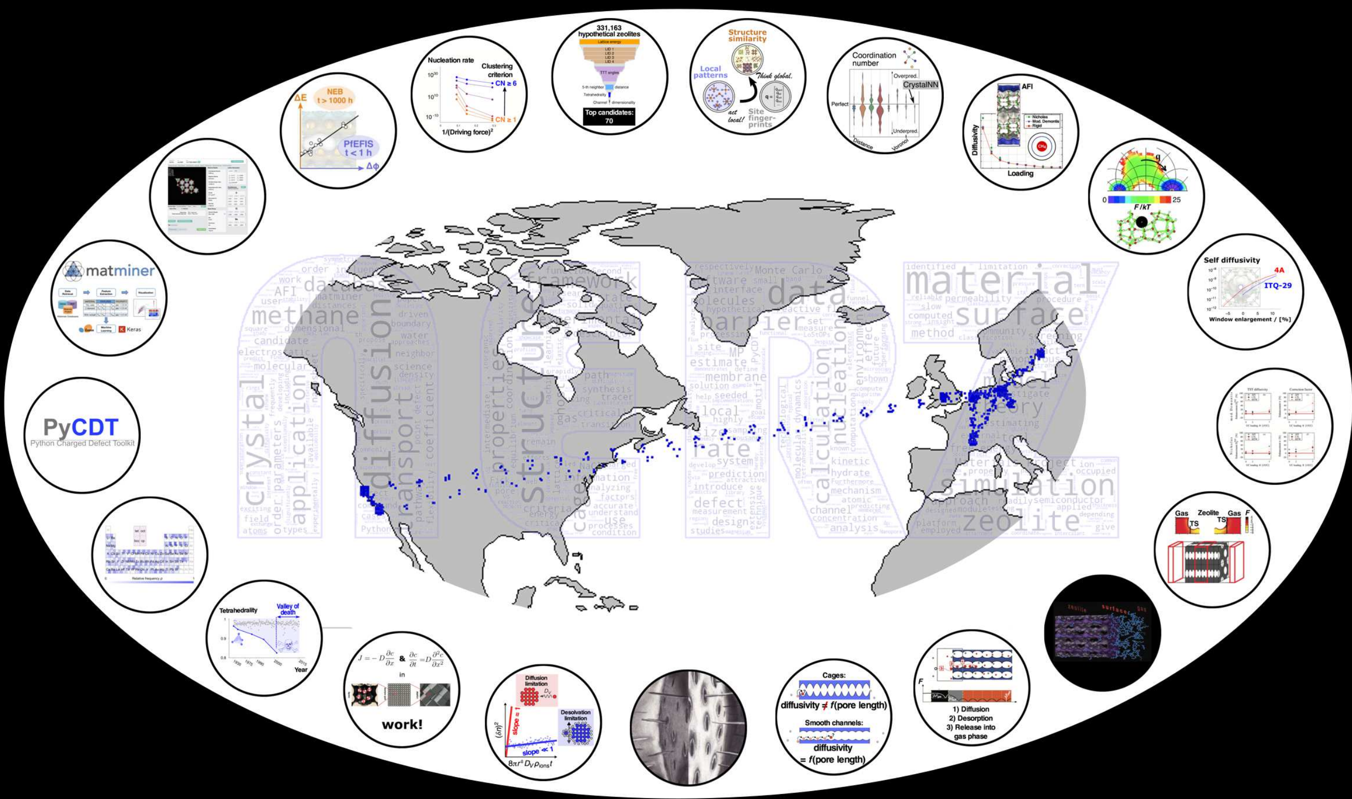
Dr.-Ing.
Nils Zimmermann

Engineer
Physical chemist
Materials scientist
Data scientist
Visualizer

nils.e.r.zimmermann@gmail.com


331,163 hypothetical zeolites
Top candidates: 70
Nucleation rate
Clustering criterion
CN ≥ 6
CN ≥ 1
1/(Driving force)²
Structure similarity
Local patterns
Think global.
act local!
Site fingerprints
Coordination number
Overpred.
CrystalNN
Perfect
Underpred.
AFI
Diffusivity
Loading
NEB
t > 1000 h
PIEFIS
t < 1 h
ΔE
Δϕ
F/kT
matminer
Keras
Self diffusivity
4A
ITQ-29
Window enlargement / [%]
PyCDT
Python Charged Defect Toolkit
Gas
Zeolite
Gas
TS
Tetrahedrality
Valley of death
Year
work!
Diffusion limitation
Desolvation limitation
slope ≈ 1
slope ≪ 1
Cages:
diffusivity ≠ f(pore length)
Smooth channels:
diffusivity = f(pore length)
1) Diffusion
2) Desorption
3) Release into gas phase
crystal
application
methane
diffusion
transport
structure
properties
data
barrier
rate
calculation
nucleation
material
surface
simulation
zeolite
defect
Monte Carlo

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Contents

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Curriculum Vitae

Personal Data

Name	Nils Edvin Richard Zimmermann
Birthday	May 24, 1979
Place of birth	Buchholz in der Nordheide, Germany
Citizenship	Germany
Work address	Pfaffenwaldring 9 70569 Stuttgart Germany
Website	http://www.nisseshem.de Visualization of my academic career path
LinkedIn	https://www.linkedin.com/in/nils-zimmermann-22656372/
GibHub	https://github.com/nisse3000
Google Scholar	https://scholar.google.com/citations?user=S_NflkQAAAAJ
Wikipedia	https://en.wikipedia.org/wiki/User:Nisse3333
ORCID	0000-0003-1063-5926
ResearcherID	B-1044-2018

Areas of Activity and Fields of Competence

• Physical chemistry	• Theory	• Interdisciplinarity
