

## Prof. Dr. Stefan Ringe

Assistant Professor, Korea University

Research Fellow, IBS Center for Molecular Spectroscopy and Dynamics (CMSD)

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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

- 02/2022– **Assistant Professor**, *Korea University* (Rep. of Korea).  
present | Department of Chemistry
- 02/2022– **Research Fellow**, *Institute for Basic Science (IBS)* (Rep. of Korea).  
present | Center for Molecular Spectroscopy and Dynamics
- 02/2020– **Assistant Professor**, *DGIST* (Rep. of Korea).  
02/2022 | 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:** CO<sub>2</sub> 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.

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## Awards

- 2023 **Fellowship of the Cluster of Excellence Sustainable and Energy-Efficient Aviation (SE2A)**, SE2A/TU Braunschweig, Braunschweig, Germany.
- 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).

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## Scientific Achievements

- Invited Talks
- 10/2023 Korean Chemical Society, Physical Chemistry Symposium, 2023 KCS Fall Meeting, Gwangju, Rep. of Korea
  - 07/2023 Weierstrass Institute, Seminar on Numerical Mathematics, Berlin, Germany
  - 04/2023 KPS-DPG Symposium, 2023 KPS Spring Meeting, DCC, Daejeon, Rep. of Korea
  - 03/2023 1st Y-KAST International Conference, Jeju Shinhwa World, Jeju, Rep. of Korea
  - 02/2023 139th Korean Physical Chemistry Spring Symposium, Korea University, Rep. of Korea
  - 02/2023 SIAM Conference on Computational Science and Engineering (CSE23), RAI Congress Centre, Amsterdam, Netherlands
  - 02/2023 Virtual Winterschool on Computational Chemistry (online)

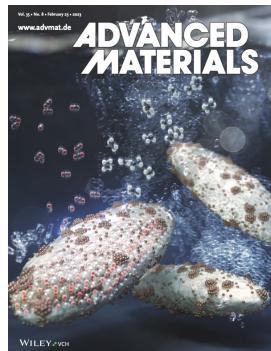
- 10/2022 IBS symposium at the 130th General Meeting of the Korea Chemical Society (KCS), Gyeongju HICO , Rep. of Korea
- 08/2022 Theory seminar, Theory department, FHI Berlin, Germany
- 11/2021 Department seminar, Department of Biomolecular and Chemical Engineering, Sogang University (online)
- 07/2021 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 General Meeting of the Korean Chemical Society (KCS), Electrochemistry Division, 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/year for various SCI journals, such as *Nature Catal.*, *Nature Energy*, *Angew. Chem. Int. Ed.*, *Joule*, *Adv. Energy Mater.*, *Nature Comm.*, etc..

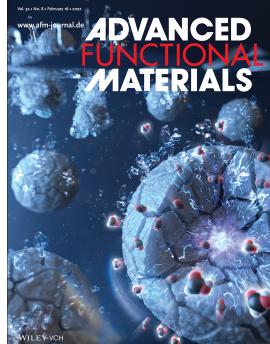
Research Stay • 10/2011–02/2012, *Synthesis of Oxygen-Evolution Catalysts*, Prof. Dr. Åkermark, Stockholm University (Sweden)

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

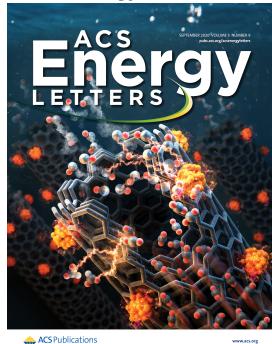
- 1 B. Kim†, Y. C. Tan†, Y. Ryu†, K. Jang, H. G. Abbas, T. Kang, H. Choi, K.-S. Lee, S. Park, W. Kim, P.-P. Choi, S. Ringe\*, J. Oh\*, *Trace-Level Cobalt Dopants Enhance CO<sub>2</sub> Electroreduction and Ethylene Formation on Copper*, *ACS Energy Lett.* **2023**, *8*, 3356–3364, DOI: 10.1021/acsenergylett.3c00418.
- 2 M. Park, S. Cho, J. Yang, V. W.-H. Lau, K. H. Kim, J. H. Park\*, S. Ringe\*, Y.-M. Kang\*, *Heterogeneous Catalyst as a Functional Substrate Governing the Shape of Electrochemical Precipitates in Oxygen-Fueled Rechargeable Batteries*, *J. Am. Chem. Soc.* **2023**, *145*, 15425–15434, DOI: 10.1021/jacs.3c03619.
- 3 S. Ringe, *The importance of a charge transfer descriptor for screening potential CO<sub>2</sub> reduction electrocatalysts*, *Nat. Commun.* **2023**, *14*, 2598, DOI: 10.1038/s41467-023-37929-4.
- 4 S. Ringe, *Cation effects on electrocatalytic reduction processes at the example of the hydrogen evolution reaction*, *Current Opinion in Electrochemistry* **2023**, *10*1268, DOI: 10.1016/j.coelec.2023.101268.
- 5 S. Hong†, H. G. Abbas†, K. Jang†, K. K. Patra, B. Kim, B.-U. Choi, H. Song, K.-S. Lee, P.-P. Choi, S. Ringe\*, J. Oh\*, *Tuning the C1 /C2 Selectivity of Electrochemical CO<sub>2</sub> Reduction on Cu-CeO<sub>2</sub> Nanorods by Oxidation State Control*, *Adv. Mater.* **2023**, *35*, e2208996, DOI: 10.1002/adma.202208996.



