

Michal Bajdich

[ˈmaɪkəl ˈbaɪdɪtʃ]

Curriculum Vitae

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Appointments

2013–present	Stanford University and SLAC, SUNCAT Center for Catalysis Department of Chemical Engineering and SLAC National Accelerator Laboratory <i>Leads:</i> Thomas F. Jaramillo and Frank Abild-Pedersen
2021–present	SLAC Full Staff Scientist, Principal Investigator Liquid Sunlight Alliance (LiSA), CleanTech-FOA, SLAC-LDRD, Principal Investigator
2016–2021	SLAC Associate Staff Scientist
2013–2016	SLAC Project Scientist

2011–2013	UC Berkeley, Joint Center for Artificial Photosynthesis Department of Chemical & Biomolecular Engineering and Lawrence Berkeley National Laboratory <i>Co-Advisors:</i> Prof. Alex T. Bell and Prof. Jens K. Nørskov Postdoctoral Fellow
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2009–2011	Oak Ridge National Laboratory, Materials Theory Group <i>Advisors:</i> Dr. G. Malcolm Stocks and Dr. Fernando A. Reboreda Postdoctoral Fellow
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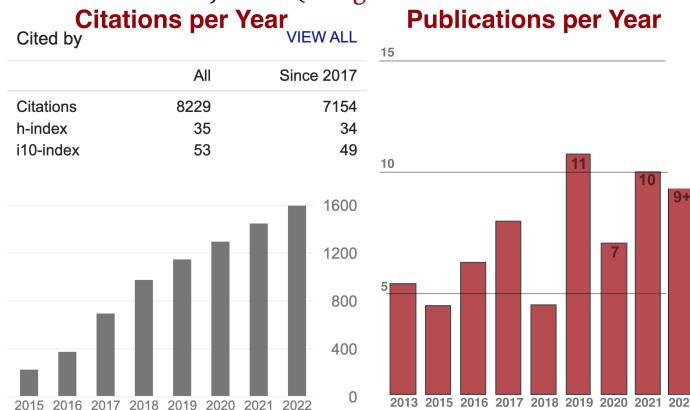
Education

2002–2007	North Carolina State University , Raleigh, NC, USA Ph.D, Physics <i>Advisor:</i> Prof. Lubos Mitas
2002–2004	M.Sc. en route, Multi-disciplinary major: Physics, Chemistry & Math

1996–2001	Comenius University , Bratislava, Slovakia M.Sc., Physics, specialization in Condensed Matter <i>Advisor:</i> Prof. Richard Hlubina
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Publications & Metric

Summary as of November 30, 2022 (Google Scholar & ORCID & Web of Science)