• Materials science	• Simulation & modeling	• Communication strength
• Engineering	• Data analysis	• Cooperation talent
• Data science	• Visualization	• Diversity competence

Research Interests

- Investigating chemicophysical processes on the atomic and electronic level by combining theory, computation, and visualization
- Designing, developing, and improving modelling methods and approaches with a focus on rare, extreme, and nonequilibrium events
- Improving our understanding of nucleation, polymorphism, defect formation, intercalation, adsorption, and (thermo-)diffusion
- Materials discovery through smart descriptor design & data mining

Dr.-Ing. Nils Zimmermann
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Education

▼ Nov. 2007–Aug. 2013 — Hamburg University of Technology (TUHH), Hamburg, Germany
Degree: Dr.-Ing. Chemical Engineering
Grade: 1.0

▼ Aug. 2003–Jun. 2006 — Hamburg University of Technology (TUHH), Hamburg, Germany
Degree: M.Sc. Chemical Engineering
Grade: 1.4

▼ Aug. 2004–Dec. 2004 — Royal Institute of Technology (KTH), Stockholm, Sweden
ERASMUS exchange studies

▼ Oct. 1999–Jul. 2003 — Hamburg University of Technology (TUHH), Hamburg, Germany
Degree: B.Sc. General Engineering Sciences
Grade: 1.7

▼ Aug. 1991–Jul. 1998 — Gymnasium Neu Wulmstorf, Neu Wulmstorf, Germany
Degree: Abitur
Grade: 1.4

- Honors courses: mathematics, chemistry

Professional Experience

▼ since Jan. 2021 — University of Stuttgart, Stuttgart, Germany
Institute of Thermodynamics and Thermal Process Engineering (ITT)
Mentor: apl. Prof. Dr.-Ing. habil. Niels Hansen
Collaborator: Prof. Dr.-Ing. Joachim Groß
Research Associate

- Investigating effects influencing thermophoresis of active pharmaceutical ingredients for characterization purposes

