

# Junseok Moon (문준석)

311–315, 1, Gwanak-ro, Gwanak-gu, Seoul, Republic of Korea  
 Cell Phone: +82-10-3635-9735 • E-Mail: jsmoon0311@snu.ac.kr

## Education

**Seoul National University (SNU), Seoul, Republic of Korea**

Ph.D. candidate in Chemical and Biological Engineering

Supervisor: Prof. Taeghwan Hyeon

Mar. 2022

– Aug. 2026 (expected)

**Seoul National University (SNU), Seoul, Republic of Korea**


B.S. in Chemical and Biological Engineering

Mar. 2017 – Feb. 2022

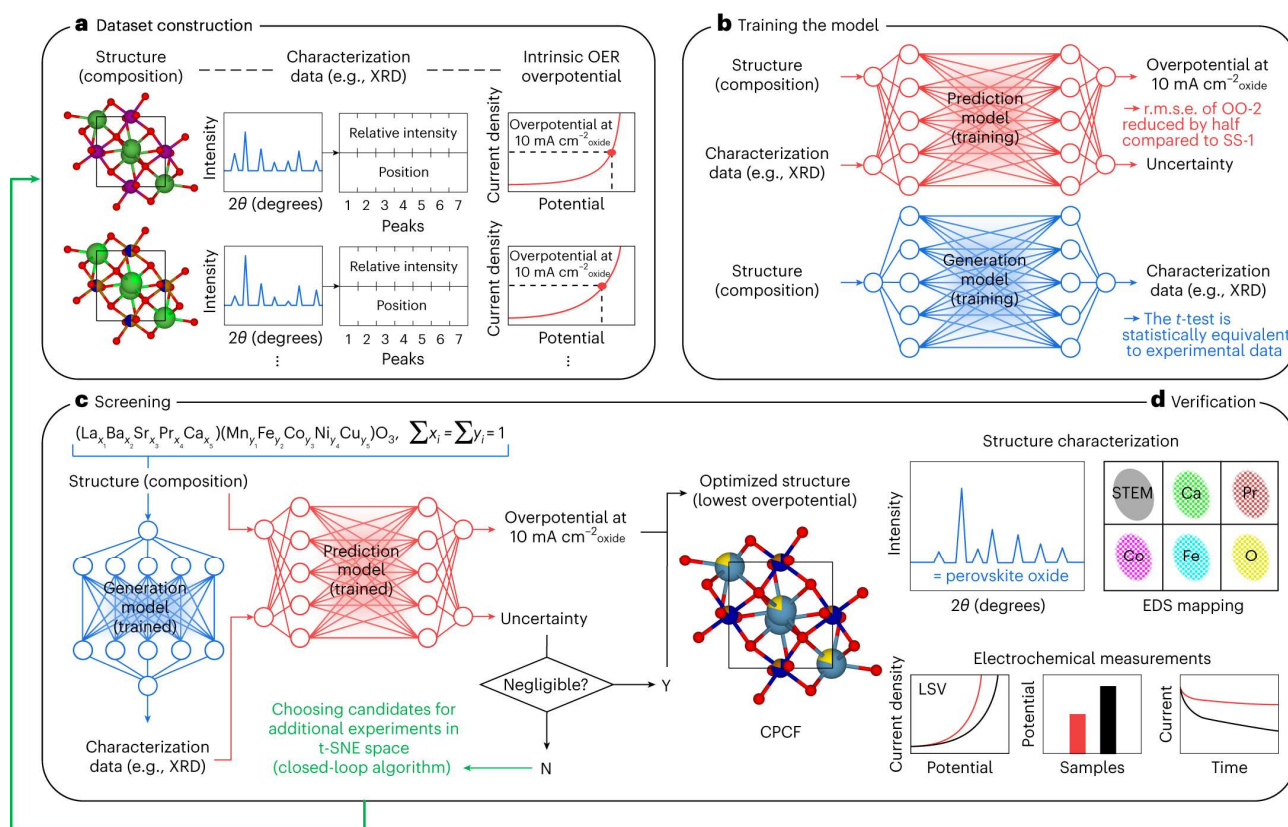
## Representative Publication

**Moon, J.<sup>#</sup>**, Beker, W., Siek, M., Kim, J., Lee, H. S., Hyeon, T.\*<sup>,</sup> Grzybowski, B. A.\*

Active learning guides discovery of a champion four-metal perovskite oxide for oxygen evolution electrocatalysis.

*Nat. Mater.* **23**, 108-115 (2024). 

*(Submission in the first year of Ph.D. course, publication in the second year as the sole first author)*



This work is a *tour de force* demonstration how appropriately “instructed” AI can enable discovery at the forefront of materials science – remarkably, in the absence of large quantities of input data. The model we develop not only reproduces several non-obvious and actively studied experimental trends but also identifies a composition of a perovskite oxide electrocatalyst exhibiting an intrinsic overpotential at  $10 \text{ mA cm}^{-2}_{\text{oxide}}$  of 391 mV for electrochemical oxygen evolution in alkaline condition, which is among the lowest known of four-metal perovskite oxides. Junseok Moon (the sole first author) designed the workflow and algorithm, collected and analyzed data and performed the materials characterization and electrochemical measurements.

