

Curriculum vitae

NILS EDVIN RICHARD ZIMMERMANN

March 21, 2017

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| Email: nerz@lbl.gov | Lawrence Berkeley National Laboratory |
| URL: http://www.nisseshem.de | Computing Sciences Area |
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| | Comp. Chemistry, Materials & Climate |
| | 1 Cyclotron Road, MS 50F-1650 |
| | Berkeley, CA 94720 |

RESEARCH INTERESTS

- Physical chemistry & materials science: nucleation, polymorph selection, defect formation, adsorbate and intercalant diffusion, adsorption
- Molecular modeling & visualization

EDUCATION

| | | |
|------|---------------------------------------|---|
| 2013 | Dr.-Ing. (Ph.D.) Chemical Engineering | Hamburg University of Technology, Germany |
| 2006 | M.Sc. Chemical Engineering | Hamburg University of Technology |
| 2004 | ERASMUS Exchange Studies | Royal Institute of Technology, Stockholm, Sweden |
| 2003 | B.Sc. General Engineering Science | Hamburg University of Technology |

PROFESSIONAL APPOINTMENTS

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|------------------|----------------------|--|---|
| 2015 –present | Postdoctoral Fellow | Lawrence Berkeley National Laboratory (LBNL) | Computational Research Division |
| 2013–2015 | Postdoctoral Scholar | University of California, Santa Barbara (UCSB) | Chemical Engineering |
| 2007–2013 | Research Fellow | Hamburg University of Technology | Chemical Engineering |
| 2006–2007 | Research Fellow | École Normale Supérieure de Lyon, France | Centre Européen de Calcul Atomique et Moléculaire (CECAM) |

PUBLICATIONS

Peer-Reviewed Journal Articles

10. N. E. R. Zimmermann and M. Haranczyk, History and Utility of Zeolite Framework-Type Discovery from a Data-Science Perspective, *Cryst. Growth Des.*, 10.1021/acs.cgd.6b00272, 2016
9. N. E. R. Zimmermann, B. Vorselaars, D. Quigley, and B. Peters, Nucleation of NaCl from Aqueous Solution: Critical Sizes, Ion-Attachment Kinetics, and Rates, *J. Am. Chem. Soc.* 137, 13352–13361, 2015
8. T. Titze, A. Lauerer, L. Heinke, C. Chmelik, N. E. R. Zimmermann, F. J. Keil, D. M. Ruthven, and J. Kärger, Transport in Nanoporous Materials Including MOFs: The Applicability of Ficks Laws, *Angew. Chem. Int. Ed.* 54, 14580–14583, 2015
German version: Transport in nanoporösen Materialien, einschließlich MOFs: über die Anwendbarkeit der Fickschen Gesetze, *Angew. Chem.* 127, 14788–14792, 2015
7. N. E. R. Zimmermann, T. J. Zabel, and F. J. Keil, Transport into Nanosheets: Diffusion Equations Put to Test, *J. Phys. Chem. C* 117, 7384–7390, 2013
6. N. E. R. Zimmermann, B. Smit, and F. J. Keil, Predicting Local Transport Coefficients at Solid–Gas Interfaces, *J. Phys. Chem. C* 116, 18878–18883, 2012
5. N. E. R. Zimmermann, S. P. Balaji, and F. J. Keil, Surface Barriers of Hydrocarbon Transport Triggered by Ideal Zeolite Structures, *J. Phys. Chem. C* 116, 3677–3683, 2012
4. N. E. R. Zimmermann, M. Haranczyk, M. Sharma, B. Liu, B. Smit, and F. J. Keil, Adsorption and Diffusion in Zeolites: the Pitfall of Isotypic Crystal Structures, *Mol. Simul.* 37, 986–989, 2011
3. N. E. R. Zimmermann, B. Smit, and F. J. Keil, On the Effects of the External Surface on the Equilibrium Transport in Zeolite Crystals, *J. Phys. Chem. C* 114, 300–310, 2010
2. B. Peters, N. E. R. Zimmermann, G. T. Beckham, J. W. Tester, and B. L. Trout, Path Sampling Calculation of Methane Diffusivity in Natural Gas Hydrates from a Water-Vacancy Assisted Mechanism, *J. Am. Chem. Soc.* 130, 17342–17350, 2008
1. N. E. R. Zimmermann, S. Jakobtorweihen, E. Beerdsen, B. Smit, and F. J. Keil, In-Depth Study of the Influence of Host-Framework Flexibility on the Diffusion of Small Gas Molecules in One-Dimensional Zeolitic Pore Systems, *J. Phys. Chem. C* 111, 17370–17381, 2007

Dissertation

N. E. R. Zimmermann, Transport at Gas–Zeolite Interfaces Probed by Molecular Simulations, Hamburg University of Technology, advised by F. J. Keil, 2013