▼ Sep. 2018–Dec. 2020 — Parental leave

▼ Feb. 2015–Sep. 2018 — Lawrence Berkeley National Laboratory (LBL), Berkeley, U. S. A.
Energy Technology Area (until Sep. 2018)
Computational Research Division (until Feb. 2017)
Mentors: Dr. Anubhav Jain (until Sep. 2018), Dr. Maciej Haranczyk (until Feb. 2017)
Collaborators: Prof. Gerbrand Ceder, Prof. Mark Asta, and Prof. Kristin A. Persson (all University of California, Berkeley (UCB))
Postdoctoral Fellow

- Developed the potential of electrostatics-finite ion size (PfEFIS) method for efficient estimations of ion migration barriers in intercalation materials using electronic density functional theory (DFT) calculations
- Designed materials descriptors for various database screening and machine learning (ML) applications
- Co-developed the Python Charged Defect Tools (PyCDT), which facilitates defect calculations with DFT
- Co-developed Matminer, which greatly facilitates machine learning of materials properties using various databases and a plethora of descriptors and algorithms

This work has resulted thus far in 8 journal papers (e.g., in The Journal of Physical Chemistry Letters and 1 invited for a special issue) and 1 book chapter.

▼ May 2017–Jul. 2017 — Parental leave

▼ Apr. 2013–Feb. 2015 — University of California, Santa Barbara (UCSB), Santa Barbara, U. S. A.
Chemical Engineering Department
Advisor: Prof. Dr. Baron Peters
Collaborators: Dr. David Quigley and Dr. Bart Vorselaars (spent 6 weeks at University of Warwick, UK)
Postdoctoral Scholar

- Demonstrated that a seeded molecular dynamics simulation approach can yield accurate solute precipitate nucleation rates for NaCl from aqueous solutions
- Developed a c++ Potts-lattice gas simulation package

This work has resulted in 2 papers: 1 in the Journal of the American Chemical Society and 1 in the Journal of Chemical Physics as part of a special issue on “Ions in Water.”

▼ Nov. 2007–Mar. 2013

Hamburg University of Technology (TUHH), Hamburg, Germany

Institute for Chemical Reaction Technology
Advisor: Prof. Dr. Prof. E.h. Dr. h.c. em. Frerich J. Keil
Co-advisor: Prof. Berend Smit (spent 3 months in 2008 and 4.5 months in 2009/2010 at University of California, Berkeley (UCB))
Research Associate

- Highlighted a limitation to Fick’s laws when guest molecules enter nanosheets that have smooth pores using non-equilibrium molecular dynamics simulations
- Unraveled various origins of surface barriers that occur at gas-zeolite interfaces using a wide variety of simulation techniques (MD, (GC)MC, reactive flux simulations, continuum calculations)
- Developed an accurate (molecular simulation-based) prediction formula for surface permeabilities, which quantify the transport through the gas-zeolite interface

This work has resulted in 4 publications in The Journal of Physical Chemistry C, 1 paper in Molecular Simulations, and 1 dissertation.

▼ Sep. 2006–Sep. 2007

École Normale Supérieure (ENS) de Lyon, Lyon, France

Centre Européen de Calcul Atomique et Moléculaire (CECAM)
Advisor: Prof. Berend Smit
Research scholarship

- Demonstrated the decisive role of water vacancies for the diffusion of methane in clathrate hydrates through a multiscale simulation study
- Reassured assumption of a frozen host structure to be reliable for diffusivity predictions of light gases in zeolites with molecular simulations

This work has resulted in 2 publications in the Journal of the American Chemical Society and in The Journal of Physical Chemistry C, respectively.

▼ Oct. 2005–May 2006

Hamburg University of Technology (TUHH), Hamburg, Germany

Institute for Chemical Reaction Technology
Advisors: Prof. Dr. Prof. E.h. Dr. h.c. em. Frerich J. Keil & Dr.-Ing. Sven Jakobtorweihen
Co-advisor: Prof. Berend Smit (University of Amsterdam (UvA), The Netherlands)
Research project

- Investigated influences of host-framework flexibility and system size in periodic zeolite structures on gas diffusion using simulations

This work resulted in my Master Thesis.

