Dr. Stefan Ringe
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Curriculum Vitae

Personal Details

Nationality	Germany.
Place of Birth	Buxtehude (Germany).
Date of Birth	02/16/1988.

Education

06/2013–05/2017 **Ph.D. in Computational Chemistry**, *Technical University Munich* *(Germany)*.
Prof. Dr. Karsten Reuter, *"Summa Cum Laude" ("With Highest Honor")*

10/2010–03/2013 **M.Sc. in Chemistry**, *Georg-August University Göttingen* *(Germany)*.
Prof. Dr. Alec Wodtke, Final Grade: 1.0 (4.0 on 4 point GPA scale) *"With Honors"*

10/2007–09/2010 **B.Sc. in Chemistry**, *Georg-August University Göttingen* *(Germany)*.
Prof. Dr. Philipp Vana, Final Grade: 1.3 (3.8 on 4 point GPA scale)

Professional Experience

02/2020–present **Assistant Professor**, *DGIST* *(Rep. of Korea)*.
Department of Energy Science & Engineering

02/2019–02/2020 **Postdoctoral Research Scholar**, *KAIST* *(Rep. of Korea)*.
Prof. Dr. Hyungjun Kim

07/2017–01/2019 **Postdoctoral Research Scholar**, *Stanford University* *(USA)*.
Prof. Dr. Jens Nørskov

Research Interests

- **Computational Design for Sustainable Energy Conversion**: CO_2 reduction, water oxidation (oxygen evolution reaction – OER) and reduction (hydrogen evolution reaction – HER), oxygen reduction reaction (fuel cell), NO reduction. . . .

- **Electrified Solid-Liquid Interface Engineering**: Solid-liquid interface electrification and its influence on electrochemical reaction kinetics, via Density Functional Theory (DFT), Implicit Solvation techniques, joint quantum – molecular mechanics approaches (QM/MM)
- **Machine Learning**: Development of *ab initio*-based machine learning – neural network force field for modeling energy conversion at the electrified solid-liquid interface
- **Multi-scale Modeling of Electrochemical Systems**: Mass transport, buffer reactions, electrolyte design, porous electrodes

Awards

2019 **Award for Outstanding Oral Presentation**, 130th Physical Chemistry Summer Symposium, Busan, Rep. of Korea.

2016 **DAAD scholarship (Kongressreise)**, 67th Annual Meeting of the ISE, The Hague, Netherlands.

2014 **Selection for Global Young Scientist Summit**, *National University of Singapore (Singapore*.

2013 **Award for Outstanding Graduation**, *Georg-August University Göttingen (Germany)*, awarded by chemistry department.

2012 **Award for Outstanding Teaching**, *Georg-August University Göttingen (Germany)*, awarded by students.

2010,2011,2012 **Scholarship of Lower Saxony**.

2010 **Otto Wallach Award**, *Georg-August University Göttingen (Germany)*, best B.Sc. degree in chemistry.

2007 **GDCh Award**, *Halepaghen-Gymnasium Buxtehude*, best graduation in chemistry (German Society of Chemistry).

Teaching and Mentoring Experience

2014–present **Mentoring/Supervision**, *Technical University Munich (Germany)*, Christoph Hille (B.Ed., M.Ed.), Christoph Muschielok, Martin Deimel, Marvin Lechner (all M.Sc).

10/2013–09/2016 **Tutor**, *Technical University Munich (Germany)*, Mathematics, computational & theoretical chemistry, molecular simulations, numerical methods.

10/2008–03/2013 **Student Tutor**, *Georg-August University Göttingen (Germany)*, Mathematics, theoretical chemistry, thermodynamics and spectroscopy.

Scientific Achievements

Invited Talks
- 01/2020 Material Science & Engineering (MSE) department seminar, KAIST (Rep. of Korea)
- 12/2018 DTU Physics Seminar, Denmark Technical University (DTU) (Denmark)

- 07/2018 FHI-aims Developer & User Meeting, Technical University Munich (Germany)
- 03/2018 Seminar of the Department of Chemistry, KAIST (Rep. of Korea)

Referee for *J. Chem. Phys.*.

Research Stay
- 10/2011–02/2012, *Synthesis of Oxygen-Evolution Catalysts*, Prof. Dr. Åkermark, Stockholm University (Sweden)

Further Skills & Achievements

2013–2017 IT Admin, *Technical University Munich (Germany)*.

Software
- *Developed Software*: Implicit solvation feature in the Density Functional Theory package FHI-aims ("SMPB"), CatINT (for multi-scale kinetic/mass-transport simulations)
- *Office/General*: MS Office, LaTeX, Version Management (Git)
- *Image Processing*: GIMP, Inkscape
- *Computational Modeling*: General Mathematics/Engineering (MATLAB, Mathematica, COMSOL), Density Functional Theory (QUANTUM ESPRESSO, VASP, FHI-aims), Force Field/Molecular Mechanics (LAMMPS, cerius2), Other (ASE, CatMAP)
- *Data Processing/Visualization*: Paraview, VMD, python/matplotlib
- *Programming*: `fortran90`, `python`, `bash` (all advanced), `c` (basic)

Languages German (native), English (fluent), Korean (advanced)

Memberships German Physical Society (DPG, since 2013), German Chemical Society (GDCh, since 2008)

Internships
- 09/2008 K+S research Institute of the K+S AG, Heringen (Germany)
- 07–08/2007 Environment and Trade Laboratory "Dr. Kaiser & Dr. Woldmann GmbH", Hamburg Germany

Publications (* = The authors contributed equally to this work.)