- (76) Rao, K. Kumar, Zhou, L., Lai Y., Richter, M., Li X., Lu Y., Yano J., Gregoire J. and **Bajdich, M.** Resolving Atomistic Structure and Oxygen Evolution Activity in Nickel Antimonates Journal of Materials Chemistry A (under review).
- ‘ (75) Baek, J.; Hossain, D.; Mukherjee, P.; Lee, J.; Winther, K.; Jiang, Y.; Chueh, W.; **Bajdich, M.**; Zheng, X. Synergistic Effects of Mixing and Strain in High Entropy Spinel Oxides for Oxygen Evolution Reaction. [10.21203/rs.3.rs-1879578/v1](https://doi.org/10.21203/rs.3.rs-1879578/v1) (preprint, under review).
- (74) Carlson, E. Z., Chueh, W., Mefford, J. T., **Bajdich, M.** Ab-Initio Energetics of Electrochemical Ion Insertion into Manganese Oxides. [10.26434/CHEMRXIV-2022-9GJ75](https://doi.org/10.26434/CHEMRXIV-2022-9GJ75) (preprint under review).
- (73) Koshy, D. M., Hossain, M. D., MASUDA, R., Yoda, Y., Gee, L. B., Abiose, K., Gong, H., Davis, R. C., Seto, M., Gallo, A., Hahn, C., **Bajdich, M.**, Bao, Z., Jaramillo, T. Investigation of the structure of atomically dispersed NiNx sites in Ni, N-doped carbon electrocatalysts by 61Ni Mössbauer Spectroscopy and Simulations. *J. Am. Chem. Soc.* 144, 47, 21741–21750i [10.1021/jacs.2c09825](https://doi.org/10.1021/jacs.2c09825) (2022)
- (72) Zhou, L., Peterson, E. A., Rao, K. K., Lu, Y., Li, X., Lai, Y., Bauers, S. R., Richter, M. H., Kan, K., Wang, Y., Newhouse, P. F., Yano, J., Neaton, J. B., **Bajdich, M.**, Gregoire, J. M. Addressing solar photochemistry durability with an amorphous nickel antimonate photoanode. *Cell Reports Physical Science*, 3(7), 100959. [10.1016/j.xcrp.2022.100959](https://doi.org/10.1016/j.xcrp.2022.100959) (2022).
- (71) Shi, X., Peng, H.-J., Hersbach, T. J. P., Jiang, Y., Zeng, Y., Baek, J., Winther, K. T., Sokaras, D., Zheng, X., **Bajdich, M.***, Efficient and Stable Acidic Water Oxidation Enabled by Low-Concentration, High-Valence Iridium Sites. ***corresponding author**, *ACS Energy Letters*, 23, 2228–2235r, [10.1021/ACSENERGYLETT.2C00578](https://doi.org/10.1021/ACSENERGYLETT.2C00578) (2022).
- (70) Comer, B. M., Li, J., Abild-Pedersen, F., **Bajdich, M.***, M., Winther, K. T. Unraveling Electronic Trends in O and OH Surface Adsorption in the MO₂Transition-Metal Oxide Series. *Journal of Physical Chemistry C*, 8. [10.1021/ACS.JPCC.2C02381](https://doi.org/10.1021/ACS.JPCC.2C02381), (2022).
- (69) Zhang, Y., Wan, G., Lewis, N. H. C., Mars, J., Bone, S., Steinrück, H. G., Lukatskaya, M. R., Weadock, N. J., **Bajdich, M.**, Borodin, O., Tokmakoff, A., Toney, M. F., & Maginn, E. J. Erratum: Water or Anion? Uncovering the Zn²⁺Solvation Environment in Mixed Zn(TFSI)₂and LiTFSI Water-in-Salt Electrolytes, *ACS Energy Letters*, 7, 5, 1694–1695 [10.1021/ACSENERGYLETT.2C00775](https://doi.org/10.1021/ACSENERGYLETT.2C00775) (2022).
- (68) Lunger, J. R., Lutz, N., Peng, J., **Bajdich, M.**, & Shao-Horn, Y. Cation-Dependent Multielectron Kinetics of Metal Oxide Splitting. *Chemistry of Materials*, [10.1021/ACS.CHEMMATER.2C00602](https://doi.org/10.1021/ACS.CHEMMATER.2C00602) (2022).
- (67) Rao, K. K., Lai, Y., Zhou, L., Haber, J. A., **Bajdich, M.***, Gregoire, J. M. Overcoming Hurdles in Oxygen Evolution Catalyst Discovery via Codesign. ***corresponding author**, *Chemistry of Materials*, [10.1021/ACS.CHEMMATER.1C04120](https://doi.org/10.1021/ACS.CHEMMATER.1C04120) (2022).
- (66) dos Santos, E. C., Araujo, R. B., Valter, M., Salazar-Alvarez, G., Johnsson, M., **Bajdich, M.**, Abild-Pedersen, F., Pettersson, L. G. M. Efficient Screening of Bi-Metallic Electrocatalysts for Glycerol Valorization. *Electrochimica Acta*, [10.1016/J.ELECTACTA.2021.139283](https://doi.org/10.1016/J.ELECTACTA.2021.139283) (2021).
- (65) Zhang, Y., Wan, G., Lewis, N. H. C., Mars, J., Bone, S. E., Steinrück, H.-G., Lukatskaya, M. R., Weadock, N. J., **Bajdich, M.**, Borodin, O., Tokmakoff, A., Toney, M. F., Maginn, E. J. (2021). Water or Anion? Uncovering the Zn²⁺ Solvation Environment in Mixed Zn(TFSI)₂ and LiTFSI Water-in-Salt Electrolytes. *ACS Energy Letters* [10.1021/ACSENERGYLETT.1C01624](https://doi.org/10.1021/ACSENERGYLETT.1C01624) (2021).

