbaten in nanoskaligen Poren“, Universität des Saarlandes, Saarbrücken 2006
  - Diplomarbeit: „FT-Infrarotspektroskopie an Stickstoff adsorbiert in nanoporösen Gläsern“, Universität des Saarlandes, Saarbrücken 1998
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## Vorträge und Konferenzbeiträge

- 12<sup>th</sup> International workshop on sample environment, Nasu (Japan), Talk: *In operando sample environment dedicated to studies in gas- and electro-catalytic processes using x-ray spectroscopy*
- SNI 2022 German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities, Berlin 2022, Poster: *Sample Environment at BESSY-II*
- 10<sup>th</sup> International workshop on sample environment, Berlin, 2018, Talk: *Sample Environment at BESSY-II: Gas Atmospheres and More ...*
- 10<sup>th</sup> International workshop on sample environment, Berlin, 2018, Poster: *Cryostat for High-Resolution X-ray Emission spectroscopy*
- SNI 2018 German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities, München-Garching 2018, Poster: *Specialized Sample Environment at BESSY-II*
- 30<sup>th</sup> European Crystallographic Meeting, 28<sup>th</sup> August - 1<sup>st</sup> September 2016, Congress Center Basel, Switzerland: *FALCON - A Laue diffractometer for ambient and non-ambient neutron structural analysis*, M. Tovar, L. Diestel, H.-J. Bleif, K. Fritsch, K. Habicht, D. Wallacher, G.N. Iles and S. Schorr, *Acta Cryst A*. A72, 415, (2016)
- 30<sup>th</sup> European Crystallographic Meeting, 28<sup>th</sup> August - 1<sup>st</sup> September

2016, Congress Center Basel, Switzerland: *Neutron diffraction on methane and hydrogen hydrates under high pressure*, U. Ranieri, L.E. Bove, S. Klotz, T.C. Hansen, M.M. Koza, P. Gillet, D. Wallacher, A. Falenty, W.F. Kuhs, *Acta Cryst A*. A72, 415, (2016)

- 8<sup>th</sup> International Workshop on Sample Environment at Neutron Scattering Facilities, Eynsham Hall – Oxfordshire (UK), 2014, Talk: *The next generation humidity chamber for neutron scattering*
- Workshop Innovative Methoden der Sorptionsmessung, Fraunhofer IWS Dresden, 2014, Invited Talk: *In-situ Gasadsorptionsmethoden kombiniert mit Röntgen- und Neutronenstreuung*
- ICNS 2013, Edinburgh (Scotland), 2013, Talk: *Innovations in Sample Environment for Soft Matter Science and Material Research at HZB*
- ESS Science Symposium: Neutrons for Future Energy Strategy, PSI-Switzerland, 2013, Invited Talk: *Dedicated Sample Environment for Energy Research*
- DN 2012, Bonn, 2012, Poster: *Standard, Advanced and Complementary Sample Environment at the Helmholtz-Centre Berlin*
- ESS Science Symposium: Time-resolved, in-situ Chemistry using neutrons, Gothenburg, Sweden 2012, Invited Talk: *Sample Environment and investigations under controlled gas atmospheres and humidity*
- Science and Scientists @ ESS, Berlin, 2012, Poster: *Standard, Advanced and Complementary Sample Environment at the Helmholtz-Centre Berlin*
- PNI in-house research “2nd Soft Matter & Life Science Workshop”, Potsdam 2012, Talk: *Soft Matter SANS Sample Environment at the HZB*
- ESS Science Symposium: The Future of Soft Matter SANS, Lund, Sweden 2012, Poster: *Soft Matter SANS Sample environment at the Helmholtz-Zentrum Berlin*
- 5<sup>th</sup> European Conference on Neutron Scattering, Prague, 2011, Talk: *In-situ Gas Adsorption Techniques in Neutron Scattering*
- 6<sup>th</sup> International workshop on sample environment, Munich, 2010, Talk: *Multi-purpose gas handling for automated in-situ gas adsorption measurements*

- ICNS 2009, Knoxville (Tennessee), 2009, Invited Talk: *Methods and Instrumentation for Neutron Scattering combined with In-Situ Gas Adsorption*
- 21. Deutsche Zeolith-Tagung, Kiel, 2009, Poster: *Combined Neutron Scattering and Gas Adsorption at the Berlin Neutron Scattering Centre*
- MOF08 - 1st International Conference on Metal Organic Frameworks, Augsburg 2008, Poster
- DN 2008, München, 2008, Poster: *Neutron Scattering under Controlled Gas Atmospheres - The CGA-Sample Environment*
- 20. Deutsche Zeolith-Tagung, Halle, 2008, Poster: *In-situ-SANS investigations of C<sub>5</sub>F<sub>12</sub> condensation in mesoporous silicas with a hierarchical pore structure Scattering; Poster: Experiments under controlled gas pressure: New experimental possibilities for the study of porous materials*
- European Conference on Neutron Scattering (ECNS 2007), Lund, Sweden, 2007, Poster: *Sample Environment at BENSC - New Developments on Magnetic Field and Temperature; Poster: Combined Neutron Scattering and In-situ Gas Adsorption Experiments under controlled PVT-Conditions*
- Fundamental of Adsorption (FOA 9), Giardini Naxos, Italy, 2007, Vortrag: *On the Nitrogen Sorption Mechanism in Silica with hierarchical mesoporosity studied by in-situ Small-Angle Neutron Scattering*
- 19. Deutsche Zeolith-Tagung, Leipzig, 2007, Vortrag: *Combined Neutron Scattering and In-situ Gas Adsorption Experiments under controlled PVT-conditions*
- SNI 2006, Hamburg, 2006, Poster: *Probenumgebung für Neutronenstreuung in Kombination mit in situ Gasadsorption unter kontrollierten PVT-Bedingungen*
- Berliner Tieftemperatur-Kolloquium, Berlin, 23. Mai 2006, Vortrag: *Neutronendiffraktion an festem 4He in porösem Glas*
- Dynamics in Confinement 2003, Grenoble, France, 2003, Poster: *Dielectric investigations of some pore condensates*
- Klausurtagung des SFB 277 „Grenzflächenbestimmte Materialien“, Homburg, November 2001, Vortrag: *Schmelzen von Argon in Nanoporen*
- Dynamics in Confinement, Grenoble, France, 2000, Poster: *Thermodynamics*

*and structure of Ar, N<sub>2</sub>, CO solidified in nanopores*

- DISMOS 6, Garchy, France, 1999, Poster: *Pore condensed molecules*
- DPG-Frühjahrstagung, Münster, 1997, Poster: *Infrarot und Strukturuntersuchungen in nanoporösem Vycor Glas*

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## Preise

- Universität des Saarlandes, Saarbrücken, Oktober 2007:  
Dr. Eduard-Martin-Preis für die beste Dissertation im akademisch Jahr 2006 in der Naturwissenschaftlich-Technischen Fakultät II der Universität des Saarlandes