

Prof. Dr. Stefan Ringe

Assistant Professor

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Curriculum Vitae

Education

- 06/2013– **Ph.D. in Computational Chemistry**, *Technical University Munich (Germany)*.
05/2017 | Prof. Dr. Karsten Reuter, “*Summa Cum Laude*”
- 10/2010– **M.Sc. in Chemistry**, *Georg-August University Göttingen (Germany)*.
03/2013 | Prof. Dr. Alec Wodtke, “*With Honors*”
- 10/2007– **B.Sc. in Chemistry**, *Georg-August University Göttingen (Germany)*.
09/2010 | Prof. Dr. Philipp Vana,

Professional Experience

- 02/2020– **Assistant Professor**, *DGIST (Rep. of Korea)*.
present | Department of Energy Science & Engineering
- 02/2019– **Postdoctoral Research Scholar**, *KAIST (Rep. of Korea)*.
02/2020 | Prof. Dr. Hyungjun Kim
- 07/2017– **Postdoctoral Research Scholar**, *Stanford University (USA)*.
01/2019 | Prof. Dr. Jens Nørskov

Research Interests

- **Computational Design for Sustainable Energy Conversion:** CO₂ 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.
- **Machine Learning:** Development of *ab initio*-based machine learning techniques for modeling molecular dynamics at electrified solid-liquid interfaces and high-throughput screening of electrocatalysts.

- **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

- 2020– **Mentoring/Supervision**, *Technical University Munich (Germany)*, Master students (2).
- 2014–2020 **Mentoring/Supervision**, *Technical University Munich (Germany)*, Master students (4), PhD students (2).
- 2020– **Lecturer**, *Technical University Munich (Germany)*, Thermodynamics, Advanced computational chemistry.
- 10/2013– **Tutor**, *Technical University Munich (Germany)*,
09/2016 Mathematics, computational & theoretical chemistry, molecular simulations, thermodynamics, numerical methods, spectroscopy.

Scientific Achievements

- Invited Talks
- 11/2021 Department seminar, Department of Biomolecular and Chemical Engineering, Sogang University
 - 07/2021 17th KIAS Electronic Structure Meeting, Online
 - 04/2021 2021 Spring Meeting of the Korean Physical Society, Sono Moon Resort, Yangpyeong, (Rep. of Korea)
 - 02/2021 BK21 Seminar of the Department of Chemical Engineering, University of Seoul, Online

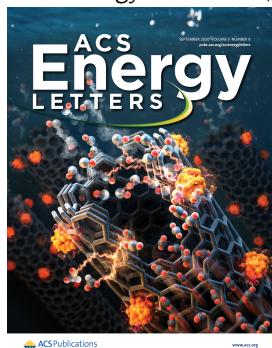
- 11/2020 6th International Conference on Electronic Materials and Nanotechnology for Green Environment (ENGE), Jeju (Rep. of Korea)
- 10/2020 Annual Meeting of the Korean Chemical Society (KCS), Suwon (Rep. of Korea)
- 09/2020 2020 Pacific Rim Meeting of electrochemical and solid state science (PRIME), Online
- 09/2020 Department seminar, Department of Chemistry, KAIST (Rep. of Korea)
- 06/2020 2020 Spring Meeting of the Korean Electrochemical Society (KECS), ICE Jeju Island (Rep. of Korea)
- 03/2020 BK21 Creation of New Materials Section Seminar, Department of Material Science and Engineering, Korea University (Rep. of Korea)
- 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 Department seminar, Department of Chemistry, KAIST (Rep. of Korea)

Paper reviews Over 20 peer reviews for various SCI journals, such as *Nature Catal.*, *Nature Energy*, *Angew. Chem. Int. Ed.*, *Joule*, *Adv. Energy Mater.*, *Nature Comm.*, etc..

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

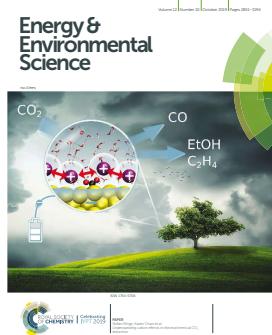
Publications ([†] = The authors contributed equally to this work; * = Corresponding author.)