▼ Jan. 2005 –Jul. 2005

Stockholm Vatten AB, Stockholm, Sweden

Advisor: Dr. Daniel Hellström
Industry internship

- Investigated various parameters in different process lines for wastewater treatment within the sustainable Hammarby Sjöstad Project

This work resulted in a technical report (requirement for Master’s degree).

▼ Jun. 2004 –Jul. 2004

Hamburg University of Technology (TUHH), Hamburg, Germany

Institute for Process Systems Engineering
Advisors: Prof. Jobst Hapke & Dr.-Ing. Antoni Sutiono
Research project

- Developed a model for calculating a metal hydrid-based cooling/air conditioning cycle

This project resulted in my Project Thesis (requirement for Master’s degree).

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▾ Jan. 2003–Mar. 2003 **Hamburg University of Technology (TUHH), Hamburg, Germany**
Institute for Fluid Mechanics
Advisors: Prof. Dr.-Ing. Lutz Friedel & Dr.-Ing. Robert Surma
Research project
- Unraveled unexpected variability of two descriptors in turbulent horizontal two-phase-flow water-air free jets

This work resulted in my Bachelor Thesis.

Honors, Awards, & Travel Grants

▾ 2020 Travel grant for participation at 34th Molecular Modelling Workshop
▾ 2012 Prize (tied 1st) for best student talk at 35th Annual British Zeolite Association Meeting
▾ 1998 Prize (tied 1st) for best high school graduation at Gymnasium Neu Wulmstorf

Fellowships

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

Professional Service & Outreach

▾ 2016–2017 Webmaster of Berkeley Lab Postdoc Association (BLPA) at LBL
▾ 2015–2016 Organizer of Postdoc Coordination Program in Computing Sciences at LBL
▾ 2015 Science Ambassador for LBL at Solano Avenue Stroll in Albany (CA, U. S. A.)
▾ 2014 Organizer of bi-weekly group meetings in Peters group
▾ 2006–2007 Organizer of weekly group meetings at CECAM
▾ 2003–2004 Advising of foreign exchange students at TUHH

Volunteering

▾ 2016–2018 Campus Chair of University of California Postdoc Union UAW Local 5810 at LBL
▾ 2016 Member of bargaining team of UAW Local 5810
▾ 2016 Participated in a successful organizing drive of LBL postdocs to join UAW Local 5810
▾ 2014–2015 Campus Chair at UCSB and Guide of Executive Board of UAW Local 5810

Languages

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

Professional Memberships

▾ since 2020 Molecular Graphics and Modeling Society - German speaking section (MGMS-DS) e.V.
▾ since 2019 German Chemical Society (Gesellschaft Deutscher Chemiker (GDCh))
International Union of Pure and Applied Chemistry (IUPAC)
▾ since 2003 Society of Alumni and Sponsors of Hamburg University of Technology

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▼ 2016	American Chemical Society (ACS)
▼ 2011–2012	
▼ 2008–2015	American Institute of Chemical Engineers (AIChE)

Dr.-Ing. Nils Zimmermann
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Publications

Peer-Reviewed Journal Articles

18. H. Pan, A. M. Ganose, M. Horton, M. Aykol, K. Persson, N. E. R. Zimmermann,* A. Jain*
Benchmarking coordination number prediction algorithms on inorganic crystal structures
Inorg. Chem., accepted, **2021** Preprint

17. N. E. R. Zimmermann,* A. Jain
Local structure order parameters and site fingerprints for quantification of coordination environment and crystal structure similarity
RSC Adv. 10, 6063–6081, **2020** OA

16. J. S. Perez, M. Haranczyk, N. E. R. Zimmermann*
High-throughput assessment of hypothetical zeolite materials for their synthesizeability and industrial deployability
Z. Kristallogr. 234, 437–450, **2019** OA