- (64) Nishimura, Y. F.; Peng, H.-J.; Nitopi, S.; **Bajdich, M.**; Wang, L.; Morales-Guio, C. G.; Abild-Pedersen, F.; Jaramillo, T. F.; Hahn, C. Guiding the Catalytic Properties of Copper for Electrochemical CO₂ Reduction by Metal Atom Decoration. *ACS Applied Materials & Interfaces* [10.1021/ACSAM.1C09128](https://doi.org/10.1021/ACSAM.1C09128) (2021).
- (63) Lee, K.; Flores, R. A.; Liu, Y.; Wang, B. Y.; Hikita, Y.; Sinclair, R.; **Bajdich, M.**; Hwang, H. Epitaxial Stabilization and Oxygen Evolution Reaction Activity of Metastable Columbite Iridium Oxide. *ACS Appl. Energy Mater.*, [10.1021/acsaem.0c02788](https://doi.org/10.1021/acsaem.0c02788) (2021).
- (62) Sanchez, J.; Stevens, M. B.; Young, R. A.; Gallo, A.; Zheng, M.; Ramos-Garcés, M. V.; Colon, J. L.; King, L. A.; **Bajdich, M.**; Jaramillo, T. F. An Active Oxygen Evolution Electrocatalyst Motif Created by Confining Transition Metal Cations within Layered Structures. *Adv. Energy Mater.*, [10.1002/aenm.202003545](https://doi.org/10.1002/aenm.202003545) (2021).
- (61) Landers, A. T.; Peng, H.; Koshy, D. M.; Lee, S. H.; Feaster, J. T.; Lin, J. C.; Beeman, J. W.; Higgins, D. C.; Yano, J.; Drisdell, W. S.; **Bajdich, M.**, et al. Dynamics and Hysteresis of Hydrogen Intercalation and Deintercalation in Palladium Electrodes: A Multimodal In Situ X-ray Diffraction, Coulometry, and Computational Study, [10.1021/acs.chemmater.1c00291](https://doi.org/10.1021/acs.chemmater.1c00291) (2021).
- (60) Zheng, X.; Tang, J.; Gallo, A.; Garrido Torres, Jose, A.; Yu, X.; Davis, R. C.; Reimer, J. A.; Vinson, J.; **Bajdich, M.***; Cui, Y. Origin of Enhanced Water Oxidation Activity in an Iridium Single Atom Catalyst., *corresponding author, *PNAS*, [10.1073/pnas.2101817118](https://doi.org/10.1073/pnas.2101817118) (2021).
- (59) Baeumer, C; Li, Jiang; Lu, Qiyang; **Bajdich, M.***; Nemsak, S.; Mefford, T.J.; Chueh, W. C.; Tuning surface composition and transformation pathways in atomically-flat LaNiO₃ thin films for enhanced water electrolysis, *corresponding author, *Nat. Mat.*, [10.1038/s41563-020-00877-1](https://doi.org/10.1038/s41563-020-00877-1) (2020).
- (58) Hubert, M. A.; Patel, Anjli, M.; Gallo, A.; Valle, E.; Ben-Naim, M.; Sanchez, J.; Liu, Y.; Dimosthenis, S.; Sinclair, R.; Nørsko;, J. K. . King, L **Bajdich, M.***, Jaramillo, T.F., Acidic Oxygen Evolution Reaction Activity-Stabilityrelationships in Ru-Based Pyrochlores, *corresponding author, *ACS Catal.*, [10.1021/acscatal.0c02252](https://doi.org/10.1021/acscatal.0c02252), (2020).
- (57) Peng, H.; Tang, M. T.; Liu, X.; Schlexer Lamoureux, P.; **Bajdich, M.**; Abild-Pedersen, F. The Role of Atomic Carbon in Directing Electrochemical CO(2)Reduction to Multicarbon Products., *Energy Environ. Sci.*, [10.1039/D0EE02826F](https://doi.org/10.1039/D0EE02826F) (2020).
- (56) Tang, M. T.; Peng, H.; Schlexer Lamoureux, P.; **Bajdich, M.**; Abild-Pedersen, F. From Electricity to Fuels: Descriptors for C1 Selectivity in Electrochemical CO₂ Reductionle. *Applied Catalysis B: Environmental*, [10.1016/j.apcatb.2020.119384](https://doi.org/10.1016/j.apcatb.2020.119384) ,(2020).
- (55) Flores, R. A.; Paolucci, C.; Winther, K. T.; Jain, A.; Garrido Torres, J. A.; Aykol, M.; Montoya, J. H.; Nørskov, J. K.; **Bajdich, M.***; Bligaard, T. Active Learning Accelerated Discovery of Stable Iridium-Oxide Polymorphs for the Oxygen Evolution Reaction., *corresponding author, *Chem. Mater.*, [10.1021/acs.chemmater.0c01894](https://doi.org/10.1021/acs.chemmater.0c01894), (2020).
- (54) Grewal, S.; Macedo Andrade, A.; Liu, Z.; Garrido Torres, J.; Nelson, A.; Kulkarni, A. R.; **Bajdich, M.***; Lee, M. H. Highly Active Bifunctional Oxygen Electrocatalytic Sites Realized in Ceria Functionalized Graphene. *corresponding author, *Advanced Sustainable Systems*, [10.1002/adsu.202000048](https://doi.org/10.1002/adsu.202000048), (2020).
- (53) Gauthier, J.; Chen, L. D.; **Bajdich, M.**; Chan, K. Implications of the Fractional Charge of Hydroxide at the Electrochemical Interface. *Phys. Chem. Chem. Phys.*, [10.1039/C9CP05952K](https://doi.org/10.1039/C9CP05952K), (2020).

