

# Junseok Moon (문 준석)

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## Education

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

Ph.D. candidate in Chemical and Biological Engineering

*Mar. 2022  
– Aug. 2026 (Expected)*

*Supervisor: Prof. Taeghwan Hyeon*

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

B.S. in Chemical and Biological Engineering

*Mar. 2017 – Feb. 2022*

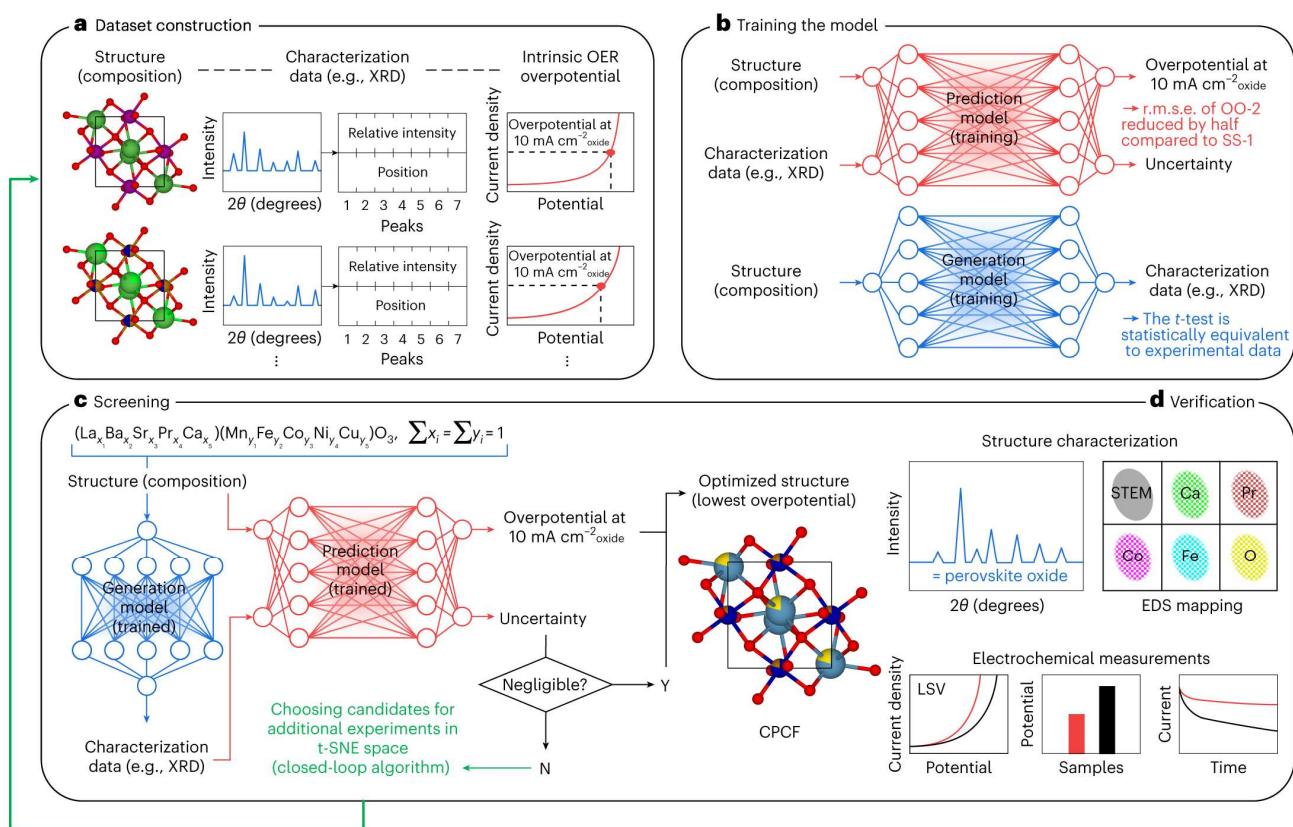
## Representative Publication

**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).

**(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  $10 \text{ mA cm}^{-2}$  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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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**

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### **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**

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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 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)

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## **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)

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### **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). 

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### **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). 

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**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.*

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**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

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**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).