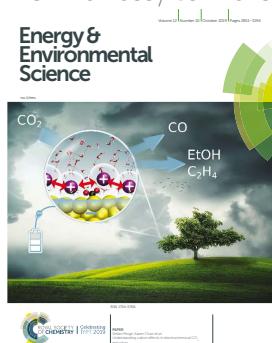
- 6 J.-H. Yu, K. P. Singh, S.-J. Kim, T.-H. Kang, K.-S. Lee, H. Kim, S. Ringe\*, J.-S. Yu\*, *Active and stable PtP2-based electrocatalysts solve the phosphate poisoning issue of high temperature fuel cells*, *J. Mater. Chem. A Mater. Energy Sustain.* **2023**, DOI: 10.1039/D2TA09110K.
- 7 S. Byun†, Z. Liu†, D. O. Shin†, K. Kim†, J. Choi, Y. Roh, D. Jin, S. Jung, K.-G. Kim, Y.-G. Lee\*, S. Ringe\*, Y. M. Lee\*, *Alkali metal ion substituted carboxymethyl cellulose as anode polymeric binders for rapidly chargeable lithium-ion batteries*, *Energy Environ. Mater.* **2022**, DOI: 10.1002/eem2.12509.
- 8 K. K. Patra†, Z. Liu†, H. Lee†, S. Hong, H. Song, H. G. Abbas, Y. Kwon\*, S. Ringe\*, J. Oh\*, *Boosting Electrochemical CO<sub>2</sub> Reduction to Methane via Tuning Oxygen Vacancy Concentration and Surface Termination on a Copper/Ceria Catalyst*, *ACS Catal.* **2022**, *12*, 10973–10983, DOI: 10.1021/acscatal.2c02669.
- 9 S.-J. Shin†, H. Choi†, S. Ringe, D. H. Won, H.-S. Oh, D. H. Kim, T. Lee, D.-H. Nam, H. Kim\*, C. H. Choi\*, *A unifying mechanism for cation effect modulating C1 and C2 productions from CO<sub>2</sub> electroreduction*, *Nat. Commun.* **2022**, *13*, 5482, DOI: 10.1038/s41467-022-33199-8.

