2. Publication List

# Academic Publications (All Peer Reviewed)

1. **Hideshi Ooka**\*, Marie E. Wintzer, Hirokazu Komatsu, Kiyohiro Adachi, Ailong Li, Shuang Kong, Daisuke Hashizume, Atsushi Mochizuki, Ryuhei Nakamura\* **"Dissipation Lifetime of Catalysis as a Dynamical System"** *ChemRxiv*, **2023**, 10.26434/chemrxiv-2023-7w3gk (*under review at Phys. Rev. Lett.*).  
**Representative Paper 1**

2. **Hideshi Ooka**\*, Yoko Chiba, Ryuhei Nakamura **"Universal Design Principle to Enhance Enzymatic Activity Using the Substrate Affinity"** *bioRxiv*, **2023**, 10.1101/2023.02.01.526728 (*under review at Nat. Commun.*).  
**Representative Paper 2**

3. Koichi Yatsuzuka, Kiyohiro Adachi, Daisuke Hashizume, Ryuhei Nakamura\*, **Hideshi Ooka**\* **"A Non-Rate-Determining Redox Process Dictates the Oxygen Evolution Tafel Slope of MnO$\_2$"** *ChemRxiv*, **2023**, 10.26434/chemrxiv-2023-lkdf3 (*submitted to J. Phys. Chem. Lett.*).

4. Yoko Chiba\*, **Hideshi Ooka**\*, Marie E. Wintzer, Nao Tsunematsu, Takehiro Suzuki, Naoshi Dohmae, Ryuhei Nakamura **"Diverse Phosphoserine Phosphatases Exhibit Maximum Activity at an Intermediate Binding Affinity in Accord With the Sabatier Principle of Catalysis"** *bioRxiv*, **2023**, 10.1101/2023.03.10.532031 (*submitted to Angew. Chem. Int. Ed.*).

5. Daoping He\*, **Hideshi Ooka**, Yamei Li, Yujeong Kim, Akira Yamaguchi, Kiyohiro Adachi, Daisuke Hashizume, Naohiro Yoshida, Sakae Toyoda, Sun Hee Kim, Ryuhei Nakamura\* **"Regulation of the Electrocatalytic Nitrogen Cycle Based on Sequential Proton-Electron Transfer"** *Nat. Catal.*, **2022**, 798-806.

6. Ailong Li, Shuang Kong, Chenxi Guo, **Hideshi Ooka**, Kiyohiro Adachi, Daisuke Hashizume, Qike Jiang, Hongxian Han, Jianping Xiao\*, Ryuhei Nakamura\* **"Enhancing the Stability of Cobalt Spinel Oxide Towards Sustainable Oxygen Evolution in Acid"** *Nat. Catal.*, **2022**, 109-118.

7. **Hideshi Ooka**\*, Jun Huang, Kai S. Exner **"The Sabatier Principle in Electrocatalysis: Basics, Limitations, and Extensions"** *Front. Energ. Res.*, **2021**, 155.

8. Thomas Kadyk\*, Jianping Xiao, **Hideshi Ooka**, Jun Huang, Kai S. Exner\* **"Material and Composition Screening Approaches in Electrocatalysis and Battery Research"** *Front. Energ. Res.*, **2021**, 227.

9. **Hideshi Ooka**\*, Marie E Wintzer, Ryuhei Nakamura **"Non-Zero Binding Enhances Kinetics of Catalysis: Machine Learning Analysis on the Experimental Hydrogen Binding Energy of Platinum"** *ACS Catal.*, **2021**, 6298-6303.  
**Representative Paper 3**

10. Ji-Eun Lee, Akira Yamaguchi, **Hideshi Ooka**, Tomohiro Kazami, Masahiro Miyauchi, Norio Kitadai, Ryuhei Nakamura\* **"In Situ FTIR Study of CO$\_2$ Reduction on Inorganic Analogues of Carbon Monoxide Dehydrogenase"** *Chem. Commun.*, **2021**, 3267-3270.

