Nicholas Marcella, Ph.D.

EDUCATION

Stony Brook University, Dep. of Materials Science and Chemical Engineering Aug. 2021
Ph.D. in Materials Science and Engineering
Dissertation: *Decoding Reactive Structures in Bimetallic Catalysts*
Focus: *X-ray absorption spectroscopy, geometric and statistical modeling of atomic distributions, machine learning*

Stony Brook University, Dep. of Chemistry May 2016
B.Sc. in Chemistry

EXPERIENCE Google Scholar

University of Massachusetts Lowell Lowell, Massachusetts
Postdoctoral Research Associate Nov 2024 – Present

The University of Illinois Urbana-Champaign Urbana-Champaign, Illinois
Postdoctoral Researcher Sep 2021 – Oct 2024

- Designed and performed in situ XAS experiments (XANES, EXAFS, HERFD-XANES) at the NSLS-II ISS, QAS, XFM, PDF, and TES beamlines.
- Developed a Python-based nanomaterials simulation framework integrating machine-learned predictive models with XAS empirical data for model validation.
- Interpreted XAS data with machine learning and materials simulation to better understand simulants for molten salt nuclear reactors.
- Led successful proposals for securing experimental and computational resources to study nanocatalysts for sustainable chemical production.
- Improved Synchrotron characterization methods via integration of data science methods in collaboration with Department of Energy Scientists from the NSLSII and CFN.
- Authored 24 technical articles and presented research that advanced stakeholder objectives, resulting in publications in leading scientific journals (Nature, Physical Review B, Journal of the American Chemical Society) and presentations at international conferences.

Stony Brook University Stony Brook, New York
Graduate Student Sep 2016 – Aug 2021

- Developed, benchmarked, and deployed neural networks for analyzing experimental XAS data.
- Crafted successful research time proposals and performed extensive literature reviews.
- Led collaborative research efforts across more than 10 universities, 5 National Labs, and international partners, contributing to global advancements in nanocatalysis and sustainable energy technologies.

ADDITIONAL AFFILIATIONS

Stony Brook University Stony Brook, New York
Adjunct Associate Professor Sep 2024 – Present

Brookhaven National Laboratory Upton, New York
Research Associate Sep 2016 – Present

TEACHING EXPERIENCE

XAFS Short Course on X-ray Absorption Fine Structure: Application to Nanomaterials 2019 - 2024

Brookhaven National Laboratory
Instructor

The BNL Workshop on XAFS 2019
Catalysis Center for Energy Innovation, University of Delaware
Instructor

Department of Materials Science and Engineering 2017 - 2020
Stony Brook University
Teaching Assistant

SERVICE

Executive Board Member, NSLS-II UEC, Brookhaven National Lab	2023 - 2024
Reviewer, Chemical Communications, Royal Society of Chemistry	2023
Reviewer, Digital Discovery, Royal Society of Chemistry	2023
Reviewer, Communications Chemistry, Nature	2023
Reviewer, The Journal of Physical Chemistry, American Chemical Society	2022
Executive Board Member, Energy Frontiers Research Center News	2020-2021
Senator, Graduate Student Organization at Stony Brook University	2016-2021
President, American Chemical Society Student Chapter	2014-2016

AWARDS AND HONORS

Award of Honor 2018
Dep. of Materials Science and Chemical Engineering, Stony Brook University

CONFERENCE PRESENTATIONS AND SEMINARS

7th International Congress on Operando Spectroscopy. 2023
"Theory-guided operando experimentation via AI-accelerated ab initio molecular dynamics and XAFS"

18th International Conference on X-Ray Absorption and Fine Structure 2022
"Linking AI-accelerated ab Initio Molecular Dynamics with XAFS to Understand Dynamic Nanomaterials"

APS March Meeting 2018- 2021
American Physical Society

DOE "Yellow team" meeting 2020
Department of Energy
"Neural network assisted analysis of bimetallic nanocatalysts using X-ray absorption near edge structure spectroscopy"

IACS Student Seminar 2019
Institute for Advanced Computational Science, Stony Brook University
"Learning real nanoparticle structure from simple synthetic models"
Chemistry Department Seminar 2017

Argonne National Laboratory
"Recent work in the application of machine learning to the analysis of X-ray absorption data for nanoparticle characterization"

PUBLICATIONS

Peer-Reviewed Articles

1. **N. Marcella**, S. Lam, V. Bryantsev, S. Roy, A. I. Frenkel
   Neural network based analysis of multimodal bond distributions using their extended X-ray absorption fine structure spectra
   Phys. Rev. B 109, 104201 (2024)

