Kaile JIANG

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ORCID: orcid.org/0009-0005-1105-990X GitHub: github.com/Kailejiang/CLRNet

PROFILE

A results-driven, final-year Master's student specializing in the intersection of machine learning (ML) and physical chemistry. My research focuses on developing innovative ML models to surpass traditional methodologies and bridge the gap between ML algorithms and physical chemistry principles. Proficient in Python, I have independently designed and built the CLRNet model. I hold first-author publications in *J. Chem. Inf. Model.* and *J. Chem. Phys.* A, and have been awarded the National Scholarship and a National Invention Patent (P.R. China). Using interdisciplinary methods to enhance the interpretability of machine learning models is also one of the key focuses of present and future research.

EDUCATION

Huaqiao University, P.R. China Sept. 2023 – Jun. 2026
Master of Optical Engineering GPA: 4.82/5.0
Capstone Thesis Project: *Efficient Cluster Structure Search Based on Machine Learning Classification-Regression Joint Model*

Huaqiao University, P.R. China Sept. 2019 – Jun. 2023
Bachelor of Optical and Electronic Information Engineering GPA: 3.91/5.0
Capstone Thesis Project: *Surgical Instrument Recognition Based on Improved YOLO*

SELECTED PUBLICATIONS

[1] **Jiang, K.-L.**, Wang, H.-Q., Li, H.-F., & Wen, Z.-X. (2025). A scalable machine learning multi-local regression framework for potential energy surface fitting across diverse chemical landscapes. ***Journal of Chemical Physics***, 163(2), 024106.

[2] **Jiang, K.-L.**, Wang, H.-Q., Li, H.-F., Pan, S.-W., Zheng, H., Zhang, Y.-H., & Zhang, J.-M. (2025). SchNet_IIA: Potential Energy Surface Fitting by Interatomic Interactions Attention Based on Transfer Learning Analysis. ***Journal of Chemical Information and Modeling***, 65(1), 92–100.

[3] Wen, Z.-X., Li, H.-F., **Jiang, K.-L.**, Wang, H.-Q. (2025) Enhancing SchNet-Based Structure Prediction for Doped Clusters via Transfer Learning and Fine-Tuning. ***Journal of Physical Chemistry A***, 129(41), 9616–9624.

[4] Zhang, Y.-H., Wang, H.-Q., Li, H.-F., Zhang, J.-M., Zheng, H., **Jiang, K.-L.**, Zhang, B., & Wu, W.-H. (2024). Discovering SnB7−: a half-sandwich structure with double aromaticity and pathways to molecular machines. ***Physical Chemistry Chemical Physics***, 26, 27106-27115.

[5] Zhang, B., Wang, H.-Q., Li, H.-F., Zheng, H., Zhang, Y.-H., Mei, X.-J., Zhang, J.-M., **Jiang, K.-L.**, & Jiang, Q.-W. (2024). The high electron mobility for spin-down channel of two-dimensional spin-polarized half-metallic ferromagnetic $EuSi_2N_4$ monolayer. ***Journal of Computational Chemistry***, 45(31), 2678.

[6] **Jiang, K.-L.**, Pan, S.-W., Yang, L., Yu, J., Lin, Y., & Wang, H.-Q. (2023). Surgical instrument recognition based on improved YOLOv5. ***Applied Sciences***, 13(21), 11709.

PATENT

A Machine Learning-Based Optimization Method and System for the Ground State Doped Clusters

Inventive Patent (Authorized), China, Patent No.: CN119314596B, Authorization Date: Jul. 2025, Assignee: Huaqiao University

PROFESSIONAL EXPERIENCE

Theoretical Study of the Structure and Electronic Properties of Semiconductor Rare Earth Doped Clusters Based on Machine Learning.

Role or Tasks: Team Member (Methodology Development, Model Construction) Dec. 2023 – Present

- Proposed the CLRNet framework (via Python) for potential energy surface fitting. Integrating clustering methods with local regression concepts, CLRNet enables more efficient adaptation to high-energy structures and noise. CLRNet achieved MAEs below 10 meV on QM9 tasks, an average MAE of 0.085 kcal/mol on MD17 tasks.
- Combined feature-representation-transfer approach with causal analysis to conduct interpretability analysis on machine learning models, addressing the difficulty in improving current machine learning frameworks caused by their high complexity and intricate interactions.
- Applied graph neural networks with graph attention mechanisms, improving cluster energy prediction accuracy by 0.015 eV/atom.

Structural Design and Property Regulation of Double Rare Earth Atom Doped Semiconductor Clusters

Role or Tasks: Team Member (Molecular Dynamic Analysis, Data Support) Nov. 2023 – Present

- Performed random searches for initial structures using the Artificial Bee Colony algorithm. Combined with DFT calculations via Gaussian 09 to obtain the Global Minimum and low-lying isomers.
- Evaluated dynamic stability through Ab Initio Molecular Dynamics (AIMD) simulations using ORCA 5.0.4. Conducted tests with the Canonical Sampling through Velocity Rescaling (CSVR) thermostat.

Research on Detection and Recognition of Surgical Instruments Based on Deep Learning

Role or Tasks: Principal Investigator (PI), Project Documents Writer Jun. 2021 – Jun. 2023

Fundings: College Students' Innovative Entrepreneurial Training Plan Program

- Integrated the Squeeze-and-Excitation channel attention module to strengthen key features, especially for overlapping surgical instruments.
  The mAP reached 88.7%, which was a 1.8% increase compared with the original YOLOv5.
- Utilizes dynamic sparsity patterns of convolutional weights to reduce computational complexity (FLOPs reduced from 16.9G to 10.3G), meeting the real-time recognition needs of surgical instruments.

ACADEMIC AWARDS & HONORS

Oct. 2025: National Scholarship for Postgraduates (Ministry of Education of China, awarded to top 5% postgraduates nationwide).

Nov. 2024: Excellent Presentation Award (Postgraduate Forum of Fujian Universities Alliance of Physics Discipline).

Oct. 2024: First-Class Academic Scholarship for Postgraduates (Huaqiao University, top 10% GPA).

SKILLS

Programming: Python, SQL, MATLAB

Simulation: Gaussian, CASTEP, SchNet

Languages: English(fluent), Mandarin(native)

Certificates: Database System Engineer (Intermediate), China Qualification of Computer and Software Professional