

Yuchen Niu

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Education

University of Maryland, College Park (UMD) 2017-2025
Ph.D., Physical Chemistry (Advisor: Janice Reutt-Robey)

University of Science and Technology of China (USTC), Hefei 2013-2017
B.S., Polymer Chemistry (Advisor: Hangxun Xu)

Research experience

University of Maryland, Department of Chemistry 01/2018 – Present
Research assistant (Advised by **Prof. Janice Reutt-Robey**)
Thesis: **Chemo-Structural Evolution of Lithium-Rich Surfaces under Driven Conditions**

- Chemo-structural evolution of $\text{LiCoO}_2(001)$ at varied $\mu(\text{O}_2)$ (Paper 1)
 - Gained new insights into $\text{LiCoO}_2(001)$ chemo-structural evolution at various O_2 chemical potentials with reported computational results
 - Reported first atomically resolved $\text{LiCoO}_2(001)$ images at room temperature, proposed an atomistic model revealing local $(\sqrt{7} \times \sqrt{7}) R19.1^\circ$ reconstruction
 - Developed a dry chemical method to prepare atomically flat stoichiometric $\text{Li}_{1.0}\text{CoO}_{2.0}(001)$
- Dynamical Li alloying and growth on $\text{Ag}(111)$ (Paper 9, in preparation)
 - Built and calibrated an *in situ* Li source to controllably deposit Li thin film
 - Comprehensive investigation of atomic structures of numerous surface $\text{Li}_x\text{Ag}(111)$ phases
 - Deciphered alloying dynamics and growth mode of Li on $\text{Ag}(111)$
- Phase-dependent oxidation of Li-Ag alloy surfaces (Paper 10, in preparation)
 - Revealed initial oxidation of $\text{Li}_x\text{Ag}(111)$ at atomic scale
 - Investigated oxidation behaviors of different surface $\text{Li}_x\text{Ag}(111)$ phases
- Work function characterization of nano phases on $\text{LiCoO}_2(001)$
 - Studied variation of valence band structure and the work function of nanoscale Co_3O_4 and Li-terminated LiCoO_2 surface phases via *in situ* XPS and UPS
 - Ongoing Kelvin probe force microscopy experiments to establish a definitive surface phase–work function relationship on $\text{LiCoO}_2(001)$
- Low-temperature cleave preparation of $\text{LiCoO}_2(104)$ and (001)
 - Designed and built a sample holder and an *in situ* cryogenic crystal cleaver

Collaborative Research, University of Maryland

2024 – present

Collaborator: **Prof. Chunsheng Wang** group

- Mechanistic study of interfaces of Li and Zn metal batteries (Paper 2, 6, 7, 11)
 - Performed extensive analysis of XPS and electrochemical data for a comprehensive understanding of interfaces– performance relationship
 - Applied the learned principle to significantly improve battery loading and lifetime

Collaborator: **Prof. Efrain E. Rodriguez** group

- Surface chemistry investigation of LuMnGaO_{4+x} (Paper 3)
 - Studied chemical variation of samples prepared by different routes via XPS

Collaborator: **Prof. Shenqiang Ren** group

- Multiferroism study of 2D CuInP_2S_6 and Fe_3GaTe_2 heterostructure (Paper 8)
 - Revealed nanoscale ferromagnetism and ferroelectricity of heterostructure via scanning probe microscopy (MFM, DART-PFM)

University of Science and Technology of China (USTC)

Research assistant (Advised by **Prof. Hangxun Xu**)

2015 – 2017

Topic: Nanomaterials for electrocatalysis and photocatalysis (Paper 4, 5)

Working Experience

Graduate assistant, Surface Analysis Center, University of Maryland

Director: **Dr. Karen Gaskell**

07/2023 – 01/2025

- 6 co-authored papers (Paper 2, 3, 6, 7, 8, 11)
- Performed repair and routine maintenance of all instruments (AFMs, XPSs, Raman)
- Developed ~100 protocols, designed and customized instruments to advance research in the fields of chemistry, physics, biology, engineering etc. from academia and industry
- Trained ~ 60 new users to independently operate AFMs and confocal Raman microscope

Teaching assistant, Department of Chemistry & Biochemistry, University of Maryland

- CHEM131 General Chemistry I Discussion 2023 Spring
- CHEM425 Instrumental Analysis Lab 2020 Fall, 2021 Spring, 2022 Spring, 2022 Fall
- CHEM132 General Chemistry I Lab 2018 Fall
- CHEM272 General Chemistry II Lab 2017 Fall, 2018 Spring