2. K. Zheng, **N. Marcella**, A. L. Smith, A. I. Frenkel
   Decoding the pair distribution function of uranium in molten fluoride salts from X-ray absorption spectroscopy data by machine learning
   J. Phys. Chem. C 128, 7635-7642 (2024)

3. **N. Marcella**, J. S. Lim, A. M. Plonka, G. Yan, C. J. Owen, J. E. S. van der Hoven, A. C. Foucher, H. T. Ngan, S. B. Torrisi, N. S. Marinkovic, E. A. Stach, J. F. Weaver, J. Aizenberg, P. Sautet, B. Kozinsky, A. I. Frenkel
   Decoding Reactive Structures in Dilute Alloy Catalysts
   Nature Commun. 13, 832 (2022)
   Featured in Editor's Highlight, 2022

4. P. K. Routh,* **N. Marcella**,* A. I. Frenkel*
   Speciation of nanocatalysts by X-ray absorption spectroscopy assisted by machine learning
   J. Phys. Chem. C (Perspective) 127, 5653-5662 (2023)
   **Equal contribution authors*
   **corresponding author*

5. **N. Marcella***, Y. Liu, J. Timoshenko, E. Guan, M. Luneau, T. Shirman, A. M. Plonka, J. E. S. v. der Hoeven, J. Aizenberg, C. M. Friend, A. I. Frenkel
   Neural network assisted analysis of bimetallic nanocatalysts using X-ray absorption near edge structure spectroscopy
   Phys. Chem. Chem. Phys. 22, 18902-18910 (2020)
   **corresponding author*

6. Y. Liu, **N. Marcella**, J. Timoshenko, A. Halder, B. Yang, L. Kolipaka, M. J. Pellin, S. Seifert, S. Vajda, P. Liu, A. I. Frenkel
   Mapping XANES spectra on structural descriptors of copper oxide clusters using supervised machine learning
   J. Chem. Phys. 151, 164201 (2019) **JCP Editors' Pick**
   Oct. 28, 2019, Cover

7. P. K. Routh,* Y. Liu,* **N. Marcella**,* B. Kozinsky, A. I. Frenkel
   Latent representation learning for structural characterization of catalysts
   J. Phys. Chem Lett. (Perspective) 12, 2086-2094 (2021)
   **Equal contribution authors*

8. A. C. Foucher, **N. Marcella**, J. D. Lee, D. J. Rosen, R. Tappero, C. B. Murray, A. I. Frenkel, E. A. Stach
   Multimodal STEM and XAS characterization of bimetallic nanocatalysts
   Microsc. Microanal. 30 (Suppl. 1), 518-519 (2024)

9. T. Pechersky-Savich, B. Xu, M. Varenik, J. Li, E. Wachtel, D. Ehre, P. K. Routh, **N. Marcella**, A. I. Frenkel, Y. Qi, I. Lubomirsky
   Correlated Displacement of Dynamic Elastic Dipoles Produces Nonclassical Electrostriction in Zr-Doped Ceria
   Chem. Mater. 16, 7665-7675 (2024)

10. R. Shimogawa, **N. Marcella**, C. R. O'Connor, T.-S. Kim, C. Reece, I. Lubomirsky, A. I. Frenkel
    Iterative Bragg peak removal on X-ray absorption spectra with automatic intensity correction
    J, Synchrotron Radiat. 31. (2024)

11. J. D. Lee, J. B. Miller, A. V. Shneidman, L. Sun, J. F. Weaver, J. Aizenberg, J. Biener, J. A. Boscoboinik, A. C. Foucher, A. I. Frenkel, B. Kozinsky, **N. Marcella**, M M. Montemore, H. T. Ngan, C. R. O'Connor, P. Sautet, D. J. Stacchiola, E. A. Stach, R. J. Madix, C. M. Friend
Dilute alloys based on Au, Ag or Cu for efficient catalysis: from synthesis to active sites
Chemical Reviews 122, 8758-8808 (2022)

12. Y. Liu, M. Xie, **N. Marcella**, A. C. Foucher, E. A. Stach, M. R. Knecht, A. I. Frenkel
Z-contrast enhancement in Au-Pt nanocatalysts by correlative X-ray absorption spectroscopy and electron microscopy: Implications for composition determination
ACS Appl. Nano Mater. 5, 8775-8782 (2022)

13. S. Xiang, P. Huang, J. Li, Y. Liu, **N. Marcella**, P. K. Routh, G. Li, A. I. Frenkel
Solving the structure of "single-atom" catalysts using machine learning – assisted XANES analysis
Phys. Chem. Chem. Phys. 24, 5116-5124 (2022)

14. A. C. Foucher, **N. Marcella**, J. D. Lee, R. Tappero, C. B. Murray, A. I. Frenkel, E. A. Stach
Dynamical change of valence states in Ni-Cu nanoparticles during redox cycling
J. Phys. Chem. C 126, 1991-2002 (2022)

