2. Publication List

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| 学術論文 (査読あり) |

# 学術論文 (査読あり)

20

1. **Hideshi Ooka**\*, Yoko Chiba, Ryuhei Nakamura **"Thermodynamic principle to enhance enzymatic activity using the substrate affinity"** *Nat. Commun.*, **2023**, *141*, 4860.  
**代表論文 1**

2. 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.*).

3. 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.*).

4. **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.*).  
**代表論文 2**

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**, *5*, 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**, *5*, 109--118.

7. **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**, *11*, 6298--6303.  
**代表論文 3**

8. 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**, *57*, 3267--3270.

9. 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**, *117*, 31631--31638.

10. 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**, *59*, 9744--9750.

11. Daoping He, **Hideshi Ooka**, Yamei Li, Fangming Jin\*, Ryuhei Nakamura\* **"Phase-Selective Hydrothermal Synthesis of Metallic MoS$\_2$ at High Temperature"** *Chem. Lett.*, **2019**, *58*, 5054--5058.

12. **Hideshi Ooka**\*, Ryuhei Nakamura **"Shift of the Optimum Binding Energy at Higher Rates of Catalysis"** *J. Phys. Chem. Lett.*, **2019**, *10*, 6706--6713.  
**代表論文 4**

13. 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**, *131*, 5108--5112.

14. **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**, *37*, 1700139.

15. 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**, *28*, 1706319.

16. 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**, *140*, 2012--2015.

17. **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**, *33*, 9307--9313.  
**代表論文 5**

18. **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**, *121*, 17873--17881.

19. **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**, *18*, 15199--15204.

20. **Hideshi Ooka**, Takumi Ishii, Kazuhito Hashimoto\*, Ryuhei Nakamura\* **"Light-Induced Cell Aggregation of Euglena Gracilis Towards Economically Feasible Biofuel Production"** *RSC Adv.*, **2014**, *4*, 20693--20698.

21. **Hideshi Ooka**\*, Jun Huang, Kai S. Exner **"The Sabatier Principle in Electrocatalysis: Basics, Limitations, and Extensions"** *Front. Energ. Res.*, **2021**, *9*, 155.

22. 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**, *9*, 227.

23. **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**, *6*, 1316--1323.

24. **Hideshi Ooka**, Toshihiro Takashima, Akira Yamaguchi, Toru Hayashi, Ryuhei Nakamura\* **"Element Strategy of Oxygen Evolution Electrocatalysis Based on In Situ Spectroelectrochemistry"** *Chem. Commun.*, **2017**, *53*, 7149--7161.

# 学会発表

## 【招待講演】

1. **大岡英史 "研究って楽しい！え、勉強も楽しいの？"** 先輩の授業を受けよう, 大阪教育大学附属中学校池田校舎, 大阪 (2023/09/16).

2. **Hideshi Ooka "Kinetic Modeling of Enzymes and Electrocatalysts"** 2023 Workshop on Bidirectional Catalysis From Molecular Machines to Enzymes, Marseille, France (2023/09/11).

3. **大岡英史 "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合宿, レクトーレ湯河原, 箱根 (2023/08/06).

4. **Hideshi Ooka "Analysis and Experimental Verification of Dissipative Chemical Reaction Networks Towards Understanding Sustainability"** 触媒・酵素・エコシステムの統合理解に向けた数理実験融合, RIKEN, Wako (2023/03/09).

5. **大岡英史 "実験データに基づく触媒反応パラメーターの推定：活性、選択性への応用"** セミナー #212203, 技術情報協会, Online (2022/12/08).

6. **大岡英史 "水の電気分解による水素製造：現状と未来"** 和光市民大学, 和光市役所, 和光 (2021/12/07).

7. **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, Japan (2020/02/03).  
**基調講演（若手枠）**

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

9. **大岡英史 "情報科学と電子移動論に基づく電極触媒に関する研究"** 第４回キャタリストインフォマティクスシンポジウム, イイノホール, 東京 (2018/11/21).

10. **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, Korea (2018/06/05).

