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Publications

PUBLICATIONS

- **Modulating coordinate site occupancy in high-entropy spinel electrocatalysts.** *Nature communications*
  Baek, J., Hamkins, K. S., Li, Y., Garcia-Esparza, A. T., Liu, T., Kuo, C. T., Lee, J. S., Potter, A. W., Kim, S., Wang, Y., Ding, H., Li, J., Zhuo, et al
  2026
- **Crossing the Oxo-Peroxo Wall for Selective Electrochemical Epoxidation.** *Advanced science (Weinheim, Baden-Wurttemberg, Germany)*
  Basera, P., Mandal, S. C., Abild-Pedersen, F., Bajdich, M.
  2025: e17229
- **The Role of Cu3+ in the Oxygen Evolution Activity of Copper Oxides.** *Journal of the American Chemical Society*
  Basera, P., Zhao, Y., Garcia-Esparza, A. T., Babbe, F., Bothra, N., Vinson, J., Sokaras, D., Yano, J., Boettcher, S. W., Bajdich, M.
  2025
- **Resolution of Selectivity Steps of CO Reduction Reaction on Copper by Quantum Monte Carlo.** *The journal of physical chemistry letters*
  Fanta, R., Bajdich, M.
  2025: 1494-1500
- **Coupling Anionic Oxygen Redox with Selenium for Stable High-Voltage Sodium Layered Oxide Cathodes** *ADVANCED FUNCTIONAL MATERIALS*
  Xue, Z., Bothra, N., Meng, D., Feng, G., Li, Y., Cui, T., Hao, H., Lee, S., Liu, Y., Bajdich, M., Nanda, J., Zheng, X.
  2024
- **In situ formation of liquid crystal interphase in electrolytes with soft templating effects for aqueous dual-electrode-free batteries** *NATURE ENERGY*
  Li, Y., Zheng, X., Carlson, E. Z., Xiao, X., Chi, X., Greenburg, L. C., Zhang, G., Zhang, E., Liu, C., Yang, Y., Kim, M., Feng, G., Zhang, et al
  2024
- **Oxidizing Role of Cu Cocatalysts in Unassisted Photocatalytic CO2Reduction Using p-GaN/Al2O3/Au/Cu Heterostructures.** *ACS nano*
  Zoric, M. R., Basera, P., Palmer, L. D., Aitbekova, A., Powers-Riggs, N., Lim, H., Hu, W., Garcia-Esparza, A. T., Sarker, H., Abild-Pedersen, F., Atwater, H. A., Cushing, S. K., Bajdich, et al
  2024
- **Tuning Two-Dimensional Phthalocyanine Dual Site Metal-Organic Framework Catalysts for the Oxygen Reduction Reaction.** *Journal of the American Chemical Society*
  Wei, L., Hossain, M. D., Chen, G., Kamat, G. A., Kreider, M. E., Chen, J., Yan, K., Bao, Z., Bajdich, M., Stevens, M. B., Jaramillo, T. F.
  2024
- **Prediction of O and OH Adsorption on Transition Metal Oxide Surfaces from Bulk Descriptors** *ACS CATALYSIS*
  Comer, B. M., Bothra, N., Lunger, J. R., Abild-Pedersen, F., Bajdich, M., Winther, K. T.
  2024
- **Synergistic effects of mixing and strain in high entropy spinel oxides for oxygen evolution reaction.** *Nature communications*
  Baek, J., Hossain, M. D., Mukherjee, P., Lee, J., Winther, K. T., Leem, J., Jiang, Y., Chueh, W. C., Bajdich, M., Zheng, X.
  2023; 14 (1): 5936
- **A Comparative Study of Electrical Double Layer Effects for CO Reduction Reaction Kinetics** *JOURNAL OF PHYSICAL CHEMISTRY C*
  Pasumarthi, V., Yu, H., Akhade, S. A., Abild-Pedersen, F., Varley, J. B., Bajdich, M.

