2. Publication List

# Academic Publications

1. **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.*).

2. **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, (*submitted to Phys. Rev. Lett.*).

3. Koichi Yatsuzuka, Kiyohiro Adachi, Daisuke Hashizume, Ryuhei Nakamura\*, **Hideshi Ooka**\* "A Non-Rate-Determining Redox Process Dictates the Oxygen Evolution Tafel Slope of MnO2", *ChemRxiv*, **2023**, 10.26434/chemrxiv-2023-lkdf3, (*submitted to J. Phys. Chem. C*).

4. Yoko Chiba\*, **Hideshi Ooka**\*, Marie 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.

10. Ji-Eun Lee, Akira Yamaguchi, **Hideshi Ooka**, Tomohiro Kazami, Masahiro Miyauchi, Norio Kitadai, Ryuhei Nakamura\* "In Situ FTIR Study of CO2 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 MoS2", *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.

14. Ailong Li, **Hideshi Ooka**, Nad{\`e}ge 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 MoS2 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, Nad{\`e}ge 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 TM 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.

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

## Invited Presentations

1. Hideshi Ooka **"Joys of Being a Scientist: Learning New Things is Fun!"** 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, including Rudolph Marcus (Nobel Prize 1992)**

3. Hideshi Ooka **"触媒理論の開拓：実験出身の理論研究者から見た研究の楽しさ"** MERIT-WINGS Seminar Camp, Lector Yugawara (2023/08/06)

4. 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**

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

6. 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)

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

8. 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, 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)

2. 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)

3. 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)

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

5. 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)

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

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

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

9. 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/)

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

11. 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/)

12. 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 Forum, Osaka University (2018/03/)

13. 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 Workshop, Osaka University (2018/03/)

14. 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/)

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

16. 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/)

17. Hideshi Ooka, Akira Yamaguchi, Kazuhito Hashimoto, Ryuhei Nakamura **"Detection of Oxygen Evolution Intermedates of Iridium Oxide Using Optical Waveguide Spectroscopy"** 第33回固体・表面光化学討論会, Kyoto University (2014/12/)

18. 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/)

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

## 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 **"Understanding Catalytic Efficiency based on the Topology of the Reaction Network"** RIKEN CSRS Interim Report, RIKEN (2019/11/)

4. 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/)

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

6. Hideshi Ooka, Ryuhei Nakamura **"The 6th International Symposium on Solar Fuels and Solar Cells"** The 6th International Symposium on Solar Fuels and Solar Cells, Dalian (2018/10/)

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

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

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/)

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/)

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/)

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

13. 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/)

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/)

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/)

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/)

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/)

# Funding

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

**2. JST FOREST Program (Principal Investigator)**Title：Theory of Non-equilibrium Catalytic Reaction Networks  
Period：2022 May - 2029 April  
Amount：50,000,000 yen

**3. JSPS Kakenhi (Early Career) (Principal Investigator)**Title：Predicting the Activity of Oxygen Evolution Electrocatalysts using Microkintics and Machine Learning  
Period：2022 May - 2024 April  
Amount：4680000 yen

**4. JSPS Kakenhi (Transformative A) (Co-Investigator)**Title：Chemistry: Demonstration of Prebiotic Metabolism in a CO-Rich Environment  
Period：2022 May - 2027 April  
Amount：252,810,000 yen

**5. JSPS Kakenhi (A) (Co-Investigator)**Title：Regulation of Catalytic Reaction Networks  
Period：2022 May - 2025 April  
Amount：30,350,000 yen

**6. RIKEN Incentive Research Project (Principal Investigator)**Title：Study on the Charge Accumulation Process Towards the Rational Development of Earth-Abundant Oxygen Evolution Catalysts  
Period：2018 May - 2020 April  
Amount：1,700,000 yen

**7. RIKEN Cluster for Science, Technology, and Innovation Hub RIKEN and Tohoku University Joint Research Program (Principal Investigator)**Title：Using Highthroughput DFT Calculations for Element Strategy of Catalysis  
Period：2022 May - 2023 April  
Amount：1,730,000 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

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

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

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

2018/03/21,Cum Laude,University of Tokyo Department of Engineering

2018/10/19,SPD Interview Declined,Japan Society for the Promotion of Science (JSPS)

2019/04/01,Special Postdoctoral Researcher,RIKEN

2020/03/25,Ohbu Award for Young Researcher,RIKEN

2021/01/18,Best SPDR Report,RIKEN