## 【口頭発表】

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

2. **大岡英史**、Marie E. Wintzer、小松弘和、足立精宏、李愛龍、孔爽、橋爪大輔、望月敦史、中村龍平 **"散逸化学反応ネットワークの寿命予測"** 2023年度日本数理生物学会年会, 奈良女子大学, 奈良 (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, Tokyo (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, The Netherlands (2023/06/21).

5. **Hideshi Ooka "Theoretical Requirements for Active and Stable Anode Materials"** Magneto Special Anodes, Schiedam, The Netherlands (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, Germany (2023/06/16).

7. **大岡英史 "一般的な化学反応ネットワークにおける自己触媒増幅率の予測"** 日本地球惑星科学連合2023年大会, 幕張メッセ, 千葉 (2023/05/21).

8. **大岡英史**、千葉洋子、中村龍平 **"酵素活性を最大化する結合性相互作用の予測"** 電気化学会第90回大会, Tohoku Institute of Technology, Sendai (2023/03/27).

9. **Hideshi Ooka "Introduction as an Experimentalist Turned Theoretician"** Lab-Theory Standing Talk, RIKEN, Wako (2023/03/16).  
**理論と実験の融合促進に向けた理研iTHEMSの第1回のセミナー**

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

11. **Hideshi Ooka "Balancing Thermodynamics and Kinetics to Achieve Maximum Rates in Catalysis"** iTHEMS Weekly Meeting, RIKEN, Wako (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, Japan (2019/11/19).

13. **大岡英史**、中村龍平 **"結合エネルギーから見た電極触媒の開発"** 電気化学会秋季大会, 山梨大学, 甲府 (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, USA (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, Japan (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, Japan (2018/03/12).

17. **大岡英史**、橋本和仁、中村龍平 **"多電子移動触媒の元素戦略：Mn,Fe,Ir酸素発生触媒のオペランド分光法に基づく3d金属触媒と5d貴金属触媒の相違"** 電気化学会秋季大会, 長崎大学, 長崎 (2017/09/10).

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

19. **大岡英史**、山口晃、橋本和仁、中村龍平 **"In situ光導波路分光法を用いた多電子水酸化反応中間体の検出"** 電気化学会第82回大会, 横浜国立大学, 横浜 (2015/03/15).

20. **大岡英史**、山口晃、橋本和仁、中村龍平 **"光導波路分光法を用いたIrOx電極触媒における酸素発生反応中間体の検出"** 第33回固体・表面光化学討論会, 京都大学, 京都 (2014/12/16).

21. **大岡英史**、山口晃、橋本和仁、中村龍平 **"水分解電極触媒における元素戦略: MnとIrの相違"** 電気化学会第81回大会, 関西大学, 吹田 (2014/03/29).

22. **大岡英史**、石居拓己、中村龍平、橋本和仁 **"ミドリムシ走光性における波長依存性"** 2013年度農芸化学会, 東北大学, 仙台 (2013/03/24).

## 【ポスター発表】

1. **大岡英史 "非平衡状態における触媒反応ネットワーク理論の開拓"** 創発研究者とマテリアル先端リサーチインフラの出会いの場, 大阪大学産業科学研究所, 大阪 (2023/03/07).

2. **Hideshi Ooka**, Yoko Chiba, Ryuhei Nakamura **"Optimum Km to Maximize Enzymatic Activity"** 第1回分子生命反応創発討論会, 金沢大学, 金沢 (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, Japan (2019/11/20).

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

5. **Hideshi Ooka "Spectral Analysis Using Machine Learning for Advanced Catalysis Development"** 第5回CSRS-ITbMジョイントワークショップ, 名古屋大学, 名古屋 (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, China (2018/10/12).

7. **大岡英史**、中村龍平 **"Informatics Approach for Understanding Multi-Electron Transfer Regulation"** エンジニアリング・ネットワークリトリート2018, 日本橋ライフサイエンスハブ, 東京 (2018/02/28).

8. **Hideshi Ooka**, Ryuhei Nakamura **"Bioinformatics Approach for Understanding Biological Electron Transfer"** RIKEN CSRS Interim Report, RIKEN, Japan (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, Korea (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, Nagoya (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, Japan (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, The Netherlands (2016/08/21).