- (52) Mefford, J. T.; Zhao, Z.; **Bajdich, M.***; Chueh, W. C. Interpreting Tafel Behavior of Consecutive Electrochemical Reactions through Combined Thermodynamic and Steady State Microkinetic Approaches, *corresponding author, *Energy Environ. Sci.*, [10.1039/C9EE02697E](https://doi.org/10.1039/C9EE02697E), (2020).
- (51) Zhou, D.; Cai, Z.; Bi, Y.; Tian, W.; Luo, M.; Zhang, Q.; Zhang, Q.; Xie, Q.; Wang, J.; Li, Y.; Kuang, Y.; Duan, X.; **Bajdich, M.**; Siahrostami, S.; Sun, X. Erratum to: Effects of Redox-Active Interlayer Anions on the Oxygen Evolution Reactivity of NiFe-Layered Double Hydroxide Nanosheets. *Nano Res.* 2019 131 2019, 13 (1), 292–292. [10.1007/S12274-019-2596-0](https://doi.org/10.1007/S12274-019-2596-0) (2020).
- (50) Gauthier, J. A.; Fields, M.; **Bajdich, M.**; Chen, L. D.; Sandberg, R. B.; Chan, K.; Nørskov, J. K. Facile Electron Transfer to CO₂ during Adsorption at the Metal|Solution Interface. *J. Phys. Chem. C*, [10.1021/acs.jpcc.9b10205](https://doi.org/10.1021/acs.jpcc.9b10205), (2019).
- (49) Strickler, A. L.; Flores, R. A.; King, L. A.; Nørskov, J. K.; **Bajdich, M.***; Jaramillo, T. F. Systematic Investigation of Iridium-Based Bimetallic Thin Film Catalysts for the Oxygen Evolution Reaction in Acidic Media, *corresponding author, *ACS Appl. Mater. Interfaces* [10.1021/acsm.9b13697](https://doi.org/10.1021/acsm.9b13697), (2019).
- (48) Schlexer Lamoureux, P.; Winther, K.; Garrido Torres, J. A.; Streibel, V.; Zhao, M.; **Bajdich, M.**; Abild-Pedersen, F.; Bligaard, T. Machine Learning for Computational Heterogeneous Catalysis. *ChemCatChem*, [10.1002/cctc.201900595](https://doi.org/10.1002/cctc.201900595), (2019).
- (47) Zhao, Wei-Wei; Bothra, P.; Lu, Z.; Li, Y.; Mei, L.-P.; Liu, K.; Zhao, Z.; Chen, G.; Back, S.; Siahrostami, S.; **Bajdich, M., ***; Cui, Y., Improved Oxygen Reduction Reaction Activity of Nanostructured CoS₂ through Electrochemical Tuning. *corresponding author, *ACS Appl. Energy Mater.* [10.1021/acs.9b01527](https://doi.org/10.1021/acs.9b01527), (2019).
- (46) Zhao, Z.; Schlexer Lamoureux, P.; Kulkarni, A.; **Bajdich, M.***, M. Trends in Oxygen Electrocatalysis of 3d-Layered (Oxy)(Hydro)Oxides., *corresponding author, *ChemCatChem*, [10.1002/cctc.201900846](https://doi.org/10.1002/cctc.201900846), (2019).
- (45) Winther, K. T.; Hoffmann, M. J.; Boes, J. R.; Mamun, O.; **Bajdich, M.**; Bligaard, T. Catalysis-Hub.Org, an Open Electronic Structure Database for Surface Reactions. *Sci. Data*, [10.1038/s41597-019-0081-y](https://doi.org/10.1038/s41597-019-0081-y) (2019).
- (44) Skafte, T.L; Guan, Z.; García-Melchor, M; **Bajdich, M.***; Chueh, W.; Graves, C; et.al; Selective High-Temperature CO₂ Electrolysis Enabled by Oxidized Carbon Intermediates., *corresponding author, *Nat. Energy*, [10.1038/s41560-019-0457-4](https://doi.org/10.1038/s41560-019-0457-4), (2019).
- (43) Patel, Anjli M.; Ringe, Stefan; Siahrostami, Samira; **Bajdich, M.**; Kulkarni, Ambarish R. and Nørskov, J.K.; Theoretical Approaches to Describing the Oxygen Reduction Reaction Activity of Single Atom Catalysts. *J. Phys. Chem. C.*, [10.1021/acs.jpcc.8b09430](https://doi.org/10.1021/acs.jpcc.8b09430) (2018).
- (42) Baker, J. G.; Schneider, J. R.; Garrido Torres, J. A.; Singh, J. A.; Mackus, A. J. M.; **Bajdich, M.**; Bent, S. F. The Role of Aluminum in Promoting Ni-Fe-OOH Electrocatalysts for the Oxygen Evolution Reaction. *ACS Appl. Energy Mater.* [10.1021/acs.9b00265](https://doi.org/10.1021/acs.9b00265) (2019).
- (41) 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.; et al. Stabilization of Reactive Co₄O₄ Cubane Oxygen-Evolution Catalysts within Porous Frameworks. *Proc. Natl. Acad. Sci. U. S. A.*, [10.1073/pnas.1815013116](https://doi.org/10.1073/pnas.1815013116), (2019).
- (40) Dickens, C.F; Montoya, J.; Kulkarni, A; **Bajdich, M.**; Nørskov, J.K.; An electronic structure descriptor for oxygen reactivity at metal and metal-oxide surfaces. *Surf. Sci.*, [10.1016/j.susc.2018.11.019](https://doi.org/10.1016/j.susc.2018.11.019) (2018).

