

# Junseok Moon (문 준 석)

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

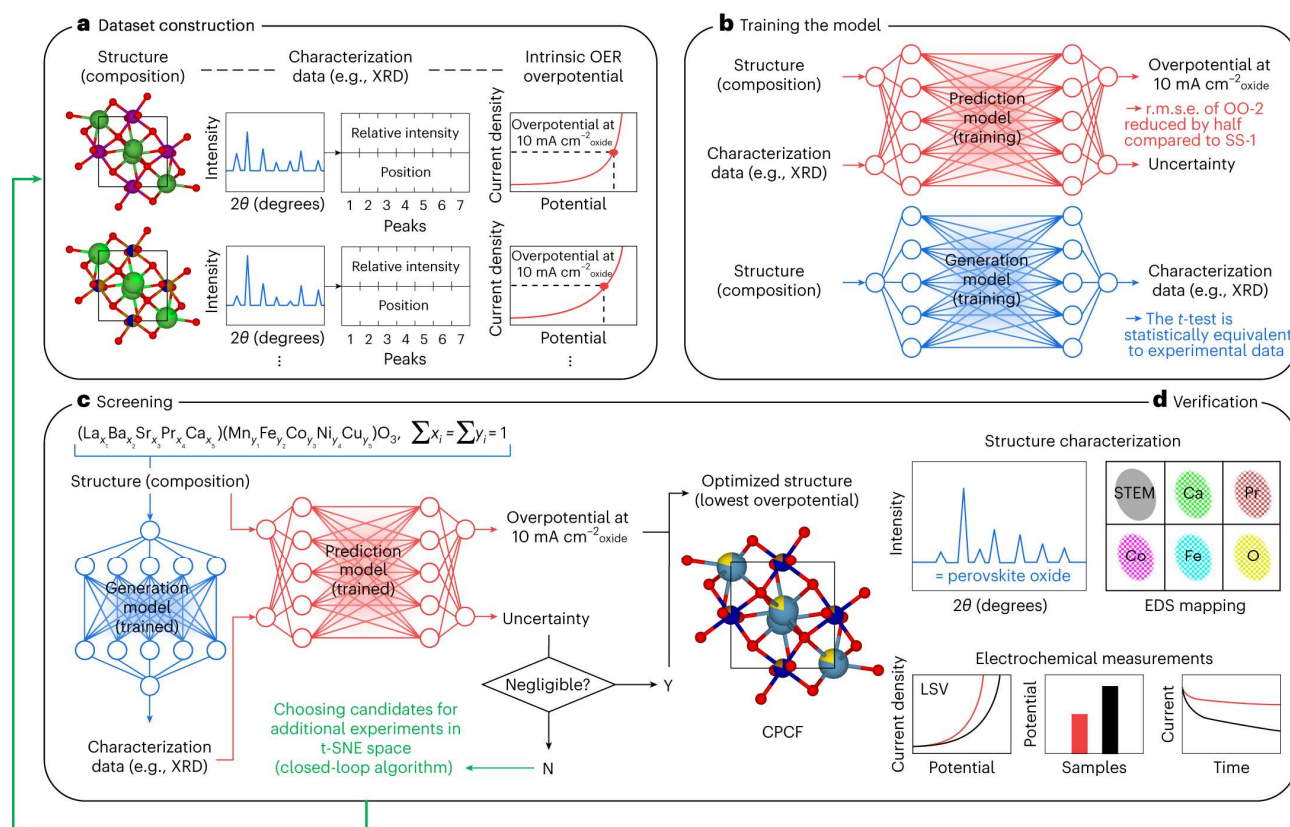
## Representative Publication

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

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

---

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
OK Bae & Jung Scholarship for Graduate Students, OK Bae & Jung Scholarship Foundation; <i>The Largest Private Scholarship Foundation in the Republic of Korea</i>	2022
Grand Prize, The 10 <sup>th</sup> Chemical Engineering Process Design Competition, The Korean Institute of Chemical Engineers	2021
Sooyoungro Scholarship for Undergraduate Students, Sooyoungro Church	2017
Presidential Science Scholarship for Undergraduate Students, President of the Republic of Korea	2017

## Research Interests

---

### Machine Learning-Driven Materials Discovery for Energy and Biomedical 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

---

### 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 Inorganic Functional Materials

Synthesis of Inorganic Bulk/Nanomaterials (Sol-Gel, Solid-State, Wet Impregnation, Hydrothermal, Heat-Up)  
Synthesis of Metal Oxides (High-Entropy Oxides, Multi-Metallic Perovskite, Spinel, and Rutile Oxides)

Synthesis of Metal Halides (Lithium Metal Halides)  
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, CO<sub>2</sub> Reduction)  
Batteries (Electrolytes for All-Solid-State Batteries, Cathode Materials for Lithium-Ion and Sodium-Ion Batteries, Anode-Free Batteries)  
Biomedicine (mRNA Delivery using Nanoparticles)

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

---

### **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, Random Forest, Gaussian)  
Text Mining (Natural Language Processing, Term Frequency-Inverse Document Frequency)  
Explainable Chatbot Development (GPT-4.1, FAISS)

### **Synthesis and Structural Characterization**

Various Techniques for Inorganic Functional Materials Synthesis (Sol-Gel, Solid-State, Wet Impregnation, Hydrothermal, Heat-Up Process)  
Air-free Schlenk Techniques for Inorganic Functional Materials Synthesis  
Glove Box Techniques for Inorganic Functional Materials Synthesis  
Ball Milling Techniques for Inorganic Functional Materials 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)

Conductivity Measurements (Electrolytes for All-Solid-State Batteries)



### Publications (Research Articles)

---

1. 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). 
2. 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). 
3. 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). 
4. **Moon, J.†**, 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). 
5. 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)

---

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)**

---

1. **Moon, J. et al.**  
Catalysts discovery across material groups by deep learning. *In Revision.*
2. **Moon, J. et al.**  
Superionic conductor discovery for all-solid-state batteries via machine learning. *In Preparation (Submission within two months).*
3. **Moon, J. et al.**  
New architecture design for anode-free solid-state batteries based on machine learning. *In Preparation (Submission within two months).*
4. **Moon, J. et al.**  
Champion catalyst discovery for proton exchange membrane water electrolysis using deep learning. *In Preparation (Submission within three months).*
5. **Moon, J. et al.**  
Design of superior fuel cell catalysts via deep learning. *In Preparation (Submission within three months).*
6. **Moon, J. et al.**  
Deep learning-driven nanoparticle design for mRNA delivery. *In Preparation.*

**Teaching Experiences**

---

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**

---

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).