

Muhammad Mominur Rahman

Weinberg Distinguished Staff Fellow, Oak Ridge National Laboratory

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Education

- **Ph.D. in chemistry (August 2016 - May 2021)**
Virginia Tech, USA; Supervisor: Prof. Feng Lin
- **M.S. in applied chemistry and chemical engineering (2016)**
University of Dhaka, Bangladesh; Supervisor: Prof. Sayed Md. Shamsuddin
- **B.S. in applied chemistry and chemical engineering (2014)**
University of Dhaka, Bangladesh

Professional experience

- Weinberg Distinguished Staff Fellow 2024, Oak Ridge National Laboratory
- Chemistry research associate (August 2021 – December 2023; worked in DOE Battery500 Consortium), Brookhaven National Laboratory
- Graduate research assistant (August 2016 - May 2021), Virginia Tech

Honors and awards

- Weinberg Distinguished Staff Fellowship 2024, Oak Ridge National Laboratory
- Electrochemical Society Battery Division Student Research Award, 2021
- Chemistry Graduate Research Award, Virginia Tech, 2020
- Graduate School Doctoral Assistantship Award, Department of Chemistry, Virginia Tech, Spring 2019
- Finalist for the Graduate Student of the Year Award, Virginia Tech, 2020
- Dean's Award, Faculty of Engineering and Technology, University of Dhaka, 2014
- Dr. Aminul Haque-Atiya Haque Memorial Gold Medal, Department of Applied Chemistry and Chemical Engineering, University of Dhaka, 2014
- Tokyo Mitsubishi UFJ Foundation Scholarship, 2013
- Dutch Bangla Bank Foundation Scholarship, 2011-2015
- Participant in JENESYS 2015, Tokyo, Japan
- Dr. Shahidullah Scholarship, Shahidullah Hall, University of Dhaka, 2014

Scholarly output

Scientific articles

- (27) **Rahman, M. M.**; Tan, S.; Yang, Y.; Zhong, H.; Ghose, S.; Waluyo, I.; Hunt, A.; Ma, L.; Yang, X.-Q.; Hu, E. An inorganic-rich but LiF-free interphase for fast charging and long cycle life lithium metal batteries. *Nat. Commun.* 2023, 14 (1), 8414.
- (26) **Rahman, M. M.**; Hu, E. Electron Delocalization Enables Sulfone-based Single-solvent Electrolyte for Lithium Metal Batteries. *Angew. Chem. Int. Ed.* 2023, e202311051.