15. 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** OA

14. N. E. R. Zimmermann,* B. Vorselaars, J. R. Espinosa, D. Quigley,* W. R. Smith,* E. Sanz, C. Vega, B. Peters*
NaCl nucleation from brine in seeded simulations: Sources of uncertainty in rate estimates
J. Chem. Phys. 148, 222838, **2018** OA

13. D. Broberg,‡,* B. Medasani,‡,* N. E. R. Zimmermann,‡,* A. Canning, M. Haranczyk, M. Asta, G. Hautier*
PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators
Comput. Phys. Commun. 226, 165–179, **2018** OA

12. N. E. R. Zimmermann,* D. C. Hannah, Z. Rong, M. Liu, G. Ceder, M. Haranczyk, K. A. Persson
Electrostatic estimation of intercalant jump-diffusion barriers using finite-size ion models
J. Phys. Chem. Lett. 9, 628–634, **2018** OA

11. N. E. R. Zimmermann,* M. K. Horton, A. Jain, M. Haranczyk
Assessing local structure motifs using order parameters for motif recognition, interstitial identification and diffusion path characterization
Front. Mater. 4, 34, **2017** OA

10. N. E. R. Zimmermann,* M. Haranczyk
History and utility of zeolite framework-type discovery from a data-science perspective
Cryst. Growth Des. 16, 3043–3048, **2016**, [video available] OA

9. N. E. R. Zimmermann, B. Vorselaars, D. Quigley, 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] OA

8. T. Titze, A. Lauerer, L. Heinke, C. Chmelik, N. E. R. Zimmermann, F. J. Keil, D. M. Ruthven, J. Kärger*
Transport in nanoporous materials including MOFs: the applicability of Fick's laws
Angew. Chem. Int. Ed. 54, 14580–14583, **2015** OA
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, F. J. Keil
Transport into nanosheets: diffusion equations put to test
J. Phys. Chem. C 117, 7384–7390, **2013**, [video available] OA

6. N. E. R. Zimmermann,* B. Smit, F. J. Keil
Predicting local transport coefficients at solid-gas interfaces
J. Phys. Chem. C 116, 18878–18883, **2012**, [video available] OA

*Corresponding author.
‡(Shared) first author.

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5. N. E. R. Zimmermann,* S. P. Balaji, F. J. Keil
Surface barriers of hydrocarbon transport triggered by ideal zeolite structures
J. Phys. Chem. C 116, 3677–3683, **2012**, [video available] OA

4. N. E. R. Zimmermann,* M. Haranczyk, M. Sharma, B. Liu, B. Smit, F. J. Keil
Adsorption and diffusion in zeolites: the pitfall of isotypic crystal structures
Mol. Simul. 37, 986–989, **2011** OA

3. N. E. R. Zimmermann,* B. Smit, 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** OA

2. B. Peters,* N. E. R. Zimmermann, G. T. Beckham, J. W. Tester, 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] OA

1. N. E. R. Zimmermann,* S. Jakobtorweihen, E. Beerdsen, B. Smit, 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** OA

Book Chapters

1. A. Jain,* J. Montoya, S. Dwaraknath, N. E. R. Zimmermann, J. Dagdelen, M. Horton, P. Huck, D. Winston, S. Cholia, S. Ping Ong, K. 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** OA

Dissertation

N. E. R. Zimmermann
Transport at gas–zeolite interfaces probed by molecular simulations
Hamburg University of Technology, advised by F. J. Keil and co-advised by B. Smit, **2013** OA

Additions and Corrections

1. N. E. R. Zimmermann,* S. Jakobtorweihen, E. Beerdsen, B. Smit, 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** OA

Open-Source Software Contributions

2015–2018	pymatgen	Local environment order parameters
		Interstitialcy Finding Tool (InFiT)
		Python Charged Defects Tools (PyCDT)
	matminer	Site and crystal structure fingerprints

Blog Posts

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

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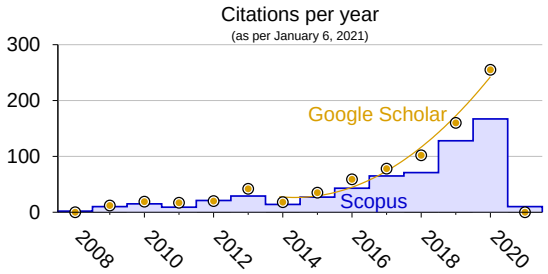
Citation Analysis

The following Google Scholar and Scopus citation analyses for Nils E. R. Zimmermann were generated on January 6, 2021.