Publications

- (1) **Niu, Y.**; Gaskell, K. J.; Reutt-Robey, J. E. Chemo-Structural Evolution of LiCoO₂(001) under Varied Oxygen Chemical Potentials. *The Journal of Physical Chemistry C* **2026**, xxx, ASAP, <https://doi.org/10.1021/acs.jpcc.6c00163>.
- (2) Dong, D.; Heo, J.; Li, Z.; Zhang, X.; Xia, K.; Zhang, Q.; **Niu, Y.**; Wang, Z.; Hu, E.; Wang, C. Beyond Water-in-Salt: Dilute Aqueous Electrolytes with Cation-Associated Hydrophilic Anions. *Nature Nanotechnology* **2026**, Accepted.
- (3) Hong, S. J.; Li, T.; Mandujano, H. C.; Manjón-Sanz, A.; Liou, S.-C.; **Niu, Y.**; Rodriguez, E. E. Reversible structural and colorimetric transitions in LuMnGaO₄ upon oxygen uptake and release. *Dalton Trans.* **2025**, 54, 13431–13442, <http://doi.org/10.1039/d5dt00798d>.
- (4) Wang, L.; Wan, Y.; Ding, Y.; **Niu, Y.**; Xiong, Y.; Wu, X.; Xu, H. Photocatalytic Oxygen Evolution from Low-Bandgap Conjugated Microporous Polymer Nanosheets: A Combined First-Principles Calculation and Experimental Study. *Nanoscale* **2017**, 9, 4090–4096, <https://doi.org/10.1039/c7nr00534b>.
- (5) Ding, Y.; **Niu, Y.**; Yang, J.; Ma, L.; Liu, J.; Xiong, Y.; Xu, H. A Metal-Amino Acid Complex-Derived Bifunctional Oxygen Electrocatalyst for Rechargeable Zinc–Air Batteries. *Small* **2016**, 12, 5414–5421, <https://doi.org/10.1002/smll.201602247>.

Under Review

- (6) Li, Z.; **Niu, Y.**; Dong, D.; Zhao, C.; Wang, T.; Chen, Y.; Li, P.; Zhang, W.; Chen, F.; Liu, Y.; Li, A.; Wang, C. Critical Aspects of Cycling Stability in Lithium-Metal Batteries, Revise and resubmit at *Science*, 2026.
- (7) Zhang, W.; Liu, Y.; Wan, H.; Wang, Z.; Liu, Y.; Song, Y.; **Niu, Y.**; Albertus, P.; Hu, L.; Wang, C. Interface Engineering Enables High Loading in All-Solid-State Batteries, Revise and resubmit at *Nature Nanotechnology*, 2026.
- (8) Wang, Z.; Hu, Y.; Fang, Z.; Wang, Y.; Yan, P.; Sun, J.; Lopez, M.; Stadel, R.; **Niu, Y.**; Little, J.; Yan, Q.; Chen, P.; Gong, C.; Bennett, J.; Gu, G.; Li, Q.; Chen, Z.; Woehl, T.; Rodriguez, E.; Liu, K.; Ren, S. Chiral Multiferroic Heterostructures, Revise and resubmit at *Nano Letters*, 2026.

In Preparation

- (9) **Niu, Y.**; Reutt-Robey, J. E. Dynamical Li Alloying and Growth on Ag(111), (Adapted from doctoral dissertation).
- (10) **Niu, Y.**; Reutt-Robey, J. E. Phase-Dependent Oxidation of Li-Ag Alloy Surfaces, (Adapted from doctoral dissertation).
- (11) Li, P.; **Niu, Y.**; Wang, C. Li battery paper, (Under PI review).

Presentations

ACS Fall 2025 (Oral)	2025
AVS 70th International Symposium and Exhibition (Oral)	2024
NC20: Celebrating 20 Years of the Maryland NanoCenter (Best Poster)	2024

Kratos XPS Workshop (Invited Talk)	2024
AVS Mid-Atlantic Chapter DC Regional Meeting (Poster)	2024
95th ACS Colloid and Surface Science Symposium (Oral)	2021

Skills

Experimental: UHV technologies, UHV instrument design, STM/STS, AFM (KPFM, MFM, PFM, AM-FM AFM, EC-AFM), XPS, UPS, Raman, LEED, Ar plasma etching, SEM, XRD, TGA

Software: CasaXPS, Gwyddion, ImageJ, LEEDpat, LabVIEW, Materials Studio, Origin, Matlab, Python, ChemDraw, SolidWorks

Honors and Awards

Best Poster Award, NC20, UMD	2024
Jacob K. Goldhaber Travel Grant, UMD	2024
Dorothy M. and Earl S. Hoffman Travel Grant, AVS	2024
Dean's Fellowship for Summer Research, UMD	2018
Dean's Fellowship for First Year, UMD	2017