- (39) Back, Seoin; Hansen, Martin; Torres, Jose ; Zhao, Zhenghang; Nørskov, J.K.; Siahrostami, Samira **Bajdich, M.***; Prediction of stable and active (oxy-hydro) oxide nanoislands on noble metal supports for electrochemical oxygen reduction reaction. ***corresponding author**, *ACS Appl. Mater. Interfaces*, [10.1021/acsami.8b15428](https://doi.org/10.1021/acsami.8b15428) (2018).
- (38) Sandberg, Robert; Hansen, Martin; Nørskov, J.K.; Abild-Pedersen, Frank; **Bajdich, M.***; Strongly Modified Scaling of CO Hydrogenation in Metal Supported TiO Nanostripes; ***corresponding author**, *ACS Catalysis*, [10.1021/acscatal.8b03327](https://doi.org/10.1021/acscatal.8b03327) (2018).
- (37) Chen L.D.*; **Bajdich, M.***; Martinez, J.M.; Krauter, C.M.; Gauthier, J.A.; Carter E.A.; Luntz, A.C., Chan, K., Nørskov, J.K.; Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. ***contributed equally**, *Nat. Comm.*, [10.1038/s41467-018-05511-y](https://doi.org/10.1038/s41467-018-05511-y) (2018).
- (36) Zhou, D.; Cai, Z.; Bi, Y.; **Bajdich, M.**; Siahrostami, S; Sun, X.; et al.; Effects of redox-active interlayer anions on the oxygen evolution reactivity of NiFe-layered double hydroxide nanosheets, *Nano Res.*, [10.1007/s12274-017-1750-9](https://doi.org/10.1007/s12274-017-1750-9) (2018).
- (35) Kirk, C.; Chen, L.; Siahrostami, S.; Karamad, M.; **Bajdich, M.**; Voss, J.; Nørskov, J.K.; Chan, K.; Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene, *ACS Cent. Sci.*, [10.1021/acscentsci.7b00442](https://doi.org/10.1021/acscentsci.7b00442) (2017).
- (34) Zhao, W.; Doyle, A.D.; Morgan, S.E.; **Bajdich, M.**; Nørskov, J. K., Campbell, Charles T.; Formic Acid Dissociative Adsorption on NiO(111): Energetics and Structure of Adsorbed Formate, *J. Phys. Chem. C.*, [10.1021/acs.jpcc.7b09405](https://doi.org/10.1021/acs.jpcc.7b09405) (2017).
- (33) Lu, Z.; Chen, G.; Li, Y.; **Bajdich, M.**, *; Cui, Y.; Identifying the Active Surfaces of Electrochemically Tuned LiCoO₂ for Oxygen Evolution Reaction, *J. Am. Chem. Soc.*, ***corresponding author**, [10.1021/jacs.7b02622](https://doi.org/10.1021/jacs.7b02622) (2017).
- (32) Doyle A.D; **Bajdich, M.**; Vojvodic, A; Theoretical Insights to Bulk Activity towards Oxygen Evolution in Oxyhydroxides, *Cat. Lett.*, [10.1007/s10562-017-2010-z](https://doi.org/10.1007/s10562-017-2010-z) (2017).
- (31) Fester, J.; García-Melchor, M.; Walton, A. S.; **Bajdich, M.**; Li, Z.; Lammich, L.; Vojvodic, A.; Lauritsen, J. V. ; Edge Reactivity and Water-Assisted Dissociation on Cobalt Oxide Nanoislands. *Nat. Comm.*, [10.1038/ncomms14169](https://doi.org/10.1038/ncomms14169) (2017).
- (30) Zhao, W.; **Bajdich, M.**; Carey, S; Vojvodic, A; Nørskov, J. K., Campbell, Charles T.; Water Dissociative Adsorption on NiO(111): Energetics and Structure of the Hydroxylated Surface, *ACS Catalysis*, [10.1021/acscatal.6b01997](https://doi.org/10.1021/acscatal.6b01997) (2016).
- (29) Siahrostami, S.; Tsai, C.; Karamad, M.; Koitz, R.; García-Melchor, M.; **Bajdich, M.**; Vojvodic, A.; Abild-Pedersen, F.; Nørskov, J. K.; Studt, F. Two-Dimensional Materials as Catalysts for Energy Conversion, *Catal. Lett.*, [10.1007/s10562-016-1837-z](https://doi.org/10.1007/s10562-016-1837-z) (2016).
- (28) Fester, J.; **Bajdich, M.**; Walton, A.S.; Sun, Z.; Plessow, P.N.; Vojvodic A; Lauritsen, J.V.; Comparative Analysis of Cobalt Oxide Nanoisland Stability on Three Related Noble Metal Surfaces: Au(111), Pt(111) and Ag(111), *Special Issue in Topics in Catalysis*, [10.1007/s11244-016-0708-6](https://doi.org/10.1007/s11244-016-0708-6) (2016).
- (27) Plessow, P.N.; **Bajdich, M.**; Greene, J.; Abild-Pedersen, F.; Trends in Thermodynamic Stability of Ultrathin Supported Oxide Films, *J. Phys. Chem. C*, [10.1021/acs.jpcc.6b01404](https://doi.org/10.1021/acs.jpcc.6b01404) (2016).
- (26) Zhang, B.; Zheng, X.; Voznyy, O.; Comin, R; **Bajdich, M.**; García-Melchor, M.; Vojvodic, A; Sargent, E.H.,*et.al.*, Homogeneously-Dispersed Multi-Metal Oxygen-Evolving Catalysts, *Science*, [10.1126/science.aaf1525](https://doi.org/10.1126/science.aaf1525) (2016).