Google Scholar

	All	Since 2016
Number of publications	22	
Citations	830	660
h-index	14	13
i10-index	17	16

Scopus

Number of publications	19
h-index	13
Sum of all citations	611
Citing documents	510

Top 5 Publications (Google Scholar)

Citations	Publication
151	Matminer: An open source toolkit for materials data mining 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* *Comput. Mater. Sci.* 152, 60–69, **2018** OA
111	Path sampling calculation of methane diffusivity in natural gas hydrates from a water-vacancy assisted mechanism B. Peters,* N. E. R. Zimmermann, G. T. Beckham, J. W. Tester, B. L. Trout* *J. Am. Chem. Soc.* 130, 17342–17350, **2008** OA
98	Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates N. E. R. Zimmermann, B. Vorselaars, D. Quigley, B. Peters* *J. Am. Chem. Soc.* 137, 13352–13361, **2015** OA
75	PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators D. Broberg,‡,* B. Medasani,‡,* N. E. R. Zimmermann,‡,* G. Yu, A. Canning, M. Haranczyk, M. Asta, G. Hautier* *Comput. Phys. Commun.* 226, 165–179, **2018** OA
65	In-depth study of the influence of host-framework flexibility on the diffusion of small gas molecules in one-dimensional zeolitic pore systems N. E. R. Zimmermann,* S. Jakobtorweihen, E. Beerdsen, B. Smit, F. J. Keil *J. Phys. Chem. C* 111, 17370–17381, **2007** OA

Citation rate [1/month]	Publication
1.45	Matminer: An open source toolkit for materials data mining 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* *Comput. Mater. Sci.* 152, 60–69, **2018** OA
0.53	PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators D. Broberg,‡,* B. Medasani,‡,* N. E. R. Zimmermann,‡,* G. Yu, A. Canning, M. Haranczyk, M. Asta, G. Hautier* *Comput. Phys. Commun.* 226, 165–179, **2018** OA
0.38	Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates N. E. R. Zimmermann, B. Vorselaars, D. Quigley, B. Peters* *J. Am. Chem. Soc.* 137, 13352–13361, **2015** OA
0.26	Local structure order parameters and site fingerprints for quantification of coordination environment and crystal structure similarity N. E. R. Zimmermann,* A. Jain *RSC Adv.* 10, 6063–6081, **2020** OA
0.25	Assessing local structure motifs using order parameters for motif recognition, interstitial identification, and diffusion path characterization N. E. R. Zimmermann,* M. K. Horton, A. Jain, M. Haranczyk *Front. Mater.* 4, 34, **2017** OA

Specific citation rate [1/week/author]	Publication
0.56	Local structure order parameters and site fingerprints for quantification of coordination environment and crystal structure similarity N. E. R. Zimmermann,* A. Jain *RSC Adv.* 10, 6063–6081, **2020** OA
0.42	Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates N. E. R. Zimmermann, B. Vorselaars, D. Quigley, B. Peters* *J. Am. Chem. Soc.* 137, 13352–13361, **2015** OA
0.39	Matminer: An open source toolkit for materials data mining L. Ward,* A. Dunn, A. Faghaninia, N. E. R. Zimmermann, S. Bajaj, Q. Wang, J. Montoya, J. Chen, /mboxK. Bystrom, M. Dylla, K. Chard, M. Asta, K. A. Persson, G. J. Snyder, I. Foster, A. Jain* *Comput. Mater. Sci.* 152, 60–69, **2018** OA
0.29	PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators D. Broberg,‡,* B. Medasani,‡,* N. E. R. Zimmermann,‡,* G. Yu, A. Canning, M. Haranczyk, M. Asta, G. Hautier* *Comput. Phys. Commun.* 226, 165–179, **2018** OA
0.27	Assessing local structure motifs using order parameters for motif recognition, interstitial identification, and diffusion path characterization N. E. R. Zimmermann,* M. K. Horton, A. Jain, M. Haranczyk *Front. Mater.* 4, 34, **2017** OA