- 10 S.-J. Kim, S. Lebègue, S. Ringe\*, H. Kim\*, *GW Quasiparticle Energies and Bandgaps of Two-Dimensional Materials Immersed in Water*, *J. Phys. Chem. Lett.* **2022**, *13*, 7574–7582, DOI: 10.1021/acs.jpclett.2c01808.
- 11 S. Ringe†\*, N. G. Hörmann†, H. Oberhofer, K. Reuter\*, *Implicit Solvation Methods for Catalysis at Electrified Interfaces*, *Chem. Rev.* **2022**, *122*, 10777–10820, DOI: 10.1021/acs.chemrev.1c00675.
- 12 E. B. Tetteh†, C. Gyan-Barimaht, H.-Y. Lee†, T.-H. Kang, S. Kang, S. Ringe\*, J.-S. Yu\*, *Strained Pt(221) Facet in a PtCo@Pt-Rich Catalyst Boosts Oxygen Reduction and Hydrogen Evolution Activity*, *ACS Appl. Mater. Interfaces* **2022**, *14*, 25246–25256, DOI: 10.1021/acsami.2c00398.
- 13 G. Kastlunger\*, L. Wang, N. Govindarajan, H. H. Heenen, S. Ringe, T. Jaramillo, C. Hahn\*, K. Chan, *Using pH Dependence to Understand Mechanisms in Electrochemical CO Reduction*, *ACS Catal.* **2022**, *12*, 4344–4357, DOI: 10.1021/acscatal.1c05520.
- 14 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.
- 15 S. Ringe\*, *Approaching in-depth mechanistic understanding of electrochemical hydrogen conversion from computational simulations*, *Chem Catalysis* **2021**, *1*, 1160–1162, DOI: 10.1016/j.chelet.2021.10.019.
- 16 H. Song, Y. C. Tan, B. Kim, S. Ringe\*, J. Oh\*, *Tunable Product Selectivity in Electrochemical CO<sub>2</sub> Reduction on Well-Mixed Ni-Cu Alloys*, *ACS Appl. Mater. Interfaces* **2021**, *13*, 55272–55280, DOI: 10.1021/acsami.1c19224.
- 17 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 SnO<sub>2</sub> Nanoparticles for High-Performance Electrochemical CO<sub>2</sub> Reduction*, *Adv. Funct. Mater.* **2021**, *n/a*, 2107349, DOI: 10.1002/adfm.202107349.
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- 18 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.
- 19 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.
- 20 Y. J. Sa†, H. Jung†, D. Shin†, H. Y. Jeong, S. Ringe, H. Kim\*, Y. J. Hwang\*, S. H. Joo\*, *Thermal Transformation of Molecular Ni<sup>2+</sup>-N<sub>4</sub> Sites for Enhanced CO<sub>2</sub> Electroreduction Activity*, *ACS Catalysis* **2020**, *10*, 10920–10931, DOI: 10.1021/acscatal.0c02325.

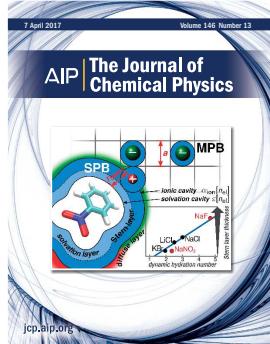
- 21 M.-Y. Lee<sup>†</sup>, S. Ringe<sup>†</sup>, H. Kim\*, S. Kang\*, Y. Kwon\*, *Electric field mediated selectivity switching of electrochemical CO<sub>2</sub> reduction from formate to CO on carbon supported Sn*, *ACS Energy Lett.* **2020**, *5*, 2987–2994, DOI: 10.1021/acsenergylett.0c01387.



- 22 S. Ringe<sup>†\*</sup>, C. G. Morales-Guio<sup>†</sup>, 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.
- 23 C. Xia<sup>†</sup>, S. Back<sup>†</sup>, S. Ringe<sup>†</sup>, 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.
- 24 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.
- 25 J. A. Gauthier<sup>†</sup>, C. F. Dickens<sup>†</sup>, S. Ringe, K. Chan, *Practical Considerations for Continuum Models Applied to Surface Electrochemistry*, *Chemphyschem* **2019**, *20*, 3074–3080, DOI: 10.1002/cphc.201900536.
- 26 S. Ringe<sup>†\*</sup>, E. L. Clark<sup>†</sup>, J. Resasco, A. Walton, B. Seger, A. T. Bell, K. Chan\*, *Understanding cation effects in electrochemical CO<sub>2</sub> 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.



- 27 Y. Wu<sup>†</sup>, S. Ringe<sup>†</sup>, C.-L. Wu, W. Chen, A. Yang, H. Chen, M. Tang, G. Zhou, H. Y. Hwang, K. Chan\*, Y. Cui\*, *A Two-Dimensional MoS<sub>2</sub> Catalysis Transistor by Solid-State Ion Gating Manipulation and Adjustment (SIGMA)*, *Nano Lett.* **2019**, *19*, 7293–7300, DOI: 10.1021/acs.nanolett.9b02888.
- 28 E. L. Clark<sup>†</sup>, S. Ringe<sup>†</sup>, 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<sub>2</sub> to CO*, *ACS Catal.* **2019**, 4006–4014, DOI: 10.1021/acscatal.9b00260.
- 29 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.
- 30 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.
- 31 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.
- 32 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<sub>2</sub> towards C<sub>2</sub> products on stepped copper*, *Nat. Commun.* **2019**, 10, 32, DOI: 10.1038/s41467-018-07970-9.
- 33 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.
- 34 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.
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- 35 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.