11. Daoping He, **Hideshi Ooka**, Yujeong Kim, Yamei Li, Fangming Jin\*, Sun Hee Kim\*, Ryuhei Nakamura\* **"Atomic-Scale Evidence for Highly Selective Electrocatalytic N- N Coupling on Metallic MoS$\_2$"** *Proc. Natl. Acad. Sci.*, **2020**, 31631-31638.

12. Yamei Li\*, Yoo Kyung Go, **Hideshi Ooka**, Daoping He, Fangming Jin, Sun Hee Kim\*, Ryuhei Nakamura\* **"Enzyme Mimetic Active Intermediates for Nitrate Reduction in Neutral Aqueous Media"** *Angew. Chem. Int. Ed.*, **2020**, 9744-9750.

13. **Hideshi Ooka**\*, Ryuhei Nakamura **"Shift of the Optimum Binding Energy at Higher Rates of Catalysis"** *J. Phys. Chem. Lett.*, **2019**, 6706-6713.  
**Representative Paper 4**

14. Ailong Li, **Hideshi Ooka**, Nadege Bonnet, Toru Hayashi, Yimeng Sun, Qike Jiang, Can Li, Hongxian Han\*, Ryuhei Nakamura\* **"Stable Potential Windows for Long-Term Electrocatalysis by Manganese Oxides Under Acidic Conditions"** *Angew. Chem. Int. Ed.*, **2019**, 5108-5112.

15. Daoping He, **Hideshi Ooka**, Yamei Li, Fangming Jin\*, Ryuhei Nakamura\* **"Phase-Selective Hydrothermal Synthesis of Metallic MoS$\_2$ at High Temperature"** *Chem. Lett.*, **2019**, 5054-5058.

16. **Hideshi Ooka**, Shawn E McGlynn, Ryuhei Nakamura\* **"Electrochemistry at Deep-Sea Hydrothermal Vents: Utilization of the Thermodynamic Driving Force Towards the Autotrophic Origin of Life"** *ChemElectroChem*, **2019**, 1316-1323.

17. **Hideshi Ooka**, Kazuhito Hashimoto, Ryuhei Nakamura\* **"Design Strategy of Multi-Electron Transfer Catalysts Based on a Bioinformatic Analysis of Oxygen Evolution and Reduction Enzymes"** *Mol. Inform.*, **2018**, 1700139.

18. Hirotaka Kakizaki, **Hideshi Ooka**, Toru Hayashi, Akira Yamaguchi, Nadege Bonnet-Mercier, Kazuhito Hashimoto, Ryuhei Nakamura\* **"Evidence That Crystal Facet Orientation Dictates Oxygen Evolution Intermediates on Rutile Manganese Oxide"** *Adv. Funct. Mater.*, **2018**, 1706319.

19. Daoping He, Yamei Li, **Hideshi Ooka**, Yoo Kyung Go, Fangming Jin\*, Sun Hee Kim\*, Ryuhei Nakamura\* **"Selective Electrocatalytic Reduction of Nitrite to Dinitrogen Based on Decoupled Proton-Electron Transfer"** *J. Am. Chem. Soc.*, **2018**, 2012-2015.

20. **Hideshi Ooka**, Marta C. Figueiredo, Marc T. M. Koper\* **"Competition Between Hydrogen Evolution and Carbon Dioxide Reduction on Copper Electrodes in Mildly Acidic Media"** *Langmuir*, **2017**, 9307-9313.

21. **Hideshi Ooka**, Toshihiro Takashima, Akira Yamaguchi, Toru Hayashi, Ryuhei Nakamura\* **"Element Strategy of Oxygen Evolution Electrocatalysis Based on In Situ Spectroelectrochemistry"** *Chem. Commun.*, **2017**, 7149-7161.  
**Representative Paper 5**

22. **Hideshi Ooka**, Akira Yamaguchi, Toshihiro Takashima, Kazuhito Hashimoto, Ryuhei Nakamura\* **"Efficiency of Oxygen Evolution on Iridium Oxide Determined From the pH Dependence of Charge Accumulation"** *J. Phys. Chem. C*, **2017**, 17873-17881.

