

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

*Corresponding author.

[‡](Shared) first author.

- 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 isotopic 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 ACA Annual Meeting, July 20–24
“Quantifying local environment and structural similarity through order
parameter-based site fingerprints and their application to machine learning”
Invited at SIAM (Materials Science), July 9–13
“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, L ^A T _E X, 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)