Elisabeth Maria Dietze
Postdoctoral researcher
Mölndal, Sweden | 079-0542077 | dietze@chalmers.se
Born: 15.04.1993, Dresden, Germany | unmarried, one child (born 2014)

Summary — Curious and self driven scientist in computational chemistry and physics with the interest to develop new methodologies to contribute to todays challenging issues by e.g. increasing the understanding about crucial environmental and energy conversion catalysts and how to approach the increasing data-mass. A proven record of scientific publications in the field of surface reactions and phenomena and presentations on international conferences.

Education

10/2016–12/2019	Doctoral studies at Karlsruhe Institute of Technology, Germany Topic: 'Theoretical investigation of catalyst stability and deactivation' Supervisors: Prof. Dr. Felix Studt, Dr. Philipp Plessow
10/2014–09/2016	Master studies Nanoscience at University of Hamburg, Germany
10/2011–09/2014	Bachelor studies Nanoscience at University of Hamburg, Germany

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Experiences

since 07/2021	CTO ContentMap AB - Code base management - Proof of concept meta data virtualization (Python) - Development meta data navigator in ContentMap (Java)
since 03/2020	Postdoc in the group of Prof. Dr. Henrik Grönbeck, Chalmers University of Technology - DFT calculations to investigate catalytic relevant reactions - Optimization and parallelization of kinetic MonteCarlo code MonteCoffee (Python) - Student supervision
01 – 02/2020	Postdoc in the group of Prof. Dr. Felix Studt
10/2016 – 12/2019	Doctoral student in the group of Prof. Dr. Felix Studt, Karlsruhe Institute of Technology, Germany under the supervision of Dr. Philipp Plessow - Development of gas-phase kinetic MonteCarlo code to simulate Ostwald ripening (Python) - Modeling of nanoparticle stability in gas-phase and on support materials - DFT calculations to build descriptor based models

11/2014 – 09/2016	Student assistant in the group of Prof. Dr. Gabriel Bester, University of Hamburg, Germany - Investigating the effect of Mn defects in Si - Unix support - Software responsible for group-own HPC cluster
07/2013 – 09/2016	Active member of the Federal Agency of Technical Relief (Bundesanstalt Technisches Hilfswerk) with additional first-aid training, training as respirators carrier and in rope rescue.

Skills

- Programming languages: Python, Bash, (Java, C++ and Fortran)
- Experience in computational work on high performance computers with compiling various quantum-chemical codes (e.g. VASP, abinit)
- Experience in working in a collaborative environment with an international team.
- Capable of writing and presenting scientific research results comprehensively.
- Flexible in adapting to knew environments and challenging situation.
- Languages: German (native), English (fluent), Swedish (fluent), French (elementary)

Teaching experiences

05/2022	Seminar on kinetic MonteCarlo methods and how-to perform simulations using MonteCoffee.
since 10/2020	Part of Cybermentor, a german language based MINT network platform for girls in the age of 14-18.
04/2017 – 07/2019	Tutor in the lab course physical chemistry for beginners at KIT (Sommersemester)
10/2016 – 01/2019	Tutor in the course 'Methods of natural sciences' at the physical chemistry department at KIT (Wintersemester)

Granted Applications & Prices

- PRACE DECI17 HPC system call 2021, Multiscale modeling of nanoparticle catalysis (NANOCAT), with Prof. Dr. Henrik Grönbeck.
- Networking Grant 2019 granted by the Karlsruhe House of Young Scientists, Germany (KHYS) to visit Prof. Dr. Henrik Grönbeck at Chalmers University of Technology, Sweden.

Publications

1. B. Habagil, E.M. Dietze, H. Grönbeck, Advancing kinetic MonteCarlo simulations by parallelization, in preparation.

2. E.M. Dietze, H. Grönbeck, Issues with the static picture of density function theory in heterogeneous catalysis, in preparation.