23. **Hideshi Ooka**, Yuanqing Wang, Akira Yamaguchi, Makoto Hatakeyama, Shinichiro Nakamura, Kazuhito Hashimoto\*, Ryuhei Nakamura\* **"Legitimate Intermediates of Oxygen Evolution on Iridium Oxide Revealed by In Situ Electrochemical Evanescent Wave Spectroscopy"** *Phys. Chem. Chem. Phys.*, **2016**, 15199-15204.

24. **Hideshi Ooka**, Takumi Ishii, Kazuhito Hashimoto\*, Ryuhei Nakamura\* **"Light-Induced Cell Aggregation of Euglena Gracilis Towards Economically Feasible Biofuel Production"** *RSC Adv.*, **2014**, 20693-20698.

# Presentations (Japanese Titles were Translated to English)

## Invited Presentations

1. **Hideshi Ooka "A Scientist's View on the Joys of Lifelong Learning"** Lecture as a Senior, Fuzoku Ikeda High School (2023/09/16).

2. **Hideshi Ooka "Kinetic Modeling of Enzymes and Electrocatalysts"** 2023 Workshop on Bidirectional Catalysis From Molecular Machines to Enzymes, Marseille (2023/09/11).  
**Youngest out of 15 invited speakers which include Rudolph Marcus (Nobel Prize 1992)**

3. **Hideshi Ooka "Development of Catalyst Theory and the Joys of Research from the Perspective of a Experimentalist Turned Theoretician"** MERIT-WINGS Seminar Camp, Lector Yugawara (2023/08/06).

4. **Hideshi Ooka "Analysis and Experimental Verification of Dissipative Chemical Reaction Networks Towards Understanding Sustainability"** Math-Experimental Collaboration Towards an Overall Understanding of Catalysis, Enzymes, and the Ecosystem, RIKEN (2023/03/09).

5. **Hideshi Ooka "Using Machine Learning in Catalysis Theory"** Seminar # 212203, Technical Information Institute Seminar (2022/12/08).

6. **Hideshi Ooka**, Ryuhei Nakamura **"From Thermodynamics to Kinetics: Predicting New Catalysts By Revisiting the Sabatier Principle"** 8th ELSI Symposium "Extending Views of Catalysis", Tokyo Institute of Technology (2020/02/03).  
**Keynote speaker on Early Career Researcher's Day**

7. **Hideshi Ooka**, Ryuhei Nakamura **"Shift of the Optimum Binding Energy at Higher Rates of Catalysis"** The 4th Solar Fuel Material Workshop, Seoul National University (2019/09/27).

8. **Hideshi Ooka "Study on Electrocatalysis based on Informatics and Electron Transfer Theory"** The 4th Catalyst Informatics Symposium, Iino Hall (2018/11/21).

9. **Hideshi Ooka "Element Strategy of Multi-Electron Transfer Catalysis: Lessons from the Oxygen Evolution Strategies of Iridium Oxide and Photosystem II"** Seminar at Nam Lab, Seoul National University (2018/06/05).

## Oral Presentations

1. **Hideshi Ooka**, Marie E. Wintzer, Ryuhei Nakamura **"Predicting the Operational Lifetime of Electrocatalysis"** 74th Annual Meeting of the International Society of Electrochemistry, Lyon (2023/09/08).

2. **Hideshi Ooka**, Marie E. Wintzer, Hirokazu Komatsu, Kiyohiro Adachi, Ailong Li, Shuang Kong, Daisuke Hashizume, Atsushi Mochizuki, Ryuhei Nakamura **"Predicting the Lifetime of Dissipative Chemical Reaction Networks"** 2023 Annual Meeting of the Japanese Society for Mathematical Biology, Nara Womens University (2023/09/04).

3. **Hideshi Ooka**, Yoko Chiba, Ryuhei Nakamura **"Mathematical Theory to Maximize Enzymatic Activity Under Thermodynamic Constraints"** 10th International Congress on Industrial and Applied Mathematics, Waseda University (2023/08/20).

4. **Hideshi Ooka "Theoretical Advancements towards Predicting the Activity and Stability of Electrocatalysts using Microkinetics and Applied Mathematics"** Seminar at Koper Lab, Leiden University (2023/06/21).