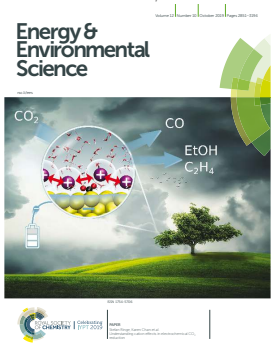
1 S. Ringe*, C. G. Morales-Guio*, L. D. Chen, M. Fields, T. F. Jaramillo, C. Hahn, K. Chan, *Double layer charging driven carbon dioxide adsorption limits the rate of electrochemical carbon dioxide reduction on Gold*, *Nat. Commun.* **2020**, *11*, 1–11, (corresponding author), DOI: 10.1038/s41467-019-13777-z.

2 C. Xia*, S. Back*, S. Ringe*, K. Jiang, F. Chen, X. Sun, S. Siahrostami, K. Chan, H. Wang, *Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide*, *Nature Catalysis* **2020**, DOI: 10.1038/s41929-019-0402-8.

3 J. A. Gauthier, C. F. Dickens, H. H. Heenen, S. Vijay, S. Ringe, K. Chan, *Unified Approach to Implicit and Explicit Solvent Simulations of Electrochemical Reaction Energetics*, *J. Chem. Theory Comput.* **2019**, *15*, 6895–6906, DOI: 10.1021/acs.jctc.9b00717.

4 J. A. Gauthier, C. F. Dickens, S. Ringe, K. Chan, *Practical Considerations for Continuum Models Applied to Surface Electrochemistry*, *Chemphyschem* **2019**, *20*, 3074–3080, DOI: 10.1002/cphc.201900536.

5 S. Ringe*, E. L. Clark*, J. Resasco, A. Walton, B. Seger, A. T. Bell, K. Chan, *Understanding cation effects in electrochemical CO_2 reduction*, *Energy Environ. Sci.* **2019**, *12*, 3001–3014, (corresponding author), inside front cover, Research Highlight in *Nature Catal.*, (DOI: 10.1038/s41929-019-0335-2) and part of the 2019 *Energy Environ. Sci.* HOT Articles, DOI: 10.1039/C9EE01341E.



6 Y. Wu*, S. Ringe*, C.-L. Wu, W. Chen, A. Yang, H. Chen, M. Tang, G. Zhou, H. Y. Hwang, K. Chan, Y. Cui, *A Two-Dimensional MoS_2 Catalysis Transistor by Solid-State Ion Gating Manipulation and Adjustment (SIGMA)*, *Nano Lett.* **2019**, *19*, 7293–7300, DOI: 10.1021/acs.nanolett.9b02888.

7 E. L. Clark*, S. Ringe*, M. Tang, A. Walton, C. Hahn, T. F. Jaramillo, K. Chan, A. T. Bell, *Influence of Atomic Surface Structure on the Activity of Ag for the Electrochemical Reduction of CO_2 to CO*, *ACS Catal.* **2019**, 4006–4014, DOI: 10.1021/acscatal.9b00260.

8 T. Ludwig, J. A. Gauthier, K. S. Brown, S. Ringe, J. K. Nørskov, K. Chan, *Solvent–Adsorbate Interactions and Adsorbate-Specific Solvent Structure in Carbon Dioxide Reduction on a Stepped Cu Surface*, *J. Phys. Chem. C* **2019**, *123*, 5999–6009, DOI: 10.1021/acs.jpcc.8b11571.

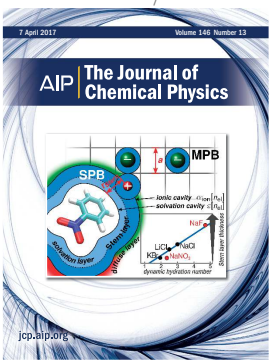
9 J. A. Gauthier, S. Ringe, C. F. Dickens, A. J. Garza, A. T. Bell, M. Head-Gordon, J. K. Nørskov, K. Chan, *Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models*, *ACS Catal.* **2019**, *9*, 920–931, DOI: 10.1021/acscatal.8b02793.

10 C. Hille*, S. Ringe*, M. Deimel, C. Kunkel, W. E. Acree, K. Reuter, H. Oberhofer, *Generalized molecular solvation in non-aqueous solutions by a single parameter implicit solvation scheme*, *J. Chem. Phys.* **2019**, *150*, 041710, (corresponding author), DOI: 10.1063/1.5050938.

11 X. Liu, P. Schlexer, J. Xiao, Y. Ji, L. Wang, R. B. Sandberg, M. Tang, K. S. Brown, H. Peng, S. Ringe, C. Hahn, T. F. Jaramillo, J. K. Nørskov, K. Chan, *pH effects on the electrochemical reduction of CO_2 towards C_2 products on stepped copper*, *Nat. Commun.* **2019**, *10*, 32, DOI: 10.1038/s41467-018-07970-9.

12 A. M. Patel, S. Ringe, S. Siahrostami, M. Bajdich, J. K. Nørskov, A. R. Kulkarni, *Theoretical Approaches to Describing the Oxygen Reduction Reaction Activity of Single-Atom Catalysts*, *J. Phys. Chem. C* **2018**, *122*, 29307–29318, DOI: 10.1021/acs.jpcc.8b09430.

13 S. Ringe, H. Oberhofer, K. Reuter, *Transferable ionic parameters for first-principles Poisson-Boltzmann solvation calculations: Neutral solutes in aqueous monovalent salt solutions*, *J. Chem. Phys.* **2017**, *146*, 134103, (corresponding author), front cover, DOI: 10.1063/1.4978850.



14 S. Ringe, H. Oberhofer, C. Hille, S. Matera, K. Reuter, *Function-Space-Based Solution Scheme for the Size-Modified Poisson-Boltzmann Equation in Full-Potential DFT*, *J. Chem. Theory Comput.* **2016**, *12*, 4052–4066, DOI: 10.1021/acs.jctc.6b00435.