- (25) **Rahman, M. M.**; Xia, K.; Yang, X.-Q.; Ariyoshi, K.; Hu, E. Asymmetric lithium extraction and insertion in high voltage spinel at fast rate. *Nano Lett.* 2023, 23 (15), 7135-7142.
- (24) **Rahman, M. M. (co-corresponding author)**; Lin, F. Reports from the Frontier-Strategies to design stable layered oxide cathode for Na-ion batteries. *Electrochem. Soc. Interface* 2022, 31 (4) (invited).
- (23) **Rahman, M. M.**; McGuigan, S.; Li, S.; Gao, L.; Hou, D.; Yang, Z.; Xu, Z.; Lee, S.-J.; Sun, C.-J.; Liu, J.; Huang, X.; Xiao, X.; Chu, Y.; Sainio, S.; Nordlund, D.; Kong, X.; Liu, Y.; Lin, F. Chemical Modulation of Local Transition Metal Environment Enables Reversible Oxygen Redox in Mn-Based Layered Cathodes. *ACS Energy Lett.* 2021, 2882–2890.
- (22) **Rahman, M. M.**; Lin, F. Oxygen Redox Chemistry in Rechargeable Li-Ion and Na-Ion Batteries. *Matter* 2021, 4 (2), 490–527.
- (21) **Rahman, M. M.**; Chen, W.-Y.; Mu, L.; Xu, Z.; Jiang, Z.; Liu, Y.; Li, M.; Bai, X.; Lin, F., Defect and structural evolution under high energy ion irradiation informs battery materials design for extreme environments. *Nat. Commun.* 2020, 11 (1), 4548.
- (20) **Rahman, M. M.**; Mao, J.; Kan, W. H.; Sun, C.-J.; Li, L.; Zhang, Y.; Avdeev, M.; Du, X.-W.; Lin, F. An Ordered P2/P3 Composite Layered Oxide Cathode with Long Cycle Life in Sodium-Ion Batteries. *ACS Mater. Lett.* 2019, 1 (5), 573–581 (one of the most downloaded papers from 2019 and 2020).
- (19) **Rahman, M. M.**; Zhang, Y.; Xia, S.; Kan, W. H.; Avdeev, M.; Mu, L.; Sokaras, D.; Kroll, T.; Du, X. W.; Nordlund, D.; et al. Surface Characterization of Li-Substituted Compositionally Heterogeneous $\text{NaLi}_{0.045}\text{Cu}_{0.185}\text{Fe}_{0.265}\text{Mn}_{0.505}\text{O}_2$ Sodium-Ion Cathode Material. *J. Phys. Chem. C* 2019, 123 (18), 11428–11435.
- (18) **Rahman, M. M.**; Xu, Y.; Cheng, H.; Shi, Q.; Kou, R.; Mu, L.; Liu, Q.; Xia, S.; Xiao, X.; Sun, C.-J.; et al. Empowering Multicomponent Cathode Materials for Sodium Ion Batteries by Exploring Three-Dimensional Compositional Heterogeneities. *Energy Environ. Sci.* 2018, 11 (9), 2496–2508.
- (17) Lu, D.; Li, R.; **Rahman, M. M.**; Lv, L.; Yang, S.; Huang, Y.; Sun, C.; Zhang, S.; Zhang, H.; Zhang, J.; Xiao, X.; Deng, T.; Fan, L.; Chen, L.; Hu, E.; Wang, C.; Fan, X. Ligand channel enabled ultra-fast Li-ion conduction. *Nature* **2023**, accepted.
- (16) Xu, X.; Li, X.-L.; **Rahman, M. M.**; Bao, J.; Luo, R.-J.; Ma, C.; Du, C.-Y.; Zeng, J.; Mei, Z.; Qian, Z. Promoting reversibility of layered potassium cathode through interstitial doping. *Chem. Eng. J.* 2023, 477, 147021.
- (15) Tan, S.; **Rahman, M. M.**; Wu, Z.; Liu, H.; Wang, S.; Ghose, S.; Zhong, H.; Waluyo, I.; Hunt, A.; Liu, P.; Yang, X.-Q.; Hu, E. Structural and Interphasial