5. **Hideshi Ooka "Theoretical Requirements for Active and Stable Anode Materials"** Magneto Special Anodes, Schiedam (2023/06/20).

6. **Hideshi Ooka "Rationalizing the Influence of the Overpotential on the Activity and Stability of Electrocatalysts "** Seminar at Exner Lab, University of Duisberg-Essen (2023/06/16).

7. **Hideshi Ooka "Predicting the Autocatalytic Feedback for a General Chemical Reaction Network"** Japan Geoscience Union Meeting 2023, Makuhari Messe (2023/05/21).

8. **Hideshi Ooka**, Yoko Chiba, Ryuhei Nakamura **"Binding Affinity to Maximize Enzymatic Activity"** Electrochemical Society of Japan 90th Annual Meeting, Tohoku Institute of Technology (2023/03/27).

9. **Hideshi Ooka "Introduction as an Experimentalist Turned Theoretician"** Lab-Theory Standing Talk, RIKEN (2023/03/16).  
**First seminar organized by iTHEMS to promote collaboration between experiments and theory.**

10. **Hideshi Ooka "Towards Quantitative Predictions of Chemical Reaction Networks"** CO World Kickoff Meeting, Tokyo Institute of Technology, Earth-Life Science Institute (2023/01/16).

11. **Hideshi Ooka "Balancing Thermodynamics and Kinetics to Achieve Maximum Rates in Catalysis"** iTHEMS Weekly Meeting, RIKEN (2020/01/17).

12. **Hideshi Ooka**, Ryuhei Nakamura **"Difference in the Binding Energy Which Optimizes the Rates and Overpotentials of Electrocatalysis"** 3rd International Solar Fuels Conference-Young, Hiroshima (2019/11/19).

13. **Hideshi Ooka**, Ryuhei Nakamura **"Catalyst Design Based on the Binding Energy"** Electrochemical Society of Japan Autumn Meeting, Yamanashi University (2019/09/05).

14. **Hideshi Ooka**, Ryuhei Nakamura **"Element Strategy of Oxygen Evolution Electrocatalysis Based on the Reaction Mechanism of Manganese Oxide, Iron Oxide, and Iridium Oxide"** 2019 North American Catalysis Society Meeting, Chicago (2019/06/23).

15. **Hideshi Ooka**, Ryuhei Nakamura **"Development Strategies of Oxygen Evolution Catalysts Based on the Reaction Kinetics of Iridium Oxide and Manganese Oxide"** The 3rd Solar Fuel Material Workshop, Osaka University (2018/03/13).

16. **Hideshi Ooka**, Ryuhei Nakamura **"From the d-band Model to Beyond: Development Strategies for Kinetically-Favorable Multi-Electron Transfer Catalysts"** The 3rd Solar Fuel Material Forum, Osaka University (2018/03/12).

17. **Hideshi Ooka**, Kazuhito Hashimoto, Ryuhei Nakamura **"Element Strategy of Multi-Electron Transfer Catalysis: Difference Between 3d and 5d Metals based on the Operando Spectroscopy of Mn, Fe, and Ir based Oxygen Evolution Catalysts"** Electrochemical Society of Japan Autumn Meeting, Nagasaki University (2017/09/10).

18. **Hideshi Ooka "Bioenergetic Restrictions on the Gene Structures of Photosynthetic and Respiratory　Enzymes"** RIKEN CSRS Interim Report, RIKEN (2015/11/26).

19. **Hideshi Ooka**, Akira Yamaguchi, Kazuhito Hashimoto, Ryuhei Nakamura **"Detection of Oxygen Evolution Intermediates Using In situ Optical Waveguide Spectroscopy"** Electrochemical Society of Japan 82nd Annual Meeting, Yokohama National University (2015/03/15).

20. **Hideshi Ooka**, Akira Yamaguchi, Kazuhito Hashimoto, Ryuhei Nakamura **"Detection of Oxygen Evolution Intermedates of Iridium Oxide Using Optical Waveguide Spectroscopy"** 3rd Meeting of Solid and Surface Photochemistry, Kyoto University (2014/12/16).

