Sangwon Lee

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Education

Korea Advanced Institute of Science and Technology (Daejeon, Korea)

Postdoctoral Researcher in Applied Science Research Institute (Apr. 2021)

Ph.D. in Chemical and Biomolecular Engineering (Feb. 2020)

Dissertation: Nanoporous Materials Discovery for Energy and Environmental Applications using Machine Learning (Advisor: Jihan Kim)

University of Seoul (Seoul, Korea)

M.S. in Chemical Engineering (Feb. 2016)

Thesis: Prediction of chemical potential and phase transition of molecular crystals using Monte Carlo simulations (Advisor: Jaeeon Chang)

B.S. in Chemical Engineering (Feb. 2014)

Research interests

- Artificial intelligence for materials
- Machine learning
- Bayesian inference
- Energy management system
- Molecular simulations
- Analytical chemistry
- Software engineering
- Numerical analysis

Publications

*The number of citations is obtained by scraping Google Scholar

First and co-first author papers

Title	Citations	Year
(Contributed Equally) Inverse design of porous materials using artificial neural networks, B Kim, S Lee, J Kim, *Science advances 6 (1), eaax9324, 2020* deep learning · molecular simulations · materials discovery	263	2020
Computational screening of trillions of metal–organic frameworks for high-performance methane storage, S Lee, B Kim, H Cho et al., *ACS Applied Materials & Interfaces 13 (20), 23647-23654, 2021* deep learning · molecular simulations · materials discovery	107	2021
User-friendly graphical user interface software for ideal adsorbed solution theory calculations, S Lee, JH Lee, J Kim, *Korean Journal of Chemical Engineering 35, 214-221, 2018* numerical analysis · software design · thermodynamics	93	2018
Predicting performance limits of methane gas storage in zeolites with an artificial neural network, S Lee, B Kim, J Kim, *Journal of Materials Chemistry A 7 (6), 2709-2716, 2019* deep learning · molecular simulations · materials discovery	44	2019
(Contributed Equally) Computational Analysis of Linker Defective Metal–Organic Frameworks for Membrane Separation Applications, H Kim, S Lee, J Kim, *Langmuir 35 (11), 3917-3924, 2019* molecular simulations · porous materials	10	2019
(Contributed Equally) Performance Evaluation of Deep Learning Architectures for Load and Temperature Forecasting under Dataset Size Constraints and Seasonality, W Choi, S Lee, *Energy and Buildings, 113027, 2023* deep learning · forecasting · energy management systems	8	2023
(Contributed Equally) Machine learning-based discovery of molecules, crystals, and composites: A perspective review, S Lee, H Byun, M Cheon, J Kim, JH Lee, *Korean Journal of Chemical Engineering, 1-12, 2021* machine learning · materials discovery	8	2021
Chemical potential and solid-solid equilibrium of near-spherical Lennard-Jones dumbbell crystal, S Lee, M Kim, J Chang, *Korean Journal of Chemical Engineering 33, 1047-1058, 2016* molecular simulations · numerical analysis · statistical mechanics	1	2016

Title	Citations	Year
(Contributed Equally) Interpretable deep learning model for load and temperature forecasting: Depending on encoding length, models may be cheating on wrong answers, W Choi, S Lee, *Energy and Buildings, 113410, 2023* deep learning forecasting energy management systems		2023
Explainable kinetic modeling for aerobic biodegradation of poly(lactic acid) using Bayesian inferences, S Lee, J Park, J Lee et al., *Under review* Bayesian inferences kinetic modeling bio-plastics		2024