- Stabilities of Sulfurized Polyacrylonitrile (SPAN) Cathode. **ACS Energy Lett.** 2023, 8 (6), 2496-2504.
- (14) Zhang, Y.; Kuai, C.; Hu, A.; Ma, L.; Tan, S.; Hwang, I.; Mu, L.; **Rahman, M. M.**; Sun, C. J.; Li, L.; Hu, E.; Lin, F. Mechanistic Insights into the Interplay between Ion Intercalation and Water Electrolysis in Aqueous Batteries. **ACS Appl. Mater. Interfaces** 2022, 14 (10), 12130–12139.
- (13) Spence, S. L.; Hu, A.; Jiang, M.; Xu, Z.; Yang, Z.; **Rahman, M. M.**; Li, L.; Chu, Y. S.; Xiao, X.; Huang, X.; Lin, F. Mapping Lattice Distortions in LiNi_{0.5}Mn_{1.5}O₄ Cathode Materials. **ACS Energy Lett.** 2022, 7 (2), 690–695.
- (12) Mu, L.; Zhang, J.; Xu, Y.; Wei, C.; **Rahman, M. M.**; Nordlund, D.; Liu, Y.; Lin, F. Resolving Charge Distribution for Compositionally Heterogeneous Battery Cathode Materials. **Nano Lett.** 2022, 22 (3), 1278–1286.
- (11) Zheng, X.; Xu, Z.; Li, S.; Zhang, Y.; Zhang, J.; Kuai, C.; Tao, L.; **Rahman, M. M.**; Zhang, Y.; Lee, S. J.; Sun, C. J.; Li, L.; Hu, W.; Nordlund, D.; Liu, J.; Liu, Y.; Lin, F. Reversible Mn/Cr Dual Redox in Cation-Disordered Li-Excess Cathode Materials for Stable Lithium Ion Batteries. **Acta Mater.** 2021, 212, 116935.
- (10) Yang, Z.; Mu, L.; Hou, D.; **Rahman, M. M.**; Xu, Z.; Liu, J.; Nordlund, D.; Sun, C.; Xiao, X.; Lin, F. Probing Dopant Redistribution, Phase Propagation, and Local Chemical Changes in the Synthesis of Layered Oxide Battery Cathodes. **Adv. Energy Mater.** 2020, 2002719.
- (9) Xu, Z.; Jiang, Z.; Kuai, C.; Xu, R.; Qin, C.; Zhang, Y.; **Rahman, M. M.**; Wei, C.; Nordlund, D.; Sun, C. J.; et al. Charge Distribution Guided by Grain Crystallographic Orientations in Polycrystalline Battery Materials. **Nat. Commun.** 2020, 11 (1).
- (8) Liu, T.; Du, Z.; Wu, X.; **Rahman, M. M.**; Nordlund, D.; Zhao, K.; Schulz, M. D.; Lin, F.; Wood, D. L.; Belharouak, I. Bulk and Surface Structural Changes in High Nickel Cathodes Subjected to Fast Charging Conditions. **Chem. Commun.** 2020, 56 (51), 6973–6976.
- (7) Wu, X.; Liu, T.; Bai, Y.; Feng, X.; **Rahman, M. M.**; Sun, C. J.; Lin, F.; Zhao, K.; Du, Z. Effects of Solvent Formulations in Electrolytes on Fast Charging of Li-Ion Cells. **Electrochim. Acta** 2020, 353, 136453.
- (6) Mu, L.; Zhang, R.; Kan, W. H.; Zhang, Y.; Li, L.; Kuai, C.; Zydlewski, B.; **Rahman, M. M.**; Sun, C. J.; Sainio, S.; et al. Dopant Distribution in Co-Free High-Energy Layered Cathode Materials. **Chem. Mater.** 2019, 31 (23), 9769–9776.
- (5) Mu, L.; Hou, Q.; Yang, Z.; Zhang, Y.; **Rahman, M. M.**; Kautz, D. J.; Sun, E.; Du, X.-W.; Du, Y.; Nordlund, D.; et al. Water-Processable P₂-Na_{0.67}Ni_{0.22}Cu_{0.11}Mn_{0.56}Ti_{0.11}O₂ Cathode Material for Sodium Ion Batteries. **J. Electrochem. Soc.** 2019, 166 (2), A251–A257.