21. **Hideshi Ooka**, Akira Yamaguchi, Kazuhito Hashimoto, Ryuhei Nakamura **"Element Strategy of Water Splitting: Difference between Mn and Ir"** Electrochemical Society of Japan 81st Annual Meeting, Kansai University (2014/03/29).

22. **Hideshi Ooka**, Takumi Ishii, Ryuhei Nakamura, Kazuhito Hashimoto **"Wavelength Dependence of Euglena Photomotility"** Japan Society for Bioscience, Biotechnology, and Agrochemistry Annual Meeting, Tohoku University (2013/03/24).

## Poster Presentations

1. **Hideshi Ooka "Development of Non-equilibrium Catalytic Network Theory"** FOREST-ARIM Joint Meeting, Osaka University (2023/03/07).

2. **Hideshi Ooka**, Yoko Chiba, Ryuhei Nakamura **"Optimum Km to Maximize Enzymatic Activity"** 1st Meeting of the Molecular Life Reactions FOREST Society, Kanazawa University (2023/02/27).

3. **Hideshi Ooka**, Ryuhei Nakamura **"Difference in the Binding Energy Which Optimizes the Rates and Overpotentials of Electrocatalysis"** 3rd International Solar Fuels Conference/International Conference on Artificial Photosynthesis 2019 (Joint symposium), Hiroshima (2019/11/20).

4. **Hideshi Ooka**, Ryuhei Nakamura **"Understanding Catalytic Efficiency based on the Topology of the Reaction Network"** RIKEN CSRS Interim Report, RIKEN (2019/11/06).

5. **Hideshi Ooka "Spectral Analysis Using Machine Learning for Advanced Catalysis Development"** The 5th CSRS-ITbM Joint Workshop, Nagoya University (2019/01/24).

6. **Hideshi Ooka**, Ryuhei Nakamura **"Element Strategy of Oxygen Evolution Catalysis Based on the Reaction Mechanism of Iridium Oxide"** The 6th International Symposium on Solar Fuels and Solar Cells, Dalian (2018/10/12).

7. **Hideshi Ooka**, Ryuhei Nakamura **"Informatics Approach for Understanding Multi-Electron Transfer Regulation"** Engineering Network Retreat 2018, Nihonbashi Life Science Hub (2018/02/28).

8. **Hideshi Ooka**, Ryuhei Nakamura **"Bioinformatics Approach for Understanding Biological Electron Transfer"** RIKEN CSRS Interim Report, RIKEN (2017/11/01).

9. **Hideshi Ooka**, Ryuhei Nakamura **"Asymmetry of Oxygen Evolution and Oxygen Reduction Catalysts Revealed by a Bioinformatic Analysis of Enzymatic Genes"** The 2nd Solar Fuel Material Workshop, Seoul National University (2017/02/23).

10. **Hideshi Ooka**, Ryuhei Nakamura **"Probing the Optimization Criteria of Biological Catalysts based on in-silico Genetic Analysis of Phylogenetically Diverse Enzymes"** The 3rd CSRS-ITbM Joint Workshop, Nagoya University (2017/01/12).

11. **Hideshi Ooka**, Marc Koper, Ryuhei Nakamura **"Differentiating Between Thermodynamic and Kinetic Rate Determining Processes for Multi-Electron Transfer Catalysis Beyond Computational Simulations"** RIKEN CSRS Interim Report, RIKEN (2016/11/02).

12. **Hideshi Ooka**, Marc Koper **"Competition of Carbon Dioxide Reduction and Hydrogen Evolution on Copper Electrodes"** 67th Annual Meeting of the International Electrochemical Society, Den Haag (2016/08/21).

13. **Hideshi Ooka**, Marc Koper **"Competition of Carbon Dioxide Reduction and Hydrogen Evolution on Copper Electrodes"** CINF Summer School 2016, Gilleleje (2016/08/07).

14. **Hideshi Ooka**, Kazuhito Hashimoto, Ryuhei Nakamura **"The Asymmetry of Multi-Electron Transfer Processes at the Enzyme Gene Structure Level"** 3rd International Workshop on Microbial Life under Extreme Energy Limitation, Sandbjerg Manor (2015/09/21).

