Junseok Moon (문 준 석)

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Education

Seoul National University (SNU), Seoul, Republic of Korea — *Mar. 2022 – Aug. 2026 (Expected)*
Ph.D. candidate in Chemical and Biological Engineering
Supervisor: **Prof. Taeghwan Hyeon**

Seoul National University (SNU), Seoul, Republic of Korea — *Mar. 2017 – Feb. 2022*
B.S. in Chemical and Biological Engineering

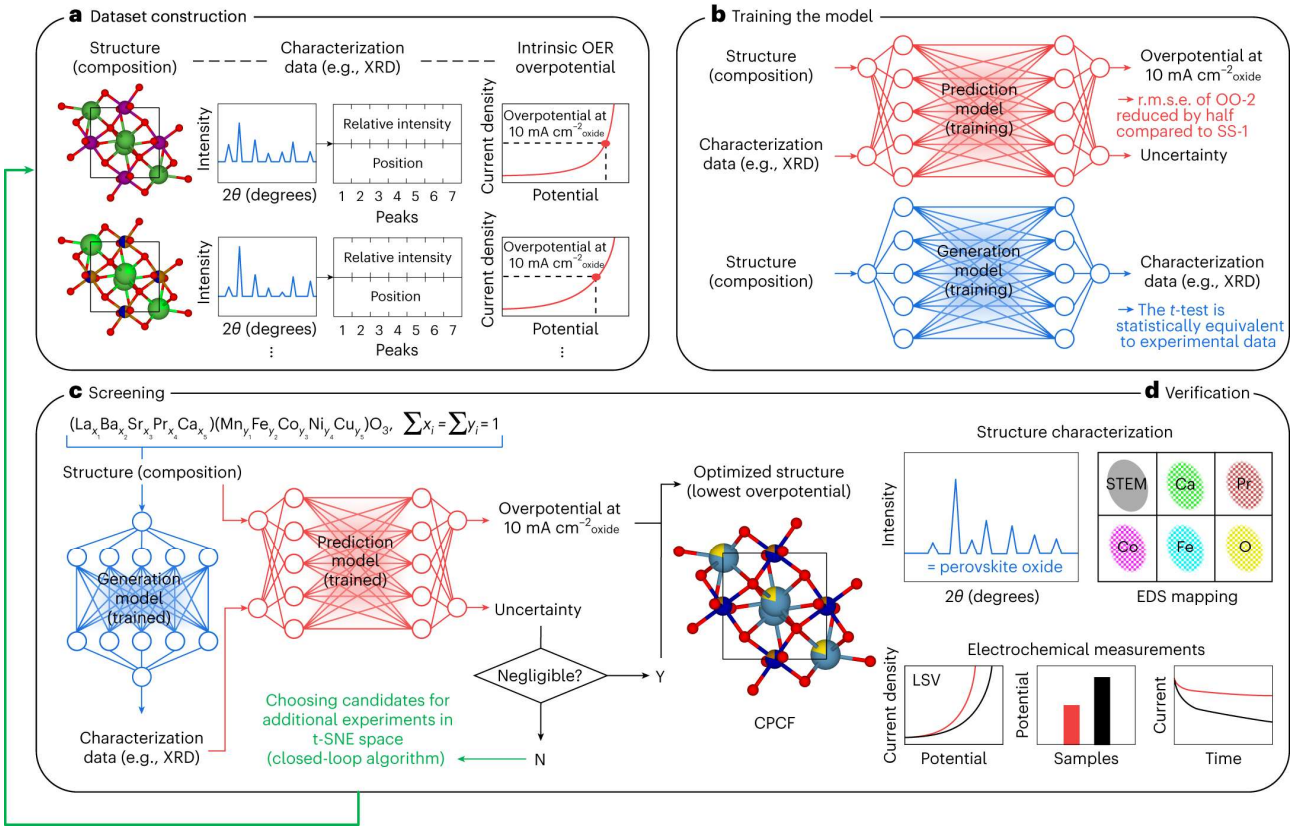
Representative Publication

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 mA cm^{-2}_{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 31st 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; *40 Students among Ph.D Candidates in All Science and Engineering Fields in the Republic of Korea*	*2024*
Silver Prize, The 29th Samsung Humantech Paper Awards, Samsung Electronics	*2023*
OK Bae & Jung Scholarship for Graduate Students, OK Bae & Jung Scholarship Foundation; *The Largest Private Scholarship Foundation in the Republic of Korea*	*2022*
Grand Prize, The 10th 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_2 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.*
   Design Principles for Non-Iridium-Based Oxygen Evolution Catalysts in Proton Exchange Membrane Water Electrolyzers
   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_2 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 (1st 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).