## Honors and Awards

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Silver Prize, The 32 <sup>nd</sup> Samsung Humantech Paper Awards, Samsung Electronics	2026
Excellent Paper Presentation Award, Spring Meeting, The Korean Society of Industrial and Engineering Chemistry	2025
Bronze Prize, The 31 <sup>st</sup> Samsung Humantech Paper Awards, Samsung Electronics	2025
Excellent Paper Presentation Award, Spring Meeting, The Korean Society of Industrial and Engineering Chemistry	2024
Presidential Science Scholarship for Graduate Students, President of the Republic of Korea; <i>40 Students among Ph.D Candidates in All Science and Engineering Fields in the Republic of Korea</i>	2024
Silver Prize, The 29 <sup>th</sup> Samsung Humantech Paper Awards, Samsung Electronics	2023
Grand Prize, The 10 <sup>th</sup> Chemical Engineering Process Design Competition, The Korean Institute of Chemical Engineers	2021
Presidential Science Scholarship for Undergraduate Students, President of the Republic of Korea	2017

## Research Interests

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### Machine Learning-Driven Materials Discovery for Energy Applications

Design of Active Learning Workflow and Algorithm  
Programming and Analyzing Machine Learning Models  
Training Dataset Generation by Experimentation and Theoretical Calculation  
Materials Synthesis, Structural and Electrochemical Characterizations  
Machine Learning Model Training and Screening  
Statistical Analysis for Model Predictions  
Experimental Validation of the Best-Performing Materials Predicted by Machine Learning  
Applications in Catalysis, Batteries, Biomedicine, and Beyond!

## Research Expertise

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### Machine Learning-Driven Materials Discovery

Design of Closed-loop Protocol and Active Learning Strategy  
Programming Deep Learning Models (Graph Neural Networks, Computer Vision, Natural Language Processing)  
Programming and Analyzing Models (Bayesian Optimization, Model Uncertainty Quantification)  
Generation of Model Training Datasets via Own Experimentation  
Explainable Artificial Intelligence (Shapley Additive Explanations, Feature Importance Analysis)  
Visualization of Exploring Chemical Spaces (t-distributed Stochastic Neighbor Embedding)

### Synthesis of Nanomaterials

Synthesis of Metal Oxides (High-Entropy Oxides, Multi-Metallic Perovskite, Spinel, and Rutile Oxides)  
Synthesis of Metal Alloys (Platinum-Group-Metal Alloys, High-Entropy Alloys)  
Synthesis of Single-Atom Catalysts (M–N–C Materials, Single-Atom Catalysts on Oxides)  
Synthesis of Metal-Organic-Frameworks

Controlling Defect of Nanomaterials (Metal Oxides, M–N–C Materials)

Surface and Bulk Modification of Nanomaterials (Facet Control, Composition and Phase Tuning)

### **Structural Characterization of Nanomaterials**

Analyzing Geometric and Electronic Structure of Nanomaterials

Discovering Structure-Property Relationships using Machine Learning and Statistics

Synchrotron-based X-ray Characterization Techniques

### **Electrochemical Characterization of Nanomaterials**

Catalytic Performance Measurements for Electrochemical Reactions (Activity, Stability)

Setting-Up Half-Cell and Single-Cell Devices

Analysis of Material Structure Changes Before and After Reactions

### **Applications of Nanomaterials in Energy Applications**

Electrochemical and Photochemical Catalysis (Oxygen Evolution, Hydrogen Evolution, Oxygen Reduction)

Batteries (Electrolytes for All-Solid-State Batteries, Cathode Materials for Lithium-Ion Batteries)

Biomedicine (mRNA Delivery using Nanoparticles)

## **Technical Skills (Self-Operating)**

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### **Machine Learning**

Design of Materials Discovery Protocols

Python Programming (Keras, PyTorch)

Model Construction and Analysis (Graph Neural Network, Convolutional Neural Network, Recurrent Neural Network, Reinforcement Learning, Text Mining Random Forest, Gaussian)

### **Synthesis and Structural Characterization**

Air-free Schlenk Techniques for Nanomaterial Synthesis

Glove Box Techniques for Nanomaterial Synthesis

Transmission Electron Microscope (JEOL JEM-2020, JEM-2100)

Synchrotron X-ray Absorption Spectroscopy

UV-Vis Spectrophotometer

BET analysis (Micromeritics)

X-ray Photoelectron Spectroscopy

Powder X-Ray Diffraction (Rigaku D/Max-3C)

### **Electrochemical Characterization**






Setting-Up Devices (PGSTAT302N)

Catalyst Ink Preparation and Electrolyte Purification

Catalytic Activity and Stability Measurements (Oxygen Evolution, Hydrogen Evolution, Oxygen Reduction)