Other papers

Title	Citations	Year
Applications of machine learning in metal-organic frameworks, S Chong, S Lee, B Kim, J Kim, *Coordination Chemistry Reviews 423, 213487, 2020*	128	2020
Finding hidden signals in chemical sensors using deep learning, SY Cho, Y Lee, S Lee et al., *Analytical chemistry 92 (9), 6529-6537, 2020*	42	2020
Size-Matching Ligand Insertion in MOF-74 for Enhanced CO2 Capture under Humid Conditions, BL Suh, S Lee, J Kim, *The Journal of Physical Chemistry C 121 (44), 24444-24451, 2017*	34	2017
Finely tuned inverse design of metal–organic frameworks with user-desired Xe/Kr selectivity, Y Lim, J Park, S Lee, J Kim, *Journal of Materials Chemistry A 9 (37), 21175-21183, 2021*	25	2021
Computational design of metal–organic frameworks with unprecedented high hydrogen working capacity and high synthesizability, J Park, Y Lim, S Lee, J Kim, *Chemistry of Materials 35 (1), 9-16, 2022*	15	2022
New model for S-shaped isotherm data and its application to process modeling using IAST, S Ga, S Lee, G Park, J Kim, M Realff, JH Lee, *Chemical Engineering Journal 420, 127580, 2021*	14	2021
Isotherm parameter library and evaluation software for CO2 capture adsorbents, S Ga, S Lee, J Kim, JH Lee, *Computers & Chemical Engineering 143, 107105, 2020*	10	2020
Deep learning-based initial guess for minimum energy path calculations, H Park, S Lee, J Kim, *Korean Journal of Chemical Engineering 38, 406-410, 2021*	1	2021
Real-time probabilistic backfill thermal property estimation method enabling estimation convergence judgment, W Choi, S Lee, BH Dinh, YS Kim, *Case Studies in Thermal Engineering 48, 103108, 2023*		2023

Title	Citations	Year
Automatic Object Extraction from Electronic Documents Using Deep Neural Network, H Jang, Y Chae, S Lee, J Jo, *KIPS Transactions on Software and Data Engineering 7 (11), 411-418, 2018*		2018

Projects

LG Chem

Predicting oxidation states and coordination numbers from XANES using deep learning (2021, with LG AI Research)

- Contributions: designed deep learning architecture, developed knowledge transfer method
- *Patent application submitted*

Building MLOps infrastructure for instance sementation models (2021-2022)

- Contributions: designed infrastructure architecture, established the infrastructure

Developmenet of a segmentation tool using segment anything model (2023)

- Contributions: worked on back-end development

Estimation of length dimension of carbon nanotubes in SEM images (2023)

- Contributions: developed a length estimation algorithm, worked on back-end development

Monocrystalinity analysis of cathodes from EBSD using machine learning (2022-2023)

- Contributions: developed the theory of monocrystallinity, designed deep learning models, worked on back-end development
- *Patent application submitted*

Tortousity estimation of bettery separators using Monte Carlo simaultions (2022)

- Contributions: developed a tortuosity calculation algorithm, created a 3D visualization tool

Predicting biodegradation of polymers using reaction kinetics and Bayesian inference (2021-2023)

- Contributions: developed a reaction kinetics model for polymer biodegradation, designed a Bayesian inference model, contributed to back-end development

EBSD orientation analysis for lithium-ion path in cathodes (2022)

- Contributions: developed the theory, contributed to back-end development

Determination of the diffusion coefficient of lithum in separators (2023)

- Contributions: developed the theory for the diffusion model

Orientation analysis of glass fibers in the engineering plastics (2021)

- Contributions: developed deep learning model

Classification of crystal phases in cathodes from 4D-STEM data (2023)

- Contributions: developed a diffraction pattern classification algorithm

Deep document understanding (2020, with LG AI Research)

- Contributions: developed a SMILES image to SMILES model using ResNet and Transformer

Softwares & Libraries

DeepTimeSeries (Python, PyTorch)

GitHub Repository

A deep learning library designed for time series forecasting, built on the PyTorch framework

PORMAKE (Python)

GitHub Repository

A Python library for the construction of porous materials using topology and building blocks

IAST++ (C++)

GitHub Repository

User-friendly software for ideal adsorbed solution theory calculations

GRIDAY (C++)

GitHub Repository

An energy shape calculator for the porous materials

PC-SAFT (Fortran)

GitHub Repository

A software tool that facilitates the calculation of chemical equilibrium using perturbed chain statistical associating fluid theory

MonteCarloSimulator (Fortran)

GitHub Repository

A molecular Monte Carlo simulator employed for free energy calculations of molecules in both fluid and solid states

dartwork-mpl (Python, Matplotlib)

GitHub Repository

A Matplotlib styling and utility package crafted for the creation of publication-ready figures

LabeledImage (Python)

(private, LG Chem)

A library designed for managing labeled images, specifically tailored for instance segmentations. This library includes tools for format conversion, patch detection aggregation, and image augmentation.

