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*

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

RESEARCH EXPERIENCE Google Scholar

The University of Illinois Urbana-Champaign Urbana-Champaign, Illinois
Postdoctoral Researcher Sep 2021 – Present
Brookhaven National Laboratory Upton, New York
Research Associate Sep 2021 – Present

- Designed and performed operando XAFS experiments (XANES, EXAFS, HERFD-XANES) to track the evolution of adsorbate-catalyzed structural changes in supported Pt nanoparticles.
- Created a novel framework for validating machine-leaned force fields with experimental X-ray absorption data.
- Integrated convolutional and transformer neural networks with a synthetic training set, generated via genetic algorithms, alongside X-ray absorption data. This approach was applied to characterize simulants for molten salt nuclear reactors.
- Developed surrogate neural networks for speeding up theoretical X-ray absorption calculations by at least 100x.
- Created autoencoder neural networks for denoising experimental signal data.
- Screened millions of frames of molecular dynamics simulations for rare atomistic events and correlated them to macroscopic materials properties.
- Authored and co-authored impactful publications in high-ranking journals, like Nature, Physical Review B, and Journal of the American Chemical Society, and presented findings at prestigious international conferences, including the 7th International Congress on Operando Spectroscopy and the 18th International Conference on X-ray Absorption and Fine Structure.

SKILLS: Python | Pytorch | Tensorflow | Molecular Dynamics | High Throughput Analysis| Computational Clusters | Parallel Computing | Linux | Git | Project Management | Leadership | Communication

Stony Brook University Stony Brook, New York
Graduate Researcher Sep 2016 – Aug 2021
Brookhaven National Laboratory Upton, New York
Gradute Student Sep 2016 – Aug 2021

- Developed, benchmarked, and deployed neural networks for mapping experimental X-ray Absorption Fine Structure spectroscopy data onto structural and catalytic descriptors.
- Utilized evolutionary algorithm, Montecarlo, molecular dynamics, and DFT to explain experimental data.
- Discovered the nature of active metals within bimetallic dilute alloy catalysts with a multimodal approach that linked experiment, theory, and computation.
- 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.

SKILLS: Materials Science | Nanomaterials | Chemistry | XAS | EXAFS | XANES | XRD/Total Scattering | Beamline experiments | Machine Learning | Autoencoders | MLP | CNNS | Neural Networks | Atomistic Simulation | Mathematica | Python | Matlab | Bash |

TEACHING EXPERIENCE

XAFS Short Course on X-ray Absorption Fine Structure: Application to Nanomaterials — 2019 - 2023
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, 2023 - 2024
Reviewer, Chemical Communications, RSC, 2023
Reviewer, Digital Discovery, RSC, 2023
Reviewer, Communications Chemistry, Nature, 2023
Reviewer, The Journal of Physical Chemistry, ACS, 2022
Executive Board Member, Energy Frontiers Research Center Newsletter, 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

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)

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)

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
**Equal contribution authors*

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*
**Co-corresponding authors*

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)
**Co-corresponding authors*

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

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*

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)

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

Chem. Mater. 16, 7665-7675 (2024)

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)

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)

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)

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)

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)

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)

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)

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)

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)

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)

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

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*

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

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*

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