

# Keqiang Yan

Ph.D. Student  
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## Research Interests

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

**AI for Drug and Material Discovery:** molecule and material property prediction, molecule, material and protein generation.

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

## Education

**Texas A&M University**, College Station, TX, USA  
Ph.D., Department of Computer Science & Engineering  
Advisor: [Prof. Shuiwang Ji](#)

Sep 2020 – Present

**Peking University**, Beijing, CHINA  
B.S., Intelligence Science and Technology  
Advisor: [Prof. Jiaying Liu](#)

Aug 2016 – Jul 2020

## Publications [\[Google Scholar\]](#)

\* indicates equal contribution.

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| [NeurIPS 2022] | <b>Periodic Graph Transformers for Crystal Material Property Prediction</b><br>Keqiang Yan, Yi Liu, Yuchao Lin, and Shuiwang Ji<br><i>Thirty-sixth Conference on Neural Information Processing Systems (NeurIPS), 2022</i><br><a href="#">[Paper]</a> <a href="#">[Code coming soon]</a>   |
| [JMLR]         | <b>DIG: A Turnkey Library for Diving into Graph Deep Learning Research</b><br>Meng Liu*, Youzhi Luo*, Limei Wang*, Yaochen Xie*, Hao Yuan*, Shurui Gui*, Haiyang Yu*, Zhao Xu, Jingtun Zhang, Yi Liu, <b>Keqiang Yan</b> , Haoran Liu, Cong Fu, Bora Oztekin, Xuan Zhang, and Shuiwang Ji<br><i>Journal of Machine Learning Research (JMLR), 2021</i><br><a href="#">[Paper]</a> <a href="#">[Code (star 1k+)]</a> <a href="#">[Documentation]</a> |
| [ICML 2021]    | <b>GraphDF: A Discrete Flow Model for Molecular Graph Generation</b><br>Youzhi Luo, <b>Keqiang Yan</b> , and Shuiwang Ji<br><i>The 38th International Conference on Machine Learning (ICML), 2021</i><br><a href="#">[Paper]</a> <a href="#">[Code]</a>  |
| [ICLR-W 2021]  | <b>GraphEBM: Molecular Graph Generation with Energy-Based Models</b><br>Meng Liu, <b>Keqiang Yan</b> , Bora Oztekin, and Shuiwang Ji<br><i>EBM Workshop at ICLR, 2021</i><br><a href="#">[Paper]</a> <a href="#">[Code]</a>  |
| [ICME 2020]    | <b>Multitask Attentive Network For Text Effects Quality Assessment</b><br>Keqiang Yan, Shuai Yang, Wenjing Wang and Jiaying Liu<br><i>2020 IEEE International Conference on Multimedia and Expo (ICME)</i><br><a href="#">[Paper]</a>  |

## **Professional Services**

### **Program Committee Member | Reviewer**

Conference on Neural Information Processing Systems ( <b>NeurIPS</b> )	2022
International Conference on Machine Learning ( <b>ICML</b> )	2022
IEEE Transactions on Pattern Analysis and Machine Intelligence ( <b>TPAMI</b> )	2022

## **Scholarships, Awards, & Honors**

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

## **Skills**

Python, Julia, Matlab, c/c++,  $\text{\LaTeX}$ , PyTorch