Curriculum vitae

NILS EDVIN RICHARD ZIMMERMANN

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URL: http://www.nisseshem.de	Energy Technology Area
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RESEARCH INTERESTS

Physical chemistry:	nucleation, polymorphism, defect formation, intercalation, adsorption, diffusion
Data mining:	materials discovery through smart descriptor design
Molecular modeling:	method development and implementation
Visualization	educational videos and intuitive method presentation

EDUCATION

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

PROFESSIONAL APPOINTMENTS

2015–present	Postdoctoral Fellow, Lawrence Berkeley National Laboratory (LBNL), Energy Technology Area (present), Computational Research Division (until Feb. 2017)
2013–2015	Postdoctoral Scholar University of California, Santa Barbara, (UCSB), Chemical Engineering
2007–2013	Research Fellow, TUHH, Chemical Engineering
2006–2007	Research Fellow, École Normale Supérieure (ENS) de Lyon, France, Centre Européen de Calcul Atomique et Moléculaire (CECAM)

PUBLICATIONS

Peer-Reviewed Journal Articles

15. N. E. R. Zimmermann,* B. Vorselaars, Jorge R. Espinosa, D. Quigley,* W. R. Smith,* E. Sanz, C. Vega, and B. Peters*
    NaCl nucleation from brine in seeded simulations: sources of uncertainty in rate estimates
    J. Chem. Phys., 148, 222838, **2018**
14. L. Ward, A. Dunn, A. Faghaninia, N. E. R. Zimmermann, S. Bajaj, Q. Wang, J. Montoya, J. Chen, K. Bystrom, M. Dylla, K. Chard, M. Asta, K. A. Persson, G. J. Snyder, I. Foster, A. Jain*
    Matminer: an open source toolkit for materials data mining
    Comput. Mater. Sci.,, 152, 60–69, **2018**
13. D. Broberg,[‡,*] B. Medasani,[‡,*] N. E. R. Zimmermann,[‡,*] A. Canning, M. Haranczyk, M. Asta, and G. Hautier*
    PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators
    Comput. Phys. Commun., 226, 165–179, **2018**
12. N. E. R. Zimmermann,* D. C. Hannah, Z. Rong, M. Liu, G. Ceder, M. Haranczyk, and K. A. Persson
    Electrostatic estimation of intercalant jump-diffusion barriers using finite-size ion models
    J. Phys. Chem. Lett. 9, 628–634, **2018**
11. N. E. R. Zimmermann,* M. K. Horton, A. Jain, and M. Haranczyk
    Assessing local structure motifs using order parameters for motif recognition, interstitial identification, and diffusion path characterization
    Front. Mater. 4, 34, **2017**
10. N. E. R. Zimmermann* and M. Haranczyk
    History and utility of zeolite framework-type discovery from a data-science perspective
    Cryst. Growth Des. 16, 3043–3048, **2016**, [video available]
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**, [video available]
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

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J. Phys. Chem. C 117, 7384–7390, **2013**, [video available]

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**, [video available]
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**, [video available]
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**, [video available]
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**

Book Chapters in Preparation

1. A. Jain,* N. E. R. Zimmermann, D. Winston, J. Dagdelen, J. H. Montoya, M. K. Horton, P. Huck, S. Cholia, S. S. Dwaraknath, S. P. Ong, and K. A. Persson
   The Materials Project: theory-driven data and tools to accelerate materials design
   in *Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling*, Springer, 2018.

Dissertation

N. E. R. Zimmermann
Transport at gas–zeolite interfaces probed by molecular simulations
Hamburg University of Technology, advised by F. J. Keil, 2013

Additions and Corrections

1. N. E. R. Zimmermann,* S. Jakobtorweihen, E. Beerdsen, B. Smit, and F. J. Keil,
   Addition/Correction: 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 114, 15546–15546, 2010

Open-Source Software Contributions

pymatgen	Local environment order parameters
	Interstitialcy Finding Tool (InFiT)
	Python Charged Defects Tools PyCDT
matminer	Site and structure fingerprints

Blog posts

2016 Call to Open Access (openaccessweek.org)
Open access publishing at Berkeley Lab (postdoc.lbl.gov)
Databases in inorganic chemistry from a publication statistics perspective (nisseshem.de)
2014 Records of some rare events (nisseshem.de)