15. A. C. Foucher, **N. Marcella**, J. D. Lee, D. Rosen, R. Tappero, C. B. Murray, A. I. Frenkel, E. A. Stach
Structural and valence state modification of cobalt in CoPt nanocatalysts in redox conditions
ACS Nano 15, 20619-20632 (2021)

16. Y. Liu, A. Halder, S. Seifert, **N. Marcella**, S. Vajda, A.I. Frenkel.
Probing active sites in Cu_xPd_y cluster catalysts by machine – learning – assisted X-ray absorption spectroscopy
ACS Appl. Mater. Interf. 13, 53363-53374 (2021)

17. M. Luneau, E. Guan, W. Chen, A. C. Foucher, **N. Marcella**, T. Shirman, D. M. A. Verbart, J. Aizenberg, M. Aizenberg, E. A. Stach, R. J. Madix, A. I. Frenkel, C. M. Friend
Enhancing catalytic performance of dilute metal alloy nanomaterials
Commun. Chem. 3, 46 (2020)

18. E. Guan, A. C. Foucher, **N. Marcella**, T. Shirman, M. Luneau, A. R. Head, D. M. A. Verbart, J. Aizenberg, C. M. Friend, D. Stachhiola, E. A. Stach, A. I. Frenkel
New role of Pd hydride as a sensor of surface Pd distributions in Pd-Au catalysts
ChemCatChem 12, 717-721 (2020)

19. S. Lapp, Z. Duan, **N. Marcella**, L. Luo, A. Genc, J. Ringnalda, A. I. Frenkel, G. Henkelman, R. M. Crooks
Experimental and theoretical structural investigation of AuPt nanoparticles synthesized using a direct electrochemical method
J. Am. Chem. Soc. 140, 6249-6259 (2018)

20. H. Nguyen, N. Xiao, S. Daniels, **N. Marcella**, J. Timoshenko, A. I. Frenkel, D. Vlachos
Role of Lewis and Brønsted acidity in metal chloride catalysis in organic media: Reductive etherification of furanics
ACS Catalysis 7, 7363-7370 (2017)

Article preprints

21. C. J. Owen,* **N. Marcella**,* Y. Xie, J. Vandermause, A. I. Frenkel, R. G. Nuzzo, B. Kozinsky*
Unraveling the catalytic effect of hydrogen adsorption on Pt nanoparticle shape-change
arXiv:2306.00901 [cond-mat.mtrl-sci], 2023
**Equal contribution authors*
**Co-corresponding authors*

22. Chen H., Gulbinski J., Jain S, Tabassum T., Lee C., Dorneles de Mello M., **Marcella, N.** et al.
The Dynamic Catalytic Activity of Phosphorus-containing Catalysts.
ChemRxiv. 2023; doi:10.26434/chemrxiv-2023-g8cb5-v2

23. C. J. Owen,* **N. Marcella**,* C. R. O'Connor,* T.-S. Kim, R. Shimogawa, C. Y. Xie, R. G. Nuzzo, A. I. Frenkel, C. Reece, B. Kozinsky
Surface roughening in nanoparticle catalysts
arXiv preprint arXiv:2407.13643
**Equal contribution authors*

24. C. J. Owen, L. Russotto, C. R. O'Connor, **N. Marcella**, A. Johansson, A. Musaelian, B. Kozinsky
Atomistic evolution of active sites in multi-component heterogeneous catalysts
arXiv preprint arXiv:2407.13607

Articles in review

C. J. Owen,* **N. Marcella,*** Y. Xie, J. Vandermause, A. I. Frenkel, R. G. Nuzzo, B. Kozinsky*
Unraveling the catalytic effect of hydrogen adsorption on Pt nanoparticle shape-change
Nature Materials (in review)
**Equal contribution authors*
**Co-corresponding authors*

C. J. Owen,* **N. Marcella**,* C. R. O'Connor,* T.-S. Kim, R. Shimogawa, C. Y. Xie, R. G. Nuzzo, A. I. Frenkel, C. Reece, B. Kozinsky
Surface roughening in nanoparticle catalysts
Science (in review)
**Equal contribution authors*

Articles in preparation

N. Marcella, Y. Xiang, R. Shimogawa, Anatoly I Frenkel
Automated First Shell EXAFS Fits via Neural Networks
Manuscript in preparation *Equal contribution authors

N. Marcella,* C. J. Owen,* Y. Xie, J. Vandermause, B. Kozinsky, A. I. Frenkel, R. G. Nuzzo
Using EXAFS to Refine Machine-Learned Force Fields
Manuscript in preparation *Equal contribution authors