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Ph.D. Student in Computer Science, admitted Autumn 2022

Publications

PUBLICATIONS

- **Spatio-Temporal Energy-Guided Diffusion Model for Zero-Shot Video Synthesis and Editing** *IEEE TRANSACTIONS ON CIRCUITS AND SYSTEMS FOR VIDEO TECHNOLOGY*
Yang, L., Zhao, Y., Yu, Z., Zeng, B., Xu, M., Hong, S., Cui, B.
2025; 35 (6): 6034-6046
- **Artificial Intelligence for Science in Quantum, Atomistic, and Continuum Systems** *FOUNDATIONS AND TRENDS IN MACHINE LEARNING*
Zhang, X., Wang, L., Helwig, J., Luo, Y., Fu, C., Xie, Y., Liu, M., Lin, Y., Xu, Z., Yan, K., Adams, K., Weiler, M., Li, et al
2025; 18 (4): 385-912
- **RetroDiff: Retrosynthesis as Multi-stage Distribution Interpolation**
Wang, Y., Song, Y., Wang, Y., Xu, M., Wang, R., Zhou, H., Ma, W.
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- **f-PO: Generalizing Preference Optimization with f-divergence Minimization**
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- **Crystal Structure Determination from Powder Diffraction Patterns with Generative Machine Learning.** *Journal of the American Chemical Society*
Riesel, E. A., Mackey, T., Nilforoshan, H., Xu, M., Badding, C. K., Altman, A. B., Leskovec, J., Freedman, D. E.
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- **An all-atom protein generative model.** *Proceedings of the National Academy of Sciences of the United States of America*
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- **An all-atom protein generative model.** *bioRxiv : the preprint server for biology*
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- **Graph and Geometry Generative Modeling for Drug Discovery**
Xu, M., Liu, M., Jin, W., Ji, S., Leskovec, J., Ermon, S., ACM
ASSOC COMPUTING MACHINERY.2023: 5833-5834
- **Scaling Riemannian Diffusion Models**
Lou, A., Xu, M., Farris, A., Ermon, S.
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- **Equivariant Flow Matching with Hybrid Probability Transport for 3D Molecule Generation**
Song, Y., Gong, J., Xu, M., Cao, Z., Lan, Y., Ermon, S., Zhou, H., Ma, W.
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- **MUDiff: Unified Diffusion for Complete Molecule Generation**
Hua, C., Luan, S., Xu, M., Ying, R., Fu, J., Ermon, S., Precup, D.
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- **When Do Graph Neural Networks Help with Node Classification? Investigating the Impact of Homophily Principle on Node Distinguishability**
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- **Infomax Neural Joint Source-Channel Coding via Adversarial Bit Flip**
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