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Editorial & Review Activity

Editorial Tasks: Journals

"Review Editor" for Mathematical and Statistical Physics in Frontiers

Reviews: Journal Articles

Total number	14
Per year	2019: 3 2018: 2 2017: 2 2016: 3 2014: 1 2013: 2 2008: 1
Journals	Angewandte Chemie, International Edition Applied Catalysis A: General Crystal Growth & Design Experimental Thermal and Fluid Science Frontiers in Chemistry Frontiers in Physics Journal of Membrane Science Journal of Physical Chemistry C Journal of Physical Chemistry Letters Molecular Simulation npj Computational Materials Physical Chemistry Chemical Physics Physical Review Letters PLOS ONE

Reviews: Research Proposals

Total number	1
Per year	2016: 1
Organization	Research Foundation – Flanders (FWO)

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Talks & Posters

2020

▼ Nov. 2–Nov. 4 — 16th German Conference on Cheminformatics and SAMPL Satellite Workshop – Virtual Edition
Guest transport in energy materials: How simulations and data-inspired approaches shape theory (T)

▼ Feb. 17–Feb. 19 — 34th Molecular Modelling Workshop 2020, Erlangen, Germany
Potential of Electrostatics-Finite Ion Size (PfEFIS) method: towards automatic ion diffusion network analysis in solids (T)

2019

▼ Nov. 3–Nov. 5 — 15th German Conference on Cheminformatics, Mainz, Germany
Fostering machine learning through coordination descriptors, site fingerprints, and structure similarity measures (T)

▼ Jul. 7–Jul. 12 — 47th IUPAC World Chemistry Congress, Paris, France
Electrostatic estimation of intercalant jump-diffusion barriers using finite-size ion models (T)
Shedding light onto homogenous NaCl nucleation from aqueous solution facilitated by molecular simulations (T)

2018

▼ Aug. 7–Aug. 8 — Workshop Artificial Intelligence for Materials Science (AIMS), Gaithersburg, MD, U. S. A.
Fostering machine learning through coordination descriptors, site fingerprints, and structure similarity measures (P)

▼ Jul. 20–Jul. 24 — ACA Annual Meeting, Toronto, Canada
Quantifying local environment and structural similarity through order parameter-based site fingerprints and their application to machine learning (T)

▼ Jul. 9–Jul. 13 — Invited at SIAM (Materials Science), Portland, OR, U. S. A.
Fostering machine learning through coordination descriptors, site fingerprints, and structure similarity measures (T)

2016

▼ Nov. 13–Nov. 18 — AIChE Annual Meeting, San Francisco, CA, U. S. A.
Descriptors and approaches for characterization and screening of inorganic materials databases (T)
NaCl nucleation from aqueous solution by a seeded simulation approach (T)

▼ Mar. 13–Mar. 17 — ACS National Meeting & Exposition, San Diego, CA, U. S. A.
Local order parameters: descriptors for databases, synthesizability, interstitial relaxation, and diffusion paths (T)
Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates (T)

2014

▼ Nov. 16–Nov. 21 — AIChE Annual Meeting, Atlanta, GA, U. S. A.
Transport into zeolite nanosheets: test of diffusion equations (T)

2012

▼ Jul. 15–Jul. 20 — Annual British Zeolite Association Meeting, Chester, U. K.
Predicting surface permeabilities via molecular simulations (T)