Deep learning architectures

MOF-NET (Tensorflow)

GitHub Repository

GitHub Repository (Graph-network version)

A deep neural network engineered for predicting MOF (Metal-Organic Framework) properties based on topology and building blocks

ZeoGAN (Tensorflow)

GitHub Repository

A generative adversarial network (GAN) designed for the inverse design of zeolites

ESGAN (Tensorflow)

GitHub Repository

A generative adversarial network (GAN) created for generating energy shapes of porous materials

XANES-Net (PyTorch)

(private, LG Chem, with LG AI Research)

An architecture developed for predicting oxidation states and coordination numbers from XANES data, leveraging knowledge transfer from crystal structures

Skills

●: Usable with some time investment

●●: Proficiently usable

●●●: Usable at an expert level

Programming languages

- C/C++ ●●●
- Python ●●●
- Fortran ●●●
- Mathematica ●●●
- Javascript ●
- Rust ●

Machine learning

- PyTorch ●●●
- Tensorflow ●●●
- PyTorch Lightning ●●●
- PyTorch Geometric ●
- Detectron2 ●●
- MMDetection ●●
- scikit-learn ●●
- XGBoost ●
- JAX ●●
- Darts ●●

Bayesian inference

- PyMC ●●●
- Pyro ●

Data visualization

- Matplotlib ●●●
- Seaborn ●●
- Plotly ●●
- Bokeh ●
- d3.js ●

Version control

- Git ●●
- GitHub ●●

CI/CD

- Github Actions ●●

Package and project management

- Poetry & Pyenv ●●●
- Conda ●●

Unit test

- pytest ●●

Data structure & numerical analysis

- Pandas ●●●
- Xarray ●●
- NumPy ●●●
- SciPy ●●●

GUI programming

- Qt, PySide6 ●●●

Symbolic computation

- Mathematica ●●●
- SymPy ●●

Computer vision

- OpenCV ●●●
- scikit-image ●●●

3D visualization

- PyVista ●●●
- OpenGL (GLSL) ●
- Panda3D ●●

Containerization

- Docker ●●
- Docker compose ●●

Back-end & ML serving

- FastAPI ●●
- MLflow models ●●

Documentation

- Sphinx ●●
- LaTeX ●●

MLOps

- MLflow ●●●
- Tensorboard ●

Reverse proxy

- Traefik ●●

Configuration management

- Hydra ●●

Operating system

- Linux (Ubuntu, CentOS) ●●

Molecular simulations

- PyMatGen ●●●
- ASE ●●●
- LAMMPS ●●●
- VASP ●
- PySCF ●

Database

- SQLite ●

Presentations

Oral presentations

- Construction of MOF Structures from Topology and Building Blocks, 2019 KIChE Fall Meeting and International Symposium
- Evaluating Performance Limits of Methane Storage Separations of Porous Materials Using Artificial Neural Network, IUMRS-ICEM 2018

Posters

- IAST++: Software for Ideal Adsorbed Solution Theory (IAST) Calculations with User-friendly Interface, 2017 KIChE Fall Meeting and International Symposium
- Sensitivity Analysis of CO2 Capture Materials in Post-combustion Flue Gas, ChemIndix 2016
- Order-disorder transition and free energy of the crystal of Lennard-Jones diatomics, 2014 KIChE Fall Meeting

Awards

Gold Prize (2nd), Engineering Mathematics Competition, University of Seoul, Nov. 2012