- (25) Desmond Ng, J. W.; García-Melchor, M.; **Bajdich, M.**; Kirk, C.; Chakthranont, P.; Vojvodic, A.; Jaramillo, T. F., Gold-supported cerium-doped NiO_x catalysts for water oxidation, *Nature Energy*, [10.1038/NENERGY.2016.53](https://doi.org/10.1038/NENERGY.2016.53) (2016).
- (24) Zhou, M.; Cai, L.; **Bajdich, M.**; García-Melchor, M.; Li, H.; He, J.; Wilcox, J.; Wu, W.; Vojvodic, A.; Zheng, X. Enhancing Catalytic CO Oxidation over Co₃O₄ Nanowires by Substituting Co²⁺ with Cu²⁺. *ACS Catal.*, [10.1021/acscatal.5b00488](https://doi.org/10.1021/acscatal.5b00488) (2015).
- (23) Walton, A.S.; A, Fester, J.; **Bajdich, M.**; Arman, M. A.; Jacek Osiecki, J; Knudsen, J.; Vojvodic, A; Lauritsen, J.V.; Interface Controlled Oxidation States in Layered Cobalt Oxide Nano-Islands on Gold. *ACS Nano*, [10.1021/acsnano.5b00158](https://doi.org/10.1021/acsnano.5b00158) (2015).
- (22) **Bajdich, M.**; Nørskov, J. K.; Vojvodic, A; Surface Energetics of Alkaline-Earth Metal Oxides: Trends in Stability and Adsorption of Small Molecules. *Phys. Rev. B*, [10.1103/PhysRevB.91.155401](https://doi.org/10.1103/PhysRevB.91.155401) (2015).
- (21) Friebel, D.*; Louie, M.*; **Bajdich, M.***; Sanwald, K.E.; Cheng, Mu-Jeng; Cai, Y.; Sokaras,D; Alonso-Mori, R; Weng, Tsu-Chien; Davis, R; Wise, A. M.; Bargar, J.; Bell, A. T.; Lercher, J. A.; Nørskov, J. K.; Nilsson, A. Identification of highly active Fe sites in (Ni,Fe)OOH for electrocatalytic water. *J. Am. Chem. Soc.*, *contributed equally, [10.1021/ja511559d](https://doi.org/10.1021/ja511559d) (2015).
- (20) Hauser, A. W.; Gomes, J.; **Bajdich, M.**; Head-Gordon, M.; Bell, A. T. Subnanometer-Sized Pt/Sn Alloy Cluster Catalysts for the Dehydrogenation of Linear Alkanes. *Phys. Chem. Chem. Phys.*, [10.1039/C3CP53796J](https://doi.org/10.1039/C3CP53796J) (2013).
- (19) Friebel, D.; **Bajdich, M.**; Yeo, B. S.; Louie, M. W.; Miller, D. J.; Casalongue, H. S.; Mbuga, F.; Weng, T.-C.; Nordlund, D.; Sokaras, D.; Alonso-Mori, R.; Bell, A. T.; Nilsson, A. On the chemical state of Co oxide electrocatalysts during alkaline water splitting. *Phys. Chem. Chem. Phys.*, [10.1039/C3CP52981A](https://doi.org/10.1039/C3CP52981A) (2013).
- (18) **Bajdich, M.**; García-Mota, M.; Vojvodic, A.; Nørskov, J. K.; Bell, A. T. Theoretical Investigation of the Activity of Cobalt Oxides for the Electrochemical Oxidation of Water. *J. Am. Chem. Soc.*, [10.1021/ja405997s](https://doi.org/10.1021/ja405997s) (2013).
- (17) Guo, S.; **Bajdich, M.**; Mitas, L.; Reynolds, P. J. Study of dipole moments of LiSr and KRb molecules by quantum Monte Carlo methods. *Mol. Phys.*, [10.1080/00268976.2013.788741](https://doi.org/10.1080/00268976.2013.788741) (2013).
- (16) García-Mota, M.; **Bajdich, M.**; Viswanathan, V.; Vojvodic, A.; Bell, A. T.; Nørskov, J. K. Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides. *J. Phys. Chem. C*, [10.1021/jp306303y](https://doi.org/10.1021/jp306303y) (2012).
- (15) **Bajdich, M.**; Kent, P. R. C.; Kim, J.; Reboreda, F. A. Simple impurity embedded in a spherical jellium: Approximations of density functional theory compared to quantum Monte Carlo benchmarks. *Phys. Rev. B*, [10.1103/PhysRevB.84.075131](https://doi.org/10.1103/PhysRevB.84.075131) (2011).
- (14) **Bajdich, M.**; Tiago, M. L.; Hood, R. Q.; Kent, P. R. C.; Reboreda, F. A. Systematic Reduction of Sign Errors in Many-Body Calculations of Atoms and Molecules. *Phys. Rev. Lett.*, [10.1103/PhysRevLett.104.193001](https://doi.org/10.1103/PhysRevLett.104.193001) (2010).
- (13) **Bajdich, M.**; Reboreda, F. A.; Kent, P. R. C. Quantum Monte Carlo calculations of dihydrogen binding energetics on Ca cations: An assessment of errors in density functionals for weakly bonded systems. *Phys. Rev. B*, [10.1103/PhysRevB.82.081405](https://doi.org/10.1103/PhysRevB.82.081405) (2010).
- (12) **Bajdich, M.**; Mitas, L. Electronic Structure Quantum Monte Carlo. *Acta Phys. Slovaca*, 59, 81–168. [ISSN 0323-0465](https://doi.org/10.1023/A:10230465) (2009).