▼ Mar. 7–Mar. 9 — German Zeolite Meeting, Magdeburg, Germany
How sensitive are adsorption and diffusion of guest molecules in zeolites towards small changes in the crystal structure? (P)

2011

▼ Sep. 15–Sep. 16 — Molecular Modeling of Thermophysical Properties – Science Meets Engineering, Dortmund, Germany

▼ Aug. 21–Aug. 24 — Diffusion Fundamentals IV, Troy, NY, U. S. A.
Transport barriers as triggered by the idealized microscopic crystal surface and the role of the evaluation protocol of diffusion experiments (P)

▼ Mar. 2–Mar. 4 — German Zeolite Meeting, Erlangen, Germany
How do chain length and pore type influence tracer transport of hydrocarbons at zeolite surfaces? (T)

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2010
▼ Jan. 8–Jan. 10 Berkeley Mini Statistical Mechanics Meeting, Berkeley, CA, U. S. A.
Crystal surface influence on equilibrium transport of guest molecules in zeolites (P)

2008
▼ Nov. 16–Nov. 21 AIChE Annual Meeting, Philadelphia, PA, U. S. A.
The influence of surface barriers on diffusion of alkane–zeolite systems—
a molecular dynamics study (T)

Dr.-Ing. Nils Zimmermann
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Third-Party Funding

▼ Feb. 2015–Sep. 2018
U. S. Department of Energy (DOE) Basic Energy Sciences (BES) program
"The Materials Project"
Grant number: EDCBEE
Main filers: Prof. Dr. Kristin Persson, Prof. Dr. Gerbrand Ceder

▼ Apr. 2013–Jan. 2015
National Science Foundation (NSF), U. S. A.
"CAREER: Nucleation from solution: a new frontier for molecular simulation"
Award number: 0955502
Filer: Prof. Dr. Baron Peters

▼ Nov. 2007–Oct. 2011
German Science Foundation (DFG)
Priority program SPP 1155
"Molecular modeling and simulation in chemical engineering"
Project: "Molecular simulations for clarifying discrepancies between microscopic and macroscopic measurements of diffusion coefficients in porous media"
Project number: 54145212
Filer: Prof. Dr. Prof. E.h. Dr. h.c. em. Frerich J. Keil
Status report securing funding continuation: Nils E. R. Zimmermann
Final report: Nils E. R. Zimmermann

▼ Sep. 2006–Sep. 2007
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Teaching Experience

2019	TUHH	Lecture “Statistical Thermodynamics and Molecular Modelling” (given jointly with Dr.-Ing. Sven Jakobtorweihen)
2018	LBL	Advised Hillary Pan during spring research internship
2016	LBL	Advised José Luis Salcedo Pérez during summer research internship
2014	UCSB	Advised research project of Julia Deacon (high school student)
2012	TUHH	Supervised and graded examinations of course “Chemical Reaction Engineering II”
2011	TUHH	Advised Bachelor Thesis of Timm Zabel
		Supervised and graded examinations of course “Chemical Reaction Engineering II”
		Instructed diffusion experiment of Master-level laboratory course “Chemical Engineering”
2010	TUHH	Advised Master Thesis of Sayee Balaji
		Supervised and graded examinations of course “Chemical Reaction Engineering II”
		Instructed diffusion experiment of Master-level laboratory course “Chemical Engineering”
2009	TUHH	Advised Bachelor Thesis of Stephan Bendt
		Advised Bachelor Thesis of Ana Popovic
		Supervised and graded examinations of course “Chemical Reaction Engineering I”
		Instructed diffusion experiment of Master-level laboratory course “Chemical Engineering”
2008	TUHH	Supervised and graded examinations of course “Chemical Reaction Engineering I”
		Instructed diffusion experiment of Master-level laboratory course “Chemical Engineering”
2007	CECAM	Instructed hands-on computer exercises of tutorial “Understanding Molecular Simulations”