13. **Hideshi Ooka**, Marc Koper **"Competition of Carbon Dioxide Reduction and Hydrogen Evolution on Copper Electrodes"** CINF Summer School 2016, Gilleleje, Denmark (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, Denmark (2015/09/21).

15. **大岡英史**、山口晃、橋本和仁、中村龍平 **"酸素発生中におけるイリジウム酸化物の電化貯蔵プロセスの評価"** 第21回シンポジウム「光触媒反応の最近の展開」, University of Tokyo, 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, Japan (2014/11/24).

17. **大岡英史**、石居拓己、中村龍平、橋本和仁 **"微生物オイル生産に向けたミドリムシの光運動性制御"** 第3回 CSJ化学フェスタ, タワーホール船堀, 東京 (2013/10/21).

# 外部資金獲得実績

1. 国立研究開発法人科学技術振興機構 創発的研究支援事業 (研究代表者)  
 **"非平衡状態における触媒反応ネットワーク理論の開拓"** (2022 April - 2029 March, 50,000,000 JPY)

2. 日本学術振興会 科学研究費助成事業 若手研究 (研究代表者)  
 **"反応速度論と機械学習による酸素発生触媒の活性予測"** (2022 April - 2024 March, 4,680,000 JPY)

3. 日本学術振興会 科学研究費助成事業 若手研究 (研究代表者)  
 **"低スピン電子配置の導入による3d金属酸素発生触媒の活性化"** (2020 April - 2022 March, 4,160,000 JPY)

4. 理研科学技術ハブ 理研-東北大 科学技術ハブ共同研究プログラム (研究代表者)  
 **"ハイスループット量子化学計算による触媒元素戦略"** (2022 April - 2023 March, 1,730,000 JPY)

5. 理研 Incentive Research Project (研究代表者)  
 **"Study on the Charge Accumulation Process Towards the Rational Development of Earth-Abundant Oxygen Evolution Catalysts"** (2018 April - 2020 March, 1,700,000 JPY)

6. 理研 CSRS次世代飛躍研究プログラム (研究代表者)  
 **"Understanding Gene Regulation based on the Informational Value of mRNA-Protein Interactions"** (2021 April - 2023 March, 2,000,000 JPY)

7. 日本学術振興会 科学研究費助成事業 学術変革領域研究(A) (研究分担者)  
 **"化学班：CO環境で駆動される前駆代謝システムの実証"** (2022 April - 2027 March, 252,810,000 JPY)

8. 日本学術振興会 科学研究費助成事業 基盤研究(A) (研究分担者)  
 **"触媒反応ネットワークの制御による持続的酸素発生触媒の創生"** (2022 April - 2025 March, 30,350,000 JPY)

# 知財・特許

1. 橋本和仁, 中村龍平, **大岡英史**, 上田巌, 松田整 "**微細藻類培養液の濃縮方法および装置**", WO2014136574A1 (登録済み).

2. 中村龍平, **大岡英史**, Bonnet Nadege, Li Ailong, Kong Shuang, Han Hongxian "**水電気分解法及び装置、並びに水電気分解の駆動電位の決定方法**", JPWO2020032256A1 (登録済み).

# 受賞歴

1. **基礎科学特別研究員 成果報告会 優秀賞**, 理化学研究所 (2021/01/18).

2. **桜舞賞**, 理化学研究所 (2020/03/25).

3. **基礎科学特別研究員 採用**, 理化学研究所 (2019/04/01).

4. **SPD面接に招待**, 日本学術振興会（JSPS) (2018/10/19).  
**理研基礎特研となるため、面接辞退**

5. **工学系研究科長賞(専攻内で最優秀賞)**, 東京大学 (2018/03/21).

6. **MERIT賞 (学年40人から優秀者4人)**, 東京大学リーディング大学院MERIT (2018/03/07).

7. **DC1 採用**, 日本学術振興会（JSPS) (2015/04/01).

8. **CSJ化学フェスタ ポスター賞**, 日本化学会 (2013/10/21).