- (4) Steiner, J. D.; Cheng, H.; Walsh, J.; Zhang, Y.; Zydlewski, B.; Mu, L.; Xu, Z.; **Rahman, M. M.**; Sun, H.; Michel, F. M.; et al. Targeted Surface Doping with Reversible Local Environment Improves Oxygen Stability at the Electrochemical Interfaces of Nickel-Rich Cathode Materials. **ACS Appl. Mater. Interfaces** 2019, 11 (41).
- (3) Mu, L.; **Rahman, M. M.**; Zhang, Y.; Feng, X.; Du, X.-W.; Nordlund, D.; Lin, F. Surface Transformation by a “Cocktail” Solvent Enables Stable Cathode Materials for Sodium Ion Batteries. **J. Mater. Chem. A** 2018, 6 (6), 2758–2766.
- (2) Steiner, J. D.; Mu, L.; Walsh, J.; **Rahman, M. M.**; Zydlewski, B.; Michel, F. M.; Xin, H. L.; Nordlund, D.; Lin, F. Accelerated Evolution of Surface Chemistry Determined by Temperature and Cycling History in Nickel-Rich Layered Cathode Materials. **ACS Appl. Mater. Interfaces** 2018, 10 (28), 23842–23850.
- (1) Xu, Z.; **Rahman, M. M.**; Mu, L.; Liu, Y.; Lin, F. Chemomechanical Behaviors of Layered Cathode Materials in Alkali Metal Ion Batteries. **J. Mater. Chem. A** 2018, 6 (44), 21859–21884.

Book chapter

- (1) **Rahman, M. M.**; Lin, F. Surface Chemistry of Alkali-Ion Battery Cathode Materials. In Encyclopedia of Inorganic and Bioinorganic Chemistry; Wiley, 2019; pp 1–23.

Disclosure of invention

- (2) Nanocomposite cathodes for sodium-ion batteries, Inventors: Feng Lin, **Muhammad Mominur Rahman** VTIP 19-006.
- (1) High entropy multi-transition metal cathodes for sodium-ion batteries, Inventors: Feng Lin, **Muhammad Mominur Rahman** VTIP 19-007.

Funding proposal (led the technical writing of the proposals)

- (2) Lin, F. Improving the Selectivity of Electrochemical Ammonia Synthesis through Defect Engineering in Vanadium Nitride Nanocatalysts: A Collaborative Project between Virginia Tech and Howard University. ICTAS Diversity Inclusion Seed Investment Award 2019 (funded).
- (1) Lin, F. Li-Ion Batteries for Applications at Extreme Temperatures: An Exploratory Study. Dean’s Discovery Fund, College of Science, Virginia Tech 2020 (funded).

DOE user facility proposals

- (5) Hu, E.; Xiao, X.; **Rahman, M. M.** Understanding the Chemomechanical Evolution of Battery Electrodes in Solid State Li Metal Batteries. NSLS-II 2023 (active).

- (4) **Rahman, M. M.**; Mu, L.; Sokaras, D.; Liu, Y.; Lin, F. Exploring the Influence of Nano/Mesoscale Distribution of Transition Metals Towards Chemomechanical Stability and Electrochemical Performance of Layered Transition Metal Oxide Cathodes for Alkali Metal Ion Batteries, SSRL 2018.
- (3) **Rahman, M. M.**; Lin, F. Exploring the Influence of Elemental Distribution at the Primary Particle Level Towards Chemomechanical Stability and Electrochemical Performance of Layered Transition Metal Oxide Cathodes for Sodium-Ion Batteries. National Synchrotron Light Source II 2018.
- (2) **Rahman, M. M.**; Lin, F. Dopants Stabilized Layered Oxide Cathodes with Enhanced Structural Stability for Sodium- Ion Batteries. Advanced Photon Source 2019.
- (1) **Rahman, M. M.**; Sun, C.-J.; Lin, F. Enhancing the Electrochemical Stability of Layered Oxide Cathodes by Controlled Crystal Defects Formation. Advanced Photon Source 2020.