2023

- **Insights into Active Sites and Mechanisms of Benzyl Alcohol Oxidation on Nickel-Iron Oxyhydroxide Electrodes** *ACS CATALYSIS*
  Wei, L., Hossain, M., Boyd, M. J., Aviles-Acosta, J., Kreider, M. E., Nielander, A. C., Stevens, M., Jaramillo, T. F., Bajdich, M., Hahn, C.
  2023: 4272-4282

- **Resolving atomistic structure and oxygen evolution activity in nickel antimonates** *JOURNAL OF MATERIALS CHEMISTRY A*
  Rao, K. K. K., Zhou, L., Lai, Y., Richter, M. H. H., Li, X., Lu, Y., Yano, J., Gregoire, J. M. M., Bajdich, M.
  2022

- **Selectivity of Electrochemical Ion Insertion into Manganese Dioxide Polymorphs.** *ACS applied materials & interfaces*
  Carlson, E. Z., Chueh, W. C., Mefford, J. T., Bajdich, M.
  2022

- **Investigation of the Structure of Atomically Dispersed NiNx Sites in Ni and N-Doped Carbon Electrocatalysts by 61Ni Mossbauer Spectroscopy and Simulations.** *Journal of the American Chemical Society*
  Koshy, D. M., Hossain, M. D., Masuda, R., Yoda, Y., Gee, L. B., Abiose, K., Gong, H., Davis, R., Seto, M., Gallo, A., Hahn, C., Bajdich, M., Bao, et al
  2022

- **Efficient and Stable Acidic Water Oxidation Enabled by Low-Concentration, High-Valence Iridium Sites** *ACS ENERGY LETTERS*
  Shi, X., Peng, H., Hersbach, T. J. P., Jiang, Y., Zeng, Y., Baek, J., Winther, K. T., Sokaras, D., Zheng, X., Bajdich, M.
  2022

- **Unraveling Electronic Trends in O* and OH* Surface Adsorption in the MO2 Transition-Metal Oxide Series** *JOURNAL OF PHYSICAL CHEMISTRY C*
  Comer, B. M., Li, J., Abild-Pedersen, F., Bajdich, M., Winther, K. T.
  2022; 126 (18): 7903-7909

- **Cation-Dependent Multielectron Kinetics of Metal Oxide Splitting** *CHEMISTRY OF MATERIALS*
  Lunger, J. R., Lutz, N., Peng, J., Bajdich, M., Shao-Horn, Y.
  2022; 34 (8): 3872-3881

- **Overcoming Hurdles in Oxygen Evolution Catalyst Discovery via Codesign** *CHEMISTRY OF MATERIALS*
  Rao, K. K., Lai, Y., Zhou, L., Haber, J. A., Bajdich, M., Gregoire, J. M.
  2022; 34 (3): 899-910

- **Water or Anion? Uncovering the Zn2+ Solvation Environment in Mixed Zn(TFSI)(2) and LiTFSI Water-in-Salt Electrolytes** *ACS ENERGY LETTERS*
  Zhang, Y., Wan, G., Lewis, N. H. C., Mars, J., Bone, S. E., Steinrueck, H., Lukatskaya, M. R., Weadock, N. J., Bajdich, M., Borodin, O., Tokmakoff, A., Toney, M. F., Maginn, et al
  2021; 6 (10): 3458-3463

- **Origin of enhanced water oxidation activity in an iridium single atom anchored on NiFe oxyhydroxide catalyst.** *Proceedings of the National Academy of Sciences of the United States of America*
  Zheng, X., Tang, J., Gallo, A., Garrido Torres, J. A., Yu, X., Athanitis, C. J., Been, E. M., Ercius, P., Mao, H., Fakra, S. C., Song, C., Davis, R. C., Reimer, et al
  2021; 118 (36)

