Keqiang Yan

Ph.D. Student
Department of Computer Science & Engineering
Texas A&M University

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Research Interests

Graph Deep Learning: graph neural networks, 3D graphs, periodic graphs.

AI for Science: Large language models and 3D geometric modeling for molecules, materials, and proteins.

Generative Modeling: energy-based models, score-based models, diffusion models, large language models.

Education

Texas A&M University, College Station, TX, USA   Sep 2020 – Present
Ph.D., Computer Science
Advisor: Prof. Shuiwang Ji

Peking University, Beijing, CHINA   Aug 2016 – Jul 2020
B.S., Intelligence Science and Technology
Advisor: Prof. Jiaying Liu

Professional Experiences

Microsoft Research, AI4Science, Seattle, WA   May 2023 – Aug 2023
Research Intern
Mentor: Dr. Jake Smith

West China Hospital Big Data Center, Chengdu, CHINA   Sep 2020 – Mar 2021
Research Intern
Mentor: Prof. Kang Li

Peking University, Beijing, CHINA   Mar 2018 – Mar 2020
Research Intern
Advisor: Prof. Jiaying Liu

Selected Publications [Google Scholar]

* indicates equal contribution.

[ICML 2024]   **A Space Group Symmetry Informed Network for O(3) Equivariant Crystal Tensor Prediction**
Keqiang Yan, Alexandra Saxton, Xiaofeng Qian, Xiaoning Qian, Shuiwang Ji
*Proceedings of the 41th International Conference on Machine Learning (**ICML**), 2024*
[Paper] [Code]

[ICLR 2024]   **Complete and Efficient Graph Transformers for Crystal Material Property Prediction**
Keqiang Yan, Cong Fu, Xiaofeng Qian, Xiaoning Qian and Shuiwang Ji
*The Twelfth International Conference on Learning Representations (**ICLR**), 2024*
[Paper] [Code]

[LoG 2023]   **A Latent Diffusion Model for Protein Structure Generation**
Cong Fu*, **Keqiang Yan***, Limei Wang, Wing Yee Au, Michael McThrow, Tao Komikado, Koji Maruhashi, Kanji Uchino, Xiaoning Qian and Shuiwang Ji
*Learning on Graphs Conference (**LoG**), 2023*
[Paper] [Code]

[under review]   **Artificial Intelligence for Science in Quantum, Atomistic, and Continuum Systems**

Xuan Zhang, Limei Wang, Jacob Helwig, Youzhi Luo, Cong Fu, Yaochen Xie, Meng Liu, Yuchao Lin, Zhao Xu, **Keqiang Yan**, Keir Adams, Maurice Weiler, Xiner Li, ···, Tommi Jaakkola, Connor W Coley, Xiaoning Qian, Xiaofeng Qian, Tess Smidt, Shuiwang Ji

A 263-page AI4Sience survey paper by 63 authors from 14 institutions, including 41 figures and 36 tables.
Keqiang Yan is the lead author of Protein Backbone Structure Generation and Material Representation Learning (Sec. 6.4 and 7.2).
[Paper] [Code (172 stars in one month))][Website]

[Sci. Advances]   **Examining graph neural networks for crystal structures: limitations and opportunities for capturing periodicity**
Sheng Gong, **Keqiang Yan**, Tian Xie, Yang Shao-Horn, Rafael Gomez-Bombarelli, Shuiwang Ji, and Jeffrey C. Grossman
Science Advances [Paper]

[Npj Computational Materials]   **Large Scale Benchmark of Materials Design Methods**

Kamal Choudhary, Daniel Wines, Kangming Li, Kevin F Garrity, Vishu Gupta, Aldo H Romero, ···, **Keqiang Yan**, ···, Hongliang Xin, Maureen Williams, Adam J Biacchi, Francesca Tavazza
A material benchmark with 152 methods, 274 benchmarks, and more than 8 million data points.
[Paper] [Code][Website]

[ICML 2023]   **Efficient Approximations of Complete Interatomic Potentials for Crystal Property Prediction**
Yuchao Lin, **Keqiang Yan**, Youzhi Luo, Yi Liu, Xiaoning Qian and Shuiwang Ji
*Proceedings of the 40th International Conference on Machine Learning (**ICML**), 2023*
[Paper] [Code]

[NeurIPS 2022]   **Periodic Graph Transformers for Crystal Material Property Prediction**
Keqiang Yan, Yi Liu, Yuchao Lin, and Shuiwang Ji
*Thirty-sixth Conference on Neural Information Processing Systems (**NeurIPS**), 2022*
[Paper] [Code]

[JMLR 2021]   **DIG: A Turnkey Library for Diving into Graph Deep Learning Research**
Meng Liu*, Youzhi Luo*, Limei Wang*, Yaochen Xie*, Hao Yuan*, Shurui Gui*, Haiyang Yu*, Zhao Xu, Jingtun Zhang, Yi Liu, **Keqiang Yan**, Haoran Liu, Cong Fu, Bora Oztekin, Xuan Zhang, and Shuiwang Ji
*Journal of Machine Learning Research (**JMLR**), 2021*
[Paper] [Code (star 1k+)] [Documentation]

[ICML 2021]   **GraphDF: A Discrete Flow Model for Molecular Graph Generation**
Youzhi Luo, **Keqiang Yan**, and Shuiwang Ji
*The 38th International Conference on Machine Learning (**ICML**), 2021*
[Paper] [Code]

[ICLR-W 2021]   **GraphEBM: Molecular Graph Generation with Energy-Based Models**
Meng Liu, **Keqiang Yan**, Bora Oztekin, and Shuiwang Ji
EBM Workshop at ICLR, 2021
[Paper] [Code]

Professional Services

Reviewer:
International Conference on Learning Representations (**ICLR**)	2023, 2024
Conference on Neural Information Processing Systems (**NeurIPS**)	2022, 2023
International Conference on Machine Learning (**ICML**)	2022, 2023, 2024
IEEE Transactions on Pattern Analysis and Machine Intelligence (**TPAMI**)	
American Chemical Society, The Journal of Physical Chemistry Letters (**JPCL**)	

Area Chair:
NeurIPS AI4Science workshop	2023
ICML AI4Science workshop	2024

Invited Talks

Topic: Material Representation Learning and Property Prediction
AIMS, National Institute of Standards and Technology   July 2023
AIMS, National Institute of Standards and Technology (up-coming)   July 2024
Topic: Machine learning approaches for novel material and protein discovery
D.E. Shaw Research   April 2024

Grant Proposals

NSF MOMS-2331036: Strain-Memory Effects on Solid-State Transformation, 5/1/2024-4/30/2027, Amount $566,858, Prorated $140,316. Note: **Keqiang Yan leads the writing of the machine learning components.**

Selected Scholarships, Awards, & Honors

D.E. Shaw Research Doctoral & Postdoctoral Fellowship	2024
NeurIPS Travel Award	2022
Texas A&M University Travel Award	2022, 2023
3rd Place of Open Catalyst Challenge	2021
Excellent Graduate, Peking University	2020

Skills

Python, Julia, Matlab, c/c++, LaTeX, PyTorch