Oral presentations

- (8) **Rahman, M. M.** Electrolyte Additive and Solvent Design for Li-metal Batteries. Frances S. Sterrett Environmental Symposium, ACS Long Island subsection, 2023 (**invited**).
- (7) **Rahman, M. M.** Electrolyte Additive and Solvent Design for Li-metal Batteries. NLS-II Lunchtime Seminar, Brookhaven National Laboratory, 2023 (**invited**).
- (6) **Rahman, M. M.**; Wang, Q.; Ge, M.; Lee, W.-K.; Yang, X.-Q.; Xiao, X.; Hu, E. Observation and Mitigation of Beam Damage Effects on the in Situ Experiment of Li-Ion Battery Cathodes: A Transmission X-Ray Microscopy Study. ECS Meet. Abstr. 2022, MA2022-02 (3), 234.
- (5) **Rahman, M. M.** (corresponding author); Lin, F. (Battery Division Student Research Award Address Sponsored by Mercedes-Benz Research & Development) Elucidating the Surface-to-Bulk Redox Chemistry and Design Principles of Stable Layered Cathode Materials. ECS October 12, 2021 (**invited**).
- (4) **Rahman, M. M.**; Lin, F (presenting author). Oxygen redox chemistry in Na-ion batteries. ACS Spring, 2021 (**invited**).
- (3) **Rahman, M. M.**; Lin, F. Multi-Site Redox Activities in Chemically Complex Sodium Layered Oxide Cathode Materials. Meet. Abstr. 2019, MA2019-01 (2), 139–139.
- (2) **Rahman, M. M.**; Lin, F. Three-Dimensional Compositional and Charge Heterogeneities in Sodium Layered Oxide Cathode Materials. Meet. Abstr. 2019, MA2019-01 (4), 469–469.

- (1) Steiner, J.; Walsh, J.; **Rahman, M. M.**; Zydlewski, B.; Mu, L.; Nordlund, D.; Xin, H.; Lin, F. Dynamics of Surface Metal-Oxygen Chemical Environments in Nickel-Rich Layered Cathode Materials. Abstr. Pap. Am. Chem. Soc. 2018, 255.

Poster presentations

- (4) **Rahman, M. M.**; Ariyoshi, K.; Hu, E. Rate Dependent Dynamic Phase Separation Behavior of Ordered-LiNi_{0.5}Mn_{1.5}O₄. IBA Meet. 2023 (**won 3rd place in the daily poster sessions**).
- (3) **Rahman, M. M.**; Chen, W.-Y.; Bai, X.; Lin, F. Defects and Structural Evolution in Layered Oxide Battery Cathodes under Extreme Conditions. Abstr. Pap. Am. Chem. Soc. 2020 (**selected for Sci-Mix**).
- (2) **Rahman, M. M.**; Lin, F. Sodium Layered Oxide Cathode Materials with Multisite Redox Centers. Virginia Energy Storage Convers. Workshop 2020.
- (1) Mu, L.; **Rahman, M. M.**; Lin, F. Transition Metal Triggered Electrochemical Interphases in Sodium-Ion Batteries. Meet. Abstr. 2017, MA2017-02 (1), 98–98.

Media release

- Engineered battery chemistry for fast charging capabilities. Link: <https://www.bnl.gov/newsroom/news.php?a=121622>
- SSRL science highlights: Empowering Multicomponent Cathode Materials for Sodium-Ion Batteries by Exploring Three-Dimensional Compositional Heterogeneities. Link: <https://www-ssrl.slac.stanford.edu/content/science/highlight/2018-08-31/empowering-multicomponent-cathode-materials-sodium-ion-batteries>
- Media release: XMUM Publication in Top Journal, Energy & Environmental Science (EES), with an Impact Factor of 30.067. Link: <http://www.xmu.edu.my/2018/0928/c18050a353395/page.html>
- Media release: Prof. Feng Lin published in Energy & Environmental Science. Link: <https://chem.vt.edu/about-us/news/2018-07-03-lin.html>
- Media release: Spring 2019 GSDA Awards Announced. Link: <https://chem.vt.edu/about-us/news/2019-01-16-gsda-awards.html>
- Media release: Chemistry professor's research shocking the battery field. Link: <https://augustafreepress.com/chemistry-professors-research-shocking-the-battery-field/>
- Media release: Chemistry professor's research shocking the battery field. Link: <https://twitter.com/doescience/status/1063159707655790592>
- Media release: Graduate Student Muhammad Mominur Rahman Published in Nature Communications. Link: <https://chem.vt.edu/about-us/news/2020-09-11-rahman.html>
- Media release: New Research on Battery Materials Published in Nature Communications. Link: <https://mse.vt.edu/About/mse-news-update/new-research-on-battery-materials-published-in-nature-communicat.html>