HONORS & AWARDS

2012 Prize (tied 1st) for best student talk at The 35th Annual British Zeolite Association Meeting

FELLOWSHIPS

2006–2007 Marie Curie Host Fellowship for Early Stage Research Training, CECAM

CONFERENCES & WORKSHOPS

Talks

- 2016 Local order parameters: Descriptors for databases, synthesizability, interstitial relaxation, and diffusion paths, 251st ACS National Meeting & Exposition, March 13–17
Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates, 251st ACS National Meeting & Exposition, March 13–17
- 2014 Transport into Zeolite Nanosheets: Test of Diffusion Equations, AIChE Annual Meeting, November 16–21
- 2012 Predicting Surface Permeabilities via Molecular Simulations, The 35th Annual British Zeolite Association Meeting, July 15–20
- 2011 How Do Chain Length and Pore Type Influence Tracer Transport of Hydrocarbons at Zeolite Surfaces?, 23rd German Zeolite Meeting, March 2–4
- 2008 The Influence of Surface Barriers on Diffusion of Alkane-Zeolite Systems—a Molecular Dynamics Study, AIChE Annual Meeting, November 16–21

Posters

- 2012 How Sensitive Are Adsorption and Diffusion of Guest Molecules in Zeolites Towards Small Changes in the Crystal Structure?, 24th German Zeolite Meeting, March 7–9
- 2011 Transport Barriers as Triggered by the Idealized Microscopic Crystal Surface and the Role of the Evaluation Protocol of Diffusion Experiments, Diffusion Fundamentals IV, August 21–24, and
Molecular Modeling of Thermophysical Properties - Science Meets Engineering, September 15–16
- 2010 Crystal Surface Influence on Equilibrium Transport of Guest Molecules in Zeolites, Berkeley Mini Statistical Mechanics Meeting, January 8–10

TEACHING EXPERIENCE

Hamburg University of Technology

Laboratory course “Chemical Engineering” spring 2008, 2009, 2010, 2011

Centre Européen de Calcul Atomique et Moléculaire (CECAM)

Tutorial “Understanding Molecular Simulations” January 2007

RESEARCH EXPERIENCE

- 2015–present Collaboration during Postdoctoral Fellowship with Mark Asta, Gerbrand Ceder, Kristin Persson, and Maciej Haranczyk at LBNL and UC Berkeley
- 2013–2015 Postdoctoral studies advised by Baron Peters
- 2013 Collaboration with David Quigley and Bart Vorselaars, University of Warwick, UK, June–July
- 2008–2010 Collaboration with Berend Smit and Maciej Haranczyk, University of California, Berkeley, October 2009–February 2010 and September–November 2008
- 2005–2006 Collaboration with Berend Smit, University of Amsterdam, The Netherlands, November 2005–May 2006
- 2003–2006 Student research and project works at Hamburg University of Technology advised by Sven Jakobtorweihen in summer 2006 and summer 2005, by Jobst Hapke in summer 2004, and by Lutz Friedel and Robert Surma June 2003–May 2004
- 2005 Industry internship with Daniel Hellström, Stockholm Vatten AB, Sweden, January–August

PROFESSIONAL SERVICE & OUTREACH

Journal Review

Angewandte Chemie International Edition, Applied Catalysis A: General, Crystal Growth & Design, Journal of Membrane Science, Journal of Physical Chemistry C, Molecular Simulation, Physical Chemistry Chemical Physics, Physical Review Letters, PLOS ONE

Campus and Departmental Services

- 2016 Advising José Luis Salcedo Pérez during summer research intern at LBNL
- 2016 Participating as Historian (webmaster) in the Berkeley Lab Postdoc Association (BLPA) at LBNL
- 2015–2016 Participating as organizer in the Postdoc Coordination Program in Computing Sciences at LBNL
- 2014 Organizing bi-weekly group meetings in Peters group
- 2014 Advising research project of Julia Deacon (highschool student)
- 2009–2012 Advising undergraduate and graduate students: Timm Zabel (B.Sc. 2012), Sayee Balaji (M.Sc. 2010), Stephan Bendt (B.Sc. 2009), Ana Popovic (B.Sc. 2009)
- 2006–2007 Organizing weekly group meetings at CECAM
- 2003–2004 Tutoring foreign exchange students at Hamburg University of Technology (winter term)

Off-Campus Services

- 2016 Participated in an organizing drive of Postdoctoral Fellows at LBNL to join the University of California postdoc union UAW Local 5810
2014 Campus Chair at UCSB and Guide of Executive Board in UAW Local 5810

COMPUTER SKILLS

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| Operating systems | Linux, MacOS, Windows |
| Programming | awk, bash, c, c++, Fortran, Java, MPI, python |
| Simulation packages | CHarMM, dl_poly, Fortran-written MD-MC package initiated by Sven Jakobtorweihen, LAMMPS, towhee, VASP |
| Analysis libraries | pymatgen |
| Mathematics | Matlab |
| Documentation | doxygen, L ^A T _E X, Microsoft Office, OpenOffice |
| Plotting | gnuplot |
| Visualization | vmd, VTK |
| Graphics | gimp, Inkscape, xfig |

LANGUAGES

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| German | native |
| English | fluent |
| Swedish | fluent in reading, excellent in speaking and writing |
| French | good in reading and speaking, can write with a dictionary |
| Arabic | beginner |

PROFESSIONAL MEMBERSHIPS

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| 2016, | American Chemical Society (ACS) |
| 2011–2012 | |
| 2008–2015 | American Institute of Chemical Engineers (AIChE) |
| 2003–present | Society of Alumni and Sponsors of Hamburg University of Technology |