## **Publications (Research Articles)**

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1. **Moon, J.**<sup>#</sup>, Yoo, S.<sup>#</sup>, Shim, J., Heo, S., Kim, J. H., Bootharaju, M. S., Lee, K.-S., Ryu, J., Sung, Y.-E., Hyeon, T.\*  
Cross-material catalyst discovery via deep learning  
*Nat. Mater. Accepted* (2026).
2. Ahn, H., Ji, H., **Moon, J.**, Bootharaju, M. S.\*, Hyeon, T.\*, Lee, B.-H.\*  
Spinel/Rock Salt Core/Shell High-Entropy Oxides for Selective CO<sub>2</sub> Hydrogenation  
*ACS Energy Lett.* **11**, 245-269 (2026). 
3. Wang, K., Lee, W., Zhang, R., Wang, Z., Zhang, Y., **Moon, J.**, Shin, D., Bootharaju, M. S., Du, J., Chen, A., Back, S.\*, Hyeon, T.\*, Song, S.\*, Zhang, H.\*, Wang, X.\*  
Spinel/Rock Salt Core/Shell High-Entropy Oxides for Selective CO<sub>2</sub> Hydrogenation  
*J. Am. Chem. Soc.* **147**, 35304-35312 (2025). 
4. Yoo, S., Lee, C. W., Lee, K., Moon, J., Ji, H., **Moon, J.**, Shin, D., Kweon, Y., Lee, J., Kim, K., Lee, J., Deng, G., Lee, B.-H., Ryu, J., Kim, M.\*, Bootharaju, M. S.\*, Hyeon, T.\*  
Low-temperature atomic metal deposition for an efficient dual-site incorporated photocatalyst  
*Adv. Mater.* **37**, e06402 (2025). 
5. **Moon, J.**<sup>#</sup>, Beker, W., Siek, M., Kim, J., Lee, H. S., Hyeon, T.\*, Grzybowski, B. A.\*  
Active learning guides discovery of a champion four-metal perovskite oxide for oxygen evolution electrocatalysis.  
*Nat. Mater.* **23**, 108-115 (2024). 
6. Jung, E., Kim, S. J., Kim, J., Koo, S., Lee, J., Kim, S. Y., Paldi, V. K., Ko, W., **Moon, J.**, Lee, K. S., Cho, S. P., Kim, D.\*, Yu, S. H.\*, Sung, Y. E.\*, Hyeon, T.\*  
Oxygen-plasma-treated Fe–N–C catalysts with dual binding sites for enhanced electrocatalytic polysulfide conversion in lithium–sulfur batteries.  
*ACS Energy Lett.* **7**, 2646-2653 (2022). 

## **Publications (Books)**

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1. Shin, H., Song, H., **Moon, J.**, Shin, I., Yang, Y., Yang, S.  
2024 Science Trends (English Edition).  
*Independently Published* (2024). 
2. Shin, H., **Moon, J.**, Kim, T., Ha, S., Lee, J., Cho, H., Shin, W., Yoon, M., Yang, S., Cho, M., Kim, M.  
2022 Science Trends.  
*PUBPLE* (2022). 

## **Manuscripts in Preparation (1<sup>st</sup> Author Publications, Manuscript Submission Plan within Two Months)**

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1. **Junseok Moon et al.**  
“Superionic conductor discovery for all-solid-state batteries via machine learning.”
2. **Junseok Moon et al.**  
“New architecture design for anode-free solid-state batteries based on machine learning.”
3. **Junseok Moon et al.**  
“Champion catalyst discovery for proton exchange membrane water electrolysis using deep learning.”

4. **Junseok Moon et al.**  
“Design of superior fuel cell catalysts via deep learning.”
5. **Junseok Moon et al.**  
“Deep learning-driven nanoparticle design for mRNA delivery.”

### **Teaching Experiences**

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| Teaching Assistant, Osaka Kongo International School (in English)   | 2023        |
| Teaching Assistant, Engineering Camp from Society of Engineering Network and Service, Seoul National University | 2017 – 2019 |

### **International Conference Presentations**

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1. **Moon, J.**; Hyeon, T. “Discovery of a best-performing perovskite oxide electrocatalyst for oxygen evolution reaction via closed-loop machine learning” Poster presentation in Inorganic Materials, 2025 KSIEC Spring Meeting and International Symposium, Jeju, Republic of Korea (2025).
2. **Moon, J.**; Hyeon, T. “Deep Learning-Driven Discovery of a Best-Performing Perovskite Oxide for Water Oxidation” Poster presentation, 2025 MRS Spring Meeting and Exhibit, Seattle, WA, USA (2025).
3. **Moon, J.**; Hyeon, T. “Machine learning-driven discovery of a best-performing oxide electrocatalyst for oxygen evolution reaction” Poster presentation in Inorganic Materials, 2024 KSIEC Spring Meeting and International Symposium, Busan, Republic of Korea (2024).