

Michal Bajdich

[ˈmaɪkəl ˈbaɪdɪtʃ]

Curriculum Vitae

919-649-9318, bajdich@stanford.edu

Appointments

2013–present	Stanford University, SUNCAT Center Department of Chemical Engineering and SLAC National Accelerator Laboratory <i>Leads:</i> Thomas F. Jaramillo and Frank Abild-Pedersen (formerly Jens K. Nørskov)
2016–present	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
2009–2011	Oak Ridge National Laboratory, Materials Theory Group <i>Advisors:</i> Dr. G. Malcolm Stocks and Dr. Fernando A. Reboredo Postdoctoral Fellow

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

Publications

Summary as of November 16, 2020 ([Google Scholar](#) & [ORCID](#) & [Web of Science](#))



- (62) 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.* (under review).
- (61) 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.* (under review).
- (60) 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. A Combined in Situ X-Ray Diffraction and Computational Study Reveals New Insight into Hydrogen Intercalation and Deintercalation in Palladium Electrodes. (under review).
- (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.*, (accepted).
- (58) 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**, *Sci. Adv.*, (in revision).
- (57) Hubert, M. A.; Patel, Anjali, M.; Gallo, A.; Valle, E.; Ben-Naim, M.; Sanchez, J.; Liu, Y.; Dimos-thenis, 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).
- (56) 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., [10.26434/CHEMRXIV.11374785.V1](https://doi.org/10.26434/CHEMRXIV.11374785.V1), *Energy Environ. Sci.*, (accepted)
- (55) 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).
- (54) 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).
- (53) 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).
- (52) 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).
- (51) 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).
- (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/acssami.9b13697](https://doi.org/10.1021/acssami.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/acsaem.9b01527](https://doi.org/10.1021/acsaem.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) Skaftø, 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, Anjali 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/acsaem.9b00265](https://doi.org/10.1021/acsaem.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/acssami.8b15428](https://doi.org/10.1021/acssami.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, *Catal. 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 NiOx 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](#) (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](#) (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](#) (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](#) (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](#) (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](#) (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](#) (2012).
- (15) **Bajdich, M.**; Kent, P. R. C.; Kim, J.; Reboredo, 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](#) (2011).
- (14) **Bajdich, M.**; Tiago, M. L.; Hood, R. Q.; Kent, P. R. C.; Reboredo, F. A. Systematic Reduction of Sign Errors in Many-Body Calculations of Atoms and Molecules. *Phys. Rev. Lett.*, [10.1103/PhysRevLett.104.193001](#) (2010).
- (13) **Bajdich, M.**; Reboredo, 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](#) (2010).
- (12) **Bajdich, M.**; Mitas, L. Electronic Structure Quantum Monte Carlo. *Acta Phys. Slovaca*, 59, 81–168. [ISSN 0323-0465](#) (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](#) (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](#) (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](#) (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](#) (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](#) (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](#) (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](#) (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](#) (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 | *Diploma Thesis under supervision of R. Hlubina: Variational Study of the Stability of the Nagaoka State in the Two-Dimensional t-t' Hubbard Model*, Comenius University, Bratislava, Slovakia (in Slovak).

Honors and Invited Talks

- 2009 | Finalist, **Eugene P. Wigner Fellowship**, Oak Ridge National Laboratory
- 2001 | Dean's List, **Comenius University**, Slovakia
- 1992-1994 | Honorable Mention, **International Physics Olympiad**

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	Pacifichem, Honollu, HI

Proposals and Grands

2020	NERSC DOE Supercomputing allocation for 2021 (applied)
2020	The Liquid Sunlight Alliance (LiSA) (21-25), Co-authored task on Photocatalyst stability and reconstruction (awarded, 60M total)
2020	Collaborating Laboratory Scientist for the Office of Science Graduate Student Research (SCGSR) Program (awared to Jaclyn Lunger, 6 mo. stay)
2019	NERSC DOE Supercomputing allocation for 2020 (20M CPU hours, awarded)
2019	SLAC LDRD proposal (500K, 2years, not awarded)
2019	Field Work Proposal SUNCAT (20-22), Task for Electro-catalysis (awarded, 3.6M)
2018	NERSC DOE Supercomputing allocation for 2019 (12M CPU hours, awarded)
2018	SLAC LDRD proposal w. Yasuyuki Hikita (300K, 2years, awarded)
2017	NERSC DOE Supercomputing allocation for 2018 (20M CPU hours, awarded)
2017	DOE Early Career Award (preposal stage only)
2017	SLAC LDRD proposal w. Yasuyuki Hikita (not awarded)
2016	NERSC DOE Supercomputing allocation for 2018 (2.5M CPU hours, awarded)
2015	NERSC DOE Supercomputing allocation for 2017 (1M CPU hours, awarded)
2013	Joint Center for Artificial Photosynthesis (Catalysis/Internal contribution)
2008	DOE INCITE Supercomputing allocation (Contributed)

Teaching and Mentoring Experience

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

2020	Xinjian Xin, PhD committee member
2019	Alaina Strickler, PhD committee member
2020–present	Jaclyn Rose Lunger, SCGSR scholar, Phd candidate at MIT w. Yang Shao-Horn
2018–present	Anjli M. Pattel, Phd candidate w. Jens K. Nørskov
2018–present	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

2020–present	Viswanath Pasumarthi, Postdoctoral associate
2019–present	Jiang Li, Postdoctoral associate
2019–present	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

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

2019 | **Currator of SUNCAT's Twitter** [SUNCAT_Center](#), 1000 followers

2018 | **Co-founder of** [Catalysis-hub.org](#), 4000 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*,
Nature, *PNAS*, *APS*, *Elsevier*, *WILEY*, *Cell Press*, *Angewandte Chemie*,

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

Thomas F. Jaramillo, Stanford University

Director of the SUNCAT Center and the Associate Professor of Chemical Engineering,
jaramillo@stanford.edu, ph. 650-498-6879, 307 Shriram Center, Stanford, CA 94305

Jens K. Nørskov, Technical University of Denmark

The Villum Kann Rasmussen Professor at the Department of Physics,
Recipient of the 2018 Niels Bohr Medal in Physics,
Founder of the SUNCAT Center
jkno@dtu.dk, ph. +45-45-25-3818, 2800, Kongens Lyngby, Denmark.

Alexis T. Bell, University of California at Berkeley

The Dow Professor of Sustainable Chemistry at Dept. of Chemical and Biomolecular Engineering,
alexbell@berkeley.edu, ph. 510-642-1536, 107 Gilman Hall, Berkeley, CA 94720

Anders Nilsson, Stockholm University, Sweden,

Professor in Chemical Physics,
andersn@fysik.su.se, ph. +4-685-537-8637, Roslagstullsbacken 21, 106 91 Stockholm, Sweden

Charles Campbell, University of Washington,

Professor and B. Seymour Rabinovitch Endowed Chair in Chemistry,
charliec@uw.edu, ph. 206-616-6085, Box 351700, Seattle, WA 98195-1700

Lubos Mitas, North Carolina State University

Full Professor at Department of Physics and Astronomy,
lmitas@ncsu.edu, ph. 919-513-0406, 2401 Stinson Rd., Raleigh, NC 27695-8202