Experience and skills

Research experience and skills

- Coprecipitation synthesis, solid state synthesis, and molten salt synthesis of metal oxide cathode materials with layered, spinel and rocksalt structures.
- Synthesis of carbon based anodes for Li-ion and Na-ion batteries.
- Electrolyte design for Li-metal and Li-S batteries.
- Experience in conducting synchrotron experiments at NSLS II Brookhaven National Laboratory, SLAC National Accelerator Laboratory and TEM experiments under ion irradiation at Argonne National Laboratory.
- *Electrochemical characterization*: galvanostatic battery cycling, galvanostatic intermittent titration technique, potentiostatic intermittent titration technique, cyclic voltammetry, linear sweep voltammetry, electrochemical impedance spectroscopy etc.
- *Materials characterization*: XRD with Rietveld refinement, ICP-OES, SEM, TEM, EDS.
- *X-ray characterization*: X-ray diffraction-pair distribution function, soft X-ray absorption spectroscopy, hard X-ray absorption spectroscopy, transmission X-ray microscopy, X-ray photoelectron spectroscopy, X-ray raman spectroscopy.

Teaching experience

- Taught General Chemistry laboratory courses (Gen Chem 1045 and 1046) from Fall 2016 to Spring 2018 and Spring 2021.
- Provided lecture help in General Chemistry Courses (Gen Chem 1035 and 1036) from Spring 2017 to Spring 2018.
- Provided guest lecture in the course titled “Fundamental of Batteries” taught by Prof. Feng Lin.

Mentorship experience

- (1) Kangxuan Xia, graduate student, Materials Science and Engineering, Stony Brook University
- (2) Dawei Xia, graduate student, Chemistry, Virginia Tech
- (3) Qianli Shi, Chemical Engineering undergrad, Virginia Tech (class of 2018; is a coauthor in a paper published in Energy & Environmental Science)
- (4) Cameron Bissel, Chemistry undergrad, Virginia Tech (class of 2021)
- (5) Hao Li, Chemical Engineering undergrad, Virginia Tech (class of 2019)
- (6) Robert Wear, Materials Science and Engineering, Virginia Tech (class of 2019)
- (7) Nick Schmal, Materials Science and Engineering, Virginia Tech (class of 2019)
- (8) Alli Whittle, Materials Science and Engineering, Virginia Tech (class of 2019)
- (9) Bitna Choi, Materials Science and Engineering, Virginia Tech (class of 2019)
- (10) Scott Mcguigan, Chemistry undergrad, Virginia Tech (class of 2019; is a coauthor in a paper published in ACS Energy Letters)
- (11) Elaine Sun, high school student
- (12) Eleonore Marcano, high school research program intern, Brookhaven National Laboratory

Outreach activities

- Delivered Virginia Tech Energy Storage Research to students at Effingham County High School, Savannah, GA as part of the Integrated Science Day, Virginia Tech
- Delivered multiple invited talks to ACS Student Chapter, University of Dhaka, Bangladesh to encourage potential graduate students to consider Virginia Tech and USA as their higher study destination
- Mentored high school students for the High School Research Program at Brookhaven National Laboratory

Professional involvement

- Member, ECS Student Chapter, Virginia Tech (2018-2021)
- Reviewed articles for Joule, Matter, Materials Today, Energy Storage Materials, Small, Small Methods, ACS Applied Materials and Interfaces, Journal of the Electrochemical Society, Chemistry-A European Journal, and Journal of Alloys and Compounds
- Reviewed multiple funding proposal for DOE SBIR projects