- **Dynamics and Hysteresis of Hydrogen Intercalation and Deintercalation in Palladium Electrodes: A Multimodal In Situ X-ray Diffraction, Coulometry, and Computational Study** *CHEMISTRY OF MATERIALS*
  Landers, A. T., Peng, H., Koshy, D. M., Lee, S., Feaster, J. T., Lin, J. C., Beeman, J. W., Higgins, D., Yano, J., Drisdell, W. S., Davis, R. C., Bajdich, M., Abild-Pedersen, et al
  2021; 33 (15): 5872-5884

- **Epitaxial Stabilization and Oxygen Evolution Reaction Activity of Metastable Columbite Iridium Oxide** *ACS APPLIED ENERGY MATERIALS*
  Lee, K., Flores, R. A., Liu, Y., Wang, B., Hikita, Y., Sinclair, R., Bajdich, M., Hwang, H. Y.
  2021; 4 (4): 3074-3082

- **Isolating the Electrocatalytic Activity of a Confined NiFe Motif within Zirconium Phosphate** *ADVANCED ENERGY MATERIALS*
  Sanchez, J., Stevens, M., Young, A. R., Gallo, A., Zhao, M., Liu, Y., Ramos-Garces, M. V., Ben-Naim, M., Colon, J. L., Sinclair, R., King, L. A., Bajdich, M., Jaramillo, et al

2021

- **Tuning electrochemially driven surface transformation in atomically flat LaNiO3 thin films for enhanced water electrolysis.** *Nature materials*
  Baeumer, C., Li, J., Lu, Q., Liang, A. Y., Jin, L., Martins, H. P., Duchon, T., GloSS, M., Gericke, S. M., Wohlgemuth, M. A., Giesen, M., Penn, E. E., Dittmann, et al
  2021

- **The role of atomic carbon in directing electrochemical CO(2) reduction to multicarbon products** *ENERGY & ENVIRONMENTAL SCIENCE*
  Peng, H., Tang, M. T., Liu, X., Schlexer Lamoureux, P., Bajdich, M., Abild-Pedersen, F.
  2021; 14 (1): 473–82

- **Guiding the Catalytic Properties of Copper for Electrochemical CO2 Reduction by Metal Atom Decoration.** *ACS applied materials & interfaces*
  Nishimura, Y. F., Peng, H. J., Nitopi, S., Bajdich, M., Wang, L., Morales-Guio, C. G., Abild-Pedersen, F., Jaramillo, T. F., Hahn, C.
  2021

- **From electricity to fuels: Descriptors for C-1 selectivity in electrochemical CO2 reduction** *APPLIED CATALYSIS B-ENVIRONMENTAL*
  Tang, M. T., Peng, H., Lamoureux, P., Bajdich, M., Abild-Pedersen, F.
  2020; 279

- **Acidic Oxygen Evolution Reaction Activity-Stability Relationships in Ru-Based Pyrochlores** *ACS CATALYSIS*
  Hubert, M. A., Patel, A. M., Gallo, A., Liu, Y., Valle, E., Ben-Naim, M., Sanchez, J., Sokaras, D., Sinclair, R., Norskov, J. K., King, L. A., Bajdich, M., Jaramillo, et al
  2020; 10 (20): 12182–96

- **Active Learning Accelerated Discovery of Stable Iridium Oxide Polymorphs for the Oxygen Evolution Reaction** *CHEMISTRY OF MATERIALS*
  Flores, R. A., Paolucci, C., Winther, K. T., Jain, A., Torres, J., Aykol, M., Montoya, J., Norskov, J. K., Bajdich, M., Bligaard, T.
  2020; 32 (13): 5854–63

- **Interpreting Tafel behavior of consecutive electrochemical reactions through combined thermodynamic and steady state microkinetic approaches** *ENERGY & ENVIRONMENTAL SCIENCE*
  Mefford, J., Zhao, Z., Bajdich, M., Chueh, W. C.
  2020; 13 (2): 622–34

