

Keqiang Yan

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Department of Computer Science & Engineering
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Research Interests

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

AI for Science: 3D geometric modeling and property prediction for molecules, materials, and proteins.

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

[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
[\[Paper\]](#) [\[Code\]](#)

[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 AI4Science 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 [\[Paper\]](#)

- [under review] **Large Scale Benchmark of Materials Design Methods**
 Kamal Choudhary, Daniel Wines, Kangming Li, Kevin F Garrity, Vishu Gupta, Aldo H Romero, Jaron T Krogel, Kayahan Saritas, Addis Fuhr, Panchapakesan Ganesh, Paul RC Kent, **Keqiang Yan**, · · ·, Andrew Dale Rohskopf, Jason Hattrick-Simpers, Shih-Han Wang, Luke EK Achenie, 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
IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)	
Area Chair: NeurIPS AI4Science workshop	2023

Invited Talks

Periodic Graph Representation Learning and Transformers for Crystal Material Property Prediction AIMS, National Institute of Standards and Technology	July 2023
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Scholarships, Awards, & Honors

3rd Place of Open Catalyst Challenge Excellent Graduate, Peking University	2021 2020
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Skills

Python, Julia, Matlab, c/c++, L^AT_EX, PyTorch