3. E.M. Dietze, L. Chen, H. Grönbeck, Surface steps dominate the water formation on Pd(111) surfaces, J. Chem. Phys 2022, 156, 6.

4. F. Garcia-Martinex, E.M. Dietze, F. Schiller, D. Gajdek, L.R. Merte, S.M. Gericke, J. Zetterberg, S. Albertin, E. Lundgren, H. Grönbeck, J.E. Ortega, Reduced CO saturation coverage on vicinal Pd surfaces: the importance of the adsorption site, J. Chem. Phys. Lett. 2021, 9508-9515.

5. E.M. Dietze, H. Grönbeck, Structure-Dependent Strain Effects. ChemPhysChem 2020, 21, 2407-2410.

6. A.H. Hakimioun, E.M. Dietze, B.D. Vandegehuchte, D. Curulla-Ferre, L. Joos, P.N. Plessow, F. Studt, Theoretical Investigation of the Size Effect on the Oxygen Adsorption Energy of Coinage Metal Nanoparticles. Catalysis Letters 2021.

7. E.D. Goodman, E.Z. Carlson, E.M. Dietze, N. Tahsini, A. Johnson, A. Aitbekova, T. Nguyen Taylor, P.N. Plessow, M. Cargnello, Size-controlled nanocrystals reveal spatial dependence and severity of nanoparticle coalescence and Ostwald ripening in sintering phenomena. Nanoscale 2021, 13, 930-938.

8. E.M. Dietze, P.N. Plessow, F. Studt, Modeling the Size-Dependency of the Stability of Metal Nanoparticles. J. Phys. Chem. C 2019, 123, 41, 25464-25469.

9. E.D. Goodman, A.C. Johnston-Peck, E.M. Dietze, C.J. Wrasman, A.S. Hoffman, F. Abild-Pedersen, S.R. Bare, P.N. Plessow, M. Cargnello, Catalyst deactivation via decomposition into single atoms and the role of metal loading. Nature Catalysis 2019, 2, 748-755.

10. E.M. Dietze, P.N. Plessow, Predicting the Strength of Metal–Support Interaction with Computational Descriptors for Adhesion Energies. J. Phys. Chem. C 2019, 123, 33, 20443-20450.

11. E.M. Dietze, F. Abild-Pedersen, P.N. Plessow, Comparison of Sintering by Particle Migration and Ripening through First-Principles-Based Simulations. J. Phys. Chem. C 2018, 122, 46, 26563-26569.

12. E.M. Dietze, P.N. Plessow, Kinetic Monte Carlo Model for Gas Phase Diffusion in Nanoscopic Systems. J. Phys. Chem. C 2018, 122, 21, 11524-11531.

List of oral presentations

1. E. Dietze, L. Chen, H. Grönbeck, Surface steps dominate the water formation on Pd(111) surfaces, German Catalysis Meeting, Weimar, Germany 2022.
2. E. Dietze, H. Grönbeck, CO oxidation kinetics on Pd/Pt alloys from first principles, ACS Spring 2021, virtual.
3. E. Dietze, P. Plessow, F. Studt, Support effect on oxygen adsorption on Pt nanocluster, EuropaCat, Aachen, Germany 2019.
4. E. Dietze, P. Plessow, Comparison of Sintering by Particle Migration and Ripening trough First Principles based Simulations, North American Catalysis Society Meeting (NAM), Chicago, USA 2019.
5. E. Dietze, P. Plessow, Modeling Ostwald ripening beyond mean-field models, DPG Spring Meeting Regensburg, Germany 2019.
6. E. Dietze, P. Plessow, Insights into the Relative Importance of Ripening and Particle Migration for Sintering of Pt Nanoparticles, Workshop Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis IV, Italian 2018.
7. E. Dietze, P. Plessow, Insights into the Relative Importance of Ripening and Particle Migration for Sintering of Pt Nanoparticles, DPG Spring Meeting Berlin, Germany 2018.

Reference persons

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