- **Improved Oxygen Reduction Reaction Activity of Nanostructured CoS2 through Electrochemical Tuning** *ACS APPLIED ENERGY MATERIALS*
  Zhao, W., Bothra, P., Lu, Z., Li, Y., Mei, L., Liu, K., Zhao, Z., Chen, G., Back, S., Siahrostami, S., Kulkarni, A., Norskov, J. K., Bajdich, et al
  2019; 2 (12): 8605–14

- **Selective high-temperature CO2 electrolysis enabled by oxidized carbon intermediates** *NATURE ENERGY*
  Skafte, T. L., Guan, Z., Machala, M. L., Gopal, C. B., Monti, M., Martinez, L., Stamate, E., Sanna, S., Torres, J., Crumlin, E. J., Garcia-Melchor, M., Bajdich, M., Chueh, et al
  2019; 4 (10): 846–55

- **Machine Learning for Computational Heterogeneous Catalysis** *CHEMCATCHEM*
  Lamoureux, P., Winther, K. T., Torres, J., Streibel, V., Zhao, M., Bajdich, M., Abild-Pedersen, F., Bligaard, T.
  2019; 11 (16): 3579–99

- **Trends in Oxygen Electrocatalysis of 3 d-Layered (Oxy)(Hydro)Oxides** *CHEMCATCHEM*
  Zhao, Z., Lamoureux, P., Kulkarni, A., Bajdich, M.
  2019; 11 (15): 3423–31

- **Stabilization of reactive Co4O4 cubane oxygen-evolution catalysts within porous frameworks** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Nguyen, A. I., van Allsburg, K. M., Terban, M. W., Bajdich, M., Oktawiec, J., Amtawong, J., Ziegler, M. S., Dombrowski, J. P., Lakshmi, K. V., Drisdell, W. S., Yano, J., Billinge, S. J. L., Tilley, et al
  2019; 116 (24): 11630–39

- **Catalysis-Hub.org, an open electronic structure database for surface reactions.** *Scientific data*
  Winther, K. T., Hoffmann, M. J., Boes, J. R., Mamun, O., Bajdich, M., Bligaard, T.