- (11) Wagner, L. K.; **Bajdich, M.**; Mitas, L. QWalk: A quantum Monte Carlo program for electronic structure. *J. Comp. Phys.*, [10.1016/j.jcp.2009.01.017](https://doi.org/10.1016/j.jcp.2009.01.017) (2009).
- (10) **Bajdich, M.**; Mitas, L.; Wagner, L. K.; Schmidt, K. E. Pfaffian pairing and backflow wavefunctions for electronic structure quantum Monte Carlo methods. *Phys. Rev. B*, [10.1103/PhysRevB.77.115112](https://doi.org/10.1103/PhysRevB.77.115112) (2008).
- (9) Esler, K. P.; Kim, J.; Ceperley, D. M.; Purwanto, W.; Walter, E. J.; Krakauer, H.; Zhang, S.; Kent, P. R. C.; Hennig, R. G.; Umrigar, C.; **Bajdich, M.**; Kolorenč, J.; Mitas, L.; Srinivasan, A. Quantum Monte Carlo algorithms for electronic structure at the petascale; the Endstation project. *J. Phys.: Conf. Ser.*, [10.1088/1742-6596/125/1/012057](https://doi.org/10.1088/1742-6596/125/1/012057) (2008).
- (8) **Bajdich, M.**; Mitas, L.; Drobný, G.; Wagner, L. K.; Schmidt, K. E. Pfaffian Pairing Wave Functions in Electronic-Structure Quantum Monte Carlo Simulations. *Phys. Rev. Lett.*, [10.1103/PhysRevLett.96.130201](https://doi.org/10.1103/PhysRevLett.96.130201) (2006).
- (7) **Bajdich, M.**; Mitas, L.; Drobný, G.; Wagner, L. K. Approximate and exact nodes of fermionic wavefunctions: Coordinate transformations and topologies. *Phys. Rev. B*, [10.1103/PhysRevB.72.075131](https://doi.org/10.1103/PhysRevB.72.075131) (2005).
- (6) Moško, M.; Vagner, P.; **Bajdich, M.**; Schäpers, T. Coherent "Metallic" Resistance and Medium Localization in a Disordered One-Dimensional Insulator. *Phys. Rev. Lett.*, [10.1103/PhysRevLett.91.136803](https://doi.org/10.1103/PhysRevLett.91.136803) (2003).
- (5) **Bajdich, M.**; Hlubina, R. Variational study of the stability of the Nagaoka state against single-spin flips in the two-dimensional t-t' Hubbard model. *Phys. Rev. B*, [10.1103/PhysRevB.63.233105](https://doi.org/10.1103/PhysRevB.63.233105) (2001).

Book Chapters and Conference Proceedings

- (4) **Bajdich, M.**; García-Mota, M.; Viswanathan, V.; Vojvodic, A.; Bell, A. T.; Nørskov, Theoretica Investigation of Oxygen Evolution Reaction in Layered Cobalt Oxides,Proceedings of Division of Energy and Fuels at 245th ACS National Meeting, *Energy & Fuels Preprints Volume 58 #1 Page: 218* (2013).
- (3) **Bajdich, M.**; Kolorenc, J., Mitas, L , Reynolds, P.J., Proceedings of the 22th workshop on computer simulation in condensed matter physics (CSP 2009), *Physics Procedia*, [10.1016/j.phpro.2010.01.199](https://doi.org/10.1016/j.phpro.2010.01.199) (2010).
- (2) Mitas, L and **Bajdich, M.**: Nodal properties of fermion wave functions, In Advances in Quantum Many-Body Theory, edited by J. Boronat et. al, *World Scientific*, vol.11, **ISBN: 978-981-277-987-8** (2008).
- (1) Mitas, L., Drobný, G., **Bajdich, M.**, L. K. Wagner: Investigation of nodes of fermionic wave functions, In Condensed Matter Theories, edited by J. W. Clark and R. Panoff, *Nova Science Publishers*, vol. 20, **ISBN: 1-59454-989-3** (2006).

Theses

- 2007 | *PhD. Thesis under supervision of L. Mitas: Generalized Pairing Wave Functions and Nodal Properties for Electronic Structure Quantum Monte Carlo*, North Carolina State University, Raleigh, NC.

2001	<i>Diploma Thesis under supervision of R. Hlubina:</i> Variational Study of the Stability of the Nagaoka State in the Two-Dimensional t-t' Hubbard Model, Comenius University, Bratislava, Slovakia (in Slovak).
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Honors and Invited Talks

2022	The 100 all-time list of Slovak scientists around the world
2009	Finalist, Eugene P. Wigner Fellowship , Oak Ridge National Laboratory
2001	Dean's List, Comenius University , Slovakia
1992-1994	Honorable Mention, International Physics Olympiad

2022	Catalysis and Modelling Symposium, Jens Nørskov's 70th birthday, DTU, Denmark
2019	University of California, Merced, Department of Materials Science, Merced, CA
2018	North Carolina State University, Department of Chemistry, Raleigh, NC
2016	University of Ostrava, Department of Physics, Czech Republic
2016	University of Nevada, Reno, Department of Chemistry, Reno, NV
2015	University of California at Santa Cruz, Department of Chemistry, CA
2015	University of Olomouc, Regional Centre of Adv. Tech. and Materials, Czech Republic
2009	University of Georgia, Recent Developments in Computer Simulation Studies in Condensed Matter Physics, Athens, GA
2005	Cornell University, Recent Developments in Electronic Structure Methods, Ithaca, NY
2005	Pacificchem, Honolulu, HI