15. **Hideshi Ooka**, Akira Yamaguchi, Kazuhito Hashimoto, Ryuhei Nakamura **"Evaluation of the Charge Accumulation Process During the Oxygen Evolution Reaction on Iridium Oxide"** 21st Symposium "Advances in Photocatalysis", University of Tokyo (2014/12/12).

16. **Hideshi Ooka**, Akira Yamaguchi, Kazuhito Hashimoto, Ryuhei Nakamura **"Charge Accumulation During Oxygen Evolution Catalysis on Iridium Oxide and Manganese Oxide"** International Conference on Artificial Photosynthesis (ICARP2014), Awajishima (2014/11/24).

17. **Hideshi Ooka**, Takumi Ishii, Ryuhei Nakamura, Kazuhito Hashimoto **"Study on Euglena Photomotility towards Microbial Biofuel Production"** The 3rd CSJ Chemistry Festa, Tower Hall Funabori (2013/10/21).

# Funding

1. JST FOREST Program ((Principal Investigator))  
 **"Theory of Non-Equilibrium Catalytic Reaction Networks",** (2022 April - 2029 March, 50,000,000 yen)

2. JSPS Kakenhi Early Career ((Principal Investigator))  
 **"Predicting the Activity of Oxygen Evolution Electrocatalysts using Microkinetics and Machine Learning",** (2022 April - 2024 March, 4,680,000 yen)

3. JSPS Kakenhi Early Career ((Principal Investigator))  
 **"Introducing Low Spin Electron Configuration to Enhance the Activity of 3d-Block Oxygen Evolution Catalysts",** (2020 April - 2022 March, 4,160,000 yen)

4. RIKEN Cluster for Science, Technology, and Innovation Hub RIKEN and Tohoku University Joint Research Program ((Principal Investigator))  
 **"Using Highthroughput DFT Calculations for Element Strategy of Catalysis",** (2022 April - 2023 March, 1,730,000 yen)

5. RIKEN Incentive Research Project ((Principal Investigator))  
 **"Study on the Charge Accumulation Process Towards the Rational Development of Earth-Abundant Oxygen Evolution Catalysts",** (2018 April - 2020 March, 1,700,000 yen)

6. RIKEN CSRS Next Generation Acceleration Research Program ((Principal Investigator))  
 **"Understanding Gene Regulation based on the Informational Value of mRNA-Protein Interactions",** (2021 April - 2023 March, 2,000,000 yen)

7. JSPS Kakenhi Transformative A ((Co-Investigator))  
 **"Chemistry: Demonstration of Prebiotic Metabolism in a CO-Rich Environment",** (2022 April - 2027 March, 252,810,000 yen)

8. JSPS Kakenhi A ((Co-Investigator))  
 **"Regulation of Catalytic Reaction Networks towards Realizing Stable Oxygen Evolution Catalysts",** (2022 April - 2025 March, 30,350,000 yen)

# Patents

1. Kazuhito Hashimoto, Ryuhei Nakamura, **Hideshi Ooka**, Iwao Ueda, Hitoshi Matsuda "**Method for concentrating microalga culture fluid and apparatus therefor**", WO2014136574A1 (Public).

2. Ryuhei Nakamura, **Hideshi Ooka**, Bonnet Nadege, Ailong Li, Shuang Kong, Hongxian Han "**Water electrolysis method and equipment, and method for determining the driving potential of water electrolysis**", JPWO2020032256A1 (Public).

# Awards

1. Best SPDR Report,RIKEN (2021/01/18)

2. Ohbu Award for Young Researcher,RIKEN (2020/03/25)

3. Special Postdoctoral Researcher,RIKEN (2019/04/01)

4. Invitation to SPD Interview,Japan Society for the Promotion of Science (2018/10/19)  
**Interview declined to accept RIKEN SPDR position**

5. Cum Laude,University of Tokyo, School of Engineering (2018/03/21)

6. Merit Award (4 awardees out of 40 candidates),University of Tokyo Leading Graduate Program MERIT (2018/03/07)

7. JSPS DC1 (no interview),Japan Society for the Promotion of Science (2015/04/01)

8. CSJ Chemistry Festa Poster Prize,Chemical Society of Japan (2013/10/21)