- 1 S.-J. Shin[†], D. H. Kim[†], G. Bae[†], S. Ringe, H. Choi, H.-K. Lim, C. H. Choi*, H. Kim*, *On the importance of the electric double layer structure in aqueous electrocatalysis*, *Nat. Commun.* **2022**, *13*, 174, DOI: 10.1038/s41467-021-27909-x.
- 2 S. Ringe^{†*}, N. G. Hörmann[†], H. Oberhofer, K. Reuter*, *Implicit Solvation Methods for Catalysis at Electrified Interfaces*, *Chem. Rev.* **2021**, DOI: 10.1021/acs.chemrev.1c00675.
- 3 S. Ringe*, *Approaching in-depth mechanistic understanding of electrochemical hydrogen conversion from computational simulations*, *Chem Catalysis* **2021**, *1*, 1160–1162, DOI: 10.1016/j.chechat.2021.10.019.
- 4 M. K. Kim, H. Lee, J. H. Won, W. Sim, S. J. Kang, H. Choi, M. Sharma, H. Oh, S. Ringe*, Y. Kwon*, H. M. Jeong*, *Design of less than 1 nm Scale Spaces on SnO₂ Nanoparticles for High-Performance Electrochemical CO₂ Reduction*, *Adv. Funct. Mater.* **2021**, *n/a*, 2107349, DOI: 10.1002/adfm.202107349.
- 5 D. H. Kim[†], S. Ringe[†], H. Kim, S. Kim, B. Kim, G. Bae, H.-S. Oh, F. Jaouen, W. Kim*, H. Kim*, C. H. Choi*, *Selective electrochemical reduction of nitric oxide to hydroxylamine by atomically dispersed iron catalyst*, *Nat. Commun.* **2021**, *12*, 1–11, DOI: 10.1038/s41467-021-22147-7.
- 6 T. Ludwig, J. A. Gauthier, C. F. Dickens, K. S. Brown, S. Ringe, K. Chan, J. K. Nørskov*, *Atomistic Insight into Cation Effects on Binding Energies in Cu-Catalyzed Carbon Dioxide Reduction*, *The Journal of Physical Chemistry C* **2020**, *124*, 24765–24775, DOI: 10.1021/acs.jpcc.0c07004.
- 7 Y. J. Sa[†], H. Jung[†], D. Shin[†], H. Y. Jeong, S. Ringe, H. Kim*, Y. J. Hwang*, S. H. Joo*, *Thermal Transformation of Molecular Ni²⁺–N₄ Sites for Enhanced CO₂ Electroreduction Activity*, *ACS Catalysis* **2020**, *10*, 10920–10931, DOI: 10.1021/acscatal.0c02325.
- 8 M.-Y. Lee[†], S. Ringe[†], H. Kim*, S. Kang*, Y. Kwon*, *Electric field mediated selectivity switching of electrochemical CO₂ reduction from formate to CO on carbon supported Sn*, *ACS Energy Lett.* **2020**, *5*, 2987–2994, DOI: 10.1021/acsenergylett.0c01387.



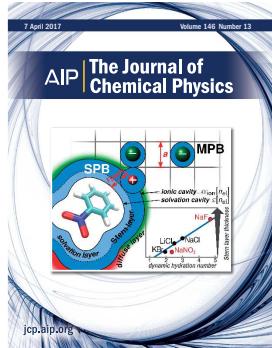
- 9 S. Ringe^{†*}, C. G. Morales-Guio[†], L. D. Chen, M. Fields, T. F. Jaramillo, C. Hahn, K. Chan*, *Double layer charging driven carbon dioxide adsorption limits the rate of electrochemical carbon dioxide reduction on Gold*, *Nat. Commun.* **2020**, *11*, 1–11, DOI: 10.1038/s41467-019-13777-z.
- 10 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.

- 11 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.
- 12 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.
- 13 S. Ringe*, E. L. Clark†, J. Resasco, A. Walton, B. Seger, A. T. Bell, K. Chan*, *Understanding cation effects in electrochemical CO₂ reduction*, *Energy Environ. Sci.* **2019**, *12*, 3001–3014, 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.



- 14 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 MoS₂ Catalysis Transistor by Solid-State Ion Gating Manipulation and Adjustment (SIGMA)*, *Nano Lett.* **2019**, *19*, 7293–7300, DOI: 10.1021/acs.nanolett.9b02888.
- 15 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 CO₂ to CO*, *ACS Catal.* **2019**, *9*, 4006–4014, DOI: 10.1021/acscatal.9b00260.
- 16 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.
- 17 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.
- 18 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, DOI: 10.1063/1.5050938.
- 19 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 CO₂ towards C₂ products on stepped copper*, *Nat. Commun.* **2019**, *10*, 32, DOI: 10.1038/s41467-018-07970-9.
- 20 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.

- 21 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, front cover, DOI: 10.1063/1.4978850.



- 22 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.