Proposals and Grants

2015–present	Lead PI for NERSC DOE Supercomputing allocation for SUNCAT FWP
2021–present	Lead PI for NERSC DOE Supercomputing allocation for LiSA
2022	DOE-BES Field Work Proposal SUNCAT (23-25) , CoPI for Task 2 for Electrocatalysis, (applied)
2022	Stanford Precourt Institute for Energy and Stanford Hydrogen Initiative seed grant , CoPI with Tyler Mefford, (awarded, 80K, 1 year)
2022	SLAC-LDRD , single PI, <i>High precision heterogeneous catalysis by QMC method</i> (awarded, \$220K, 2 years)
2022	DOE-BES Clean Tech FOA , <i>Understanding interfacial phenomena for solar H2 production and N2 reduction</i> , Co-PI with Prof. Jaramillo (awarded, \$1.5M, 3 years)
2021	FOA pre-preposals for DE-FOA-0002481, DE-FOA-0002608, DE-FOA-0002676
2020	DOE-Hub The Liquid Sunlight Alliance (LiSA) (21-25) , CoPI on Photocatalyst stability and reconstruction (awarded, \$60M total)
2020	Collaborating Laboratory Scientist for the Office of Science Graduate Student Research (SCGSR) Program (awarded to Jaclyn Lunger, 6 mo. stay)
2019	DOE-BES Field Work Proposal SUNCAT (20-22), CoPI for Task 2 for Electrocatalysis (awarded, \$3.6M)
2018	SLAC LDRD co-PI w. Yasuyuki Hikita and Harold Y. Hwang (\$300K, 2 years, awarded)
2013	Joint Center for Artificial Photosynthesis (Contributed)
2008	DOE INCITE Supercomputing allocation (Contributed)

Teaching and Mentoring Experience

2022	LiSA 101 theory series
2019	Guest lecturer for CHEMENG142/242: Basic Principles of Heterogeneous Catalysis with Applications in Energy Trans., Stanford Engineering
1999–2001	Private Tutor for Math and Science College Entry Exam, Slovakia

	Students
2021–present	Evan Zoltan Carlson, PhD student, Stanford Mat. E. w. Will C. Chueh
2022	Michael Craig, Summer Phd student, Trinity College Dublin w. Max. Garcia-Melchor
2020	Xinjian Shi, PhD committee member, Stanford Mech. E. w. Xiaolin Zheng
2019	Alaina Strickler, PhD committee member, Stanford Chem E. w. T. F. Jaramillo
2020–2021	Jaclyn Rose Lunger, SCGSR scholar, Phd candidate at MIT w. Yang Shao-Horn
2018–2021	Anjli M. Pattel, Phd candidate w. Jens K. Nørskov
2018–2021	Raul F. Flores, Phd candidate w. Jens K. Nørskov
2017–2020	Joel Gauthier, Phd candidate w. Jens K. Nørskov
2017–2019	Robert Sandberg, Phd candidate w. Jens K. Nørskov
2016–2017	Andrew Doyle, Phd candidate w. Jens K. Nørskov
	Postdoctoral Associates
2022–present	Neha Bothra, Postdoctoral associate
2021–2022	Karun Kumar Rao, Postdoctoral associate
2021–present	Md Delowar Hossain, Postdoctoral associate
2020–present	Viswanath Pasumarthi, Postdoctoral associate
2019–2021	Jiang Li, Postdoctoral associate
2019–2021	Hongie Peng, Postdoctoral associate
2018–2019	Jose A. Garrido Torres, Postdoctoral associate
2018–2019	Philomena Schlexer, Postdoctoral associate
2017–2019	Zhenghang Zhao, Postdoctoral associate
2017–2018	Seoin Back, Postdoctoral associate
2017–2018	Pallavi Bothra, Postdoctoral associate

Press and News Releases

June 2022	Optimizing iridium sites Nature Catalysis Highlight
Apr. 2022	Team creates map for production of eco-friendly metals MIT NEWS
Aug. 2021	A new approach creates an exceptional single-atom catalyst for water splitting SLAC NEWS
Jan. 2021	Study shows tweaking one layer of atoms on a catalyst's surface can make it work better SLAC NEWS
Sep. 2019	New route to carbon-neutral fuels from carbon dioxide discovered Stanford News Bioengineer.org Phys.org
	Recycling Carbon Dioxide as Fuel Could Lead to Zero-Emissions Flight Travel Inverse
	Stanford Researchers Discover a New Route to Carbon-Neutral Fuels From Carbon Dioxide Scitechdaily.com
May 2019	Ceria catalyst could help produce carbon-neutral fuels PhysicsWorld.com
	Our PNAS article on molecular-like catalysts in water-splitting devices @SLAClab

Outreach and Professional Development

2020–present	Editor Modelling, Theory and Computational Catalysis (<i>Frontiers in Catalysis</i>)
2021	Co-organizer SUNCAT Session 2022
2019	Curator of SUNCAT's Twitter SUNCAT_Center , +2K followers
2018	Co-founder of Catalysts-hub.org , +5000 active users
2017–present	AICHE programming committee , Catalysis and Reaction Engineering Division-A20
2017–2018	Guest Editor for Special Issue of Materials, MDPI Journal: Nano-based Catalysts for Renewable Energy
2009–present	Reviewer for catalysis and chemistry journals orcid.org/0000-0003-1168-8616 (13) of ACS, <i>Nature</i> , <i>PNAS</i> , <i>APS</i> , <i>Elsevier</i> , <i>WILEY</i> , <i>Cell Press</i> , <i>Angewandte Chemie</i> ,
2003–present	American Physical Society member
2013–present	American Chemical Society and Materials Research Society member
2014–present	American Institute of Chemical Engineers member
2003–2005	International Student Ambassador North Carolina State University

References

Jens K. Nørskov, Technical University of Denmark
The Villum Kann Rasmussen Professor at the Department of Physics,
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Founder of the SUNCAT Center
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