Sangjoon (Bob) Lee
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Education

Columbia University, New York, NY May 2025
M.S. in Materials Science and Engineering
- Advisor: Prof. Simon Billinge
- Department of Applied Physics and Applied Mathematics

Cooper Union, New York, NY May 2023
B.E. in Chemical Engineering, minors in Computer Science and Chemistry
- Advisor: Prof. Robert Topper
- Department of Chemical Engineering

Interests

Data-driven materials discovery, High-throughput, Experimental validation, Open-source development, DFT, Deep neural network potential

Awards

2023 American Chemical Society (ACS) New York Outstanding Student Award
2023 American Institute of Chemists (AIC) Student Award
2022 Summer STEM Teaching Fellowship, Cooper Union
4-Year Half-tuition Merit Scholarship, Cooper Union
4-Year Innovator's Merit Scholarship, Cooper Union
4-Year Corporate Scholarship, Donghwa Enterprise

Manuscripts submitted

1. Composition and structure analyzer/featurizer for explainable machine-learning models to predict solid state structures
E. I. Jaffal‡, S. Lee‡*, D. Shiryaev, A. Vtorov, N. K. Barua, H. Kleinke, A. O. Oliynyk*
10.26434/chemrxiv-2024-rrbhc

2. Recent Strides in Artificial Intelligence for Predicting Thermoelectric Properties and Materials Discovery
N. K. Barua, S. Lee, A. O. Oliynyk, H. Kleink*

Publications

Google Scholar citations: 37 from 7 peer-reviewed publications

‡ – these authors contributed equally to the work; * – corresponding author

1. Thermoelectric Materials Performance (zT) Predictions with Machine Learning
N. K. Barua, S. Lee, A. O. Oliynyk, H. Kleink*
ACS Applied Materials & Interfaces

2. cifkit: Python package for coordination geometry and atomic site analysis

S. Lee*, A. O. Oliynyk
Journal of Open Source Software

3. Machine learning descriptors in materials chemistry used in multiple experimentally validated studies: Oliynyk elemental property dataset
S. Lee*, C. Chen, G. Garcia, A. O. Oliynyk*
Data in Brief

4. The crystal and electronic structure of RE23Co6.7In20.3 (RE = Gd–Tm, Lu): A new structure type based on intergrowth of AlB2- and CsCl-type related slabs
Y. Tyvanchuk, V. Babizhetskyy, S. Baran, A. Szytula, V. Smetana, S. Lee, A. O. Oliynyk, A. Mudring*
Journal of Alloys and Compounds

5. Machine-learning prediction of thermal expansion coefficient for perovskite oxides with experimental validation
K. P. McGuinness, A. O. Oliynyk, S. Lee, B. Molero-Sanchez, P. K. Addo*
Physical Chemistry Chemical Physics

6. Electrospun nanofiber nerve guidance conduits for peripheral nerve regeneration: A review
S. Lee, M. Patel, R. Patel*
European Polymer Journal

7. TransRot: A Portable Software Package for Simulated Annealing Monte Carlo Geometry Optimization of Atomic and Molecular Clusters
R. Q. Topper*, S. L. Topper, S. Lee
ACS Symposium Series

Presentations

1.Machine-learned Features to Solve Crystal Structure Classification Problems
S. Lee, A. O. Oliynyk
ACS Northeast Regional Meeting (NERM) 2022, Computational Tools for Materials Science.
Oral, Rochester, NY, October 2022. [pdf]

2.Mag-Walking Simulated Annealing Monte Carlo Study of Nano-solvated Ammonium Chloride
S. Lee, R. Q. Topper, S. L. Topper
ACS New York 69th Annual Undergraduate Research Symposium 2022.
Oral, Virtual due to COVID-19, May 2022. [pdf]

3.TransRot: a Portable and Easy-to-Use Open Source Software Package for Simulated Annealing Monte Carlo Geometry Optimization of Nanoparticles
S. Lee, S. L. Topper, R. Q. Topper
Molecular Quantum Mechanics (MQM) 2022.
Poster, University of Virginia, June 2022. [pdf]

4.High-throughput Crystal Structure Featurizer for Binary and Ternary Compounds
S. Lee, N. K. Barua, O. Oliynyk
Gordon Research Conference (GRC) Solid State Chemistry.
Poster, New London, NH, July 2024. [pdf]

Research software

1. cifkit: open-source Python package for high-throughput CIF analysis
GitHub, 20 stars

2. CIF Bond Analyzer (CBA)
GitHub, 10 stars

3. Structure Analyzer/Featurizer (SAF)
GitHub, 9 stars