HONORS & AWARDS

2012 Prize (tied 1st) for best student talk at
The 35th Annual British Zeolite Association Meeting
1998 Prize (tied 1st) for best highschool graduation at Gymnasium Neu Wulmstorf

FELLOWSHIPS

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

CONFERENCES & WORKSHOPS

Talks

2018 Invited at SIAM Conference on Mathematical Aspects of Materials Science
"Fostering Machine Learning Through Coordination Descriptors, Site Fingerprints, and Structure Similarity Measures"
2016 AIChE Annual Meeting
"Descriptors and approaches for characterization and screening of inorganic materials databases"
"NaCl nucleation from aqueous solution by a seeded simulation approach"
ACS National Meeting & Exposition, March 13–17
"Local order parameters: descriptors for databases, synthesizability, interstitial relaxation, and diffusion paths"
"Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates"
2014 AIChE Annual Meeting, November 16–21
"Transport into zeolite nanosheets: test of diffusion equations"
2012 Annual British Zeolite Association Meeting, July 15–20
"Predicting surface permeabilities via molecular simulations"
2011 German Zeolite Meeting, March 2–4

"How do chain length and pore type influence tracer transport of hydrocarbons at zeolite surfaces?"

2008 AIChE Annual Meeting, November 16–21
"The influence of surface barriers on diffusion of alkane–zeolite systems—a molecular dynamics study"

Posters

2012 German Zeolite Meeting, March 7–9
"How sensitive are adsorption and diffusion of guest molecules in zeolites towards small changes in the crystal structure?"

2011 Diffusion Fundamentals IV, August 21–24, and
Molecular Modeling of Thermophysical Properties – Science Meets Engineering, September 15–16
"Transport barriers as triggered by the idealized microscopic crystal surface and the role of the evaluation protocol of diffusion experiments"

2010 Berkeley Mini Statistical Mechanics Meeting, January 8–10
"Crystal surface influence on equilibrium transport of guest molecules in zeolites"

TEACHING EXPERIENCE

2008–2011	Laboratory course "Chemical Engineering", TUHH
2007	Tutorial "Understanding Molecular Simulations", CECAM

RESEARCH EXPERIENCE

2015–present	Collaboration during Postdoctoral Fellowship with Mark Asta, Gerbrand Ceder, Kristin Persson, Anubhav Jain, and Maciej Haranczyk at LBNL and University of California, 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, Experimental Thermal and Fluid Science,
Frontiers in Chemistry, Journal of Membrane Science,
Journal of Physical Chemistry C, Molecular Simulation,
Physical Chemistry Chemical Physics, Physical Review Letters, PLOS ONE

Campus and Departmental Services

2016–2017	Webmaster of Berkeley Lab Postdoc Association (BLPA) at LBNL
2016	Advised José Luis Salcedo Pérez during summer research internship at LBNL
2015–2016	Organizer of Postdoc Coordination Program in Computing Sciences at LBNL
2015	Science Ambassador for LBNL at Solano Avenue Stroll in Albany (CA).
2014	Organizer of bi-weekly group meetings in Peters group
2014	Advised research project of Julia Deacon (highschool student)
2009–2011	Advised undergraduate and graduate students: Timm Zabel (B.Sc. 2011), Sayee Balaji (M.Sc. 2010), Stephan Bendt (B.Sc. 2009), Ana Popovic (B.Sc. 2009)
2006–2007	Organizer of weekly group meetings at CECAM
2003–2004	Advised foreign exchange students at TUHH

Off-Campus Services

2016–2018	Campus Chair at LBNL for University of California postdoc union UAW Local 5810
2016	Participated in a successful organizing drive of Postdoctoral Fellows at LBNL to join UAW Local 5810
2014–2015	Campus Chair at UCSB and Guide of Executive Board in UAW Local 5810

COMPUTER SKILLS

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, matminer
Mathematics	Matlab
Documentation	doxygen, LaTeX, Microsoft Office, OpenOffice
Plotting	gnuplot
Visualization	vmd, VTK
Graphics	gimp, Inkscape, xfig

LANGUAGES

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

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