2019; 6 (1): 75

- **The Role of Aluminum in Promoting Ni-Fe-OOH Electrocatalysts for the Oxygen Evolution Reaction** *ACS APPLIED ENERGY MATERIALS*
  Baker, J. G., Schneider, J. R., Torres, J., Singh, J. A., Mackus, A. J. M., Bajdich, M., Bent, S. F.
  2019; 2 (5): 3488–99
- **Catalysis-hub.org: An open electronic structure database for surface reactions and catalytic materials**
  Winther, K., Hoffmann, M., Mamun, O., Boes, J., Bajdich, M., Bligaard, T.
  AMER CHEMICAL SOC.2019
- **Systematic Investigation of Iridium-Based Bimetallic Thin Film Catalysts for the Oxygen Evolution Reaction in Acidic Media.** *ACS applied materials & interfaces*
  Strickler, A. L., Flores, R. A., King, L. A., Nørskov, J. K., Bajdich, M. n., Jaramillo, T. F.
  2019
- **Strongly Modified Scaling of CO Hydrogenation in Metal Supported TiO Nanostripes** *ACS CATALYSIS*
  Sandberg, R. B., Hansen, M. H., Norskov, J. K., Abild-Pedersen, F., Bajdich, M.
  2018; 8 (11): 10555–63
- **Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer.** *Nature communications*
  Chen, L. D., Bajdich, M., Martirez, J. M., Krauter, C. M., Gauthier, J. A., Carter, E. A., Luntz, A. C., Chan, K., Norskov, J. K.
  2018; 9 (1): 3202
- **Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer** *NATURE COMMUNICATIONS*
  Chen, L. D., Bajdich, M., Martirez, J. P., Krauter, C. M., Gauthier, J. A., Carter, E. A., Luntz, A. C., Chan, K., Norskov, J. K.
  2018; 9
- **Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene** *ACS CENTRAL SCIENCE*
  Kirk, C., Section, L., Siahrostami, S., Karamad, M., Bajdich, M., Voss, J., Norskov, J. K., Chan, K.
  2017; 3 (12): 1286–93
- **Formic Acid Dissociative Adsorption on NiO(111): Energetics and Structure of Adsorbed Formate** *JOURNAL OF PHYSICAL CHEMISTRY C*
  Zhao, W., Doyle, A. D., Morgan, S. E., Bajdich, M., Norskov, J. K., Campbell, C. T.
  2017; 121 (50): 28001–6
- **Identifying the Active Surfaces of Electrochemically Tuned LiCoO2 for Oxygen Evolution Reaction** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Lu, Z., Chen, G., Li, Y., Wang, H., Xie, J., Liao, L., Liu, C., Liu, Y., Wu, T., Li, Y., Luntz, A. C., Bajdich, M., Cui, et al
  2017; 139 (17): 6270-6276
- **Water Dissociative Adsorption on NiO(111): Energetics and Structure of the Hydroxylated Surface** *ACS CATALYSIS*
  Zhao, W., Bajdich, M., Carey, S., Vojvodic, A., Norskov, J. K., Campbell, C. T.
  2016; 6 (11): 7377-7384
- **Gold-supported cerium-doped NiOx catalysts for water oxidation** *NATURE ENERGY*
  Ng, J. W., Garcia-Melchor, M., Bajdich, M., Chakthranont, P., Kirk, C., Vojvodic, A., Jaramillo, T. F.
  2016; 1
- **Homogeneously dispersed multimetal oxygen-evolving catalysts.** *Science*
  Zhang, B., Zheng, X., Voznyy, O., Comin, R., Bajdich, M., García-Melchor, M., Han, L., Xu, J., Liu, M., Zheng, L., García de Arquer, F. P., Dinh, C. T., Fan, et al
  2016; 352 (6283): 333-337
- **Enhancing Catalytic CO Oxidation over Co3O4 Nanowires by Substituting Co2+ with Cu2+** *ACS CATALYSIS*
  Zhou, M., Cai, L., Bajdich, M., Garcia-Melchor, M., Li, H., He, J., Wilcox, J., Wu, W., Vojvodic, A., Zheng, X.
  2015; 5 (8): 4485-4491
- **Interface Controlled Oxidation States in Layered Cobalt Oxide Nanoislands on Gold** *ACS NANO*
  Walton, A. S., Fester, J., Bajdich, M., Arman, M. A., Osiecki, J., Knudsen, J., Vojvodic, A., Lauritsen, J. V.
  2015; 9 (3): 2445–53

- **Identification of Highly Active Fe Sites in (Ni,Fe)OOH for Electrocatalytic Water Splitting** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Friebel, D., Louie, M. W., Bajdich, M., Sanwald, K. E., Cai, Y., Wise, A. M., Cheng, M., Sokaras, D., Weng, T., Alonso-Mori, R., Davis, R. C., Bargar, J. R., Norskov, et al
  2015; 137 (3): 1305-1313
- **Theoretical investigation of the activity of cobalt oxides for the electrochemical oxidation of water.** *Journal of the American Chemical Society*
  Bajdich, M., García-Mota, M., Vojvodic, A., Nørskov, J. K., Bell, A. T.
  2013; 135 (36): 13521-13530
- **Theoretical investigation of oxygen evolution reaction in layered cobalt oxides**
  Bajdich, M., Garcia-Mota, M., Norskov, J. K., Bell, A. T.
  AMER CHEMICAL SOC.2013
- **Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides** *JOURNAL OF PHYSICAL CHEMISTRY C*
  Garcia-Mota, M., Bajdich, M., Viswanathan, V., Vojvodic, A., Bell, A. T., Norskov, J. K.
  2012; 116 (39): 21077-21082
- **Pfaffian pairing wave functions in electronic-structure quantum Monte Carlo simulations** *PHYSICAL REVIEW LETTERS*
  Bajdich, M., Mitas, L., Drobny, G., Wagner, L. K., Schmidt, K. E.
  2006; 96 (13): 130201