

# Prof. Truong-Son Hy

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**Research Interest** **HySonLab** is my research group. We work on graph neural networks, deep generative models on graphs, equivariant neural networks, multiresolution machine learning in the direction of **AI for Science, Bioinformatics, Drug Discovery, Drug Repurposing, and Medical AI**.

**Education** **The University of Chicago** September 2016 - June 2022  
*Illinois, USA*  
PhD. Computer Science  
Thesis: Graph representation learning, deep generative models on graphs, group equivariant molecular neural networks and multiresolution machine learning.  
Advisor: Prof. Risi Kondor

**The University of Chicago** September 2016 - December 2018  
*Illinois, USA*  
MSc. Computer Science  
Thesis: Covariant compositional networks for learning graphs and GraphFlow deep learning framework in C++/CUDA.  
Advisor: Prof. Risi Kondor

**Eötvös Loránd University** September 2013 - July 2016  
*Budapest, Hungary*  
BSc. Computer Science  
Thesis: Semi-supervised Adaptive Facial Tracking Method.  
Advisor: Prof. Lőrincz András  
GPA: **4.98/5** (in Hungary scale), **3.984/4** (in US scale)  
Award: First-class Graduation Honour  
Sponsor: Stipendium Hungaricum Full Scholarship from the Government of Hungary

**Current Position** **University of Alabama at Birmingham** **(Tenure-Track) Assistant Professor**  
Department of Computer Science August 2024 – present

- Affiliated faculty with Heersink School of Medicine (UAB), Center for Clinical and Translational Science (CCTS).
- Research and advise PhD students in AI for Science, Bioinformatics, Drug Discovery.
- Fall 2024: Teach CS 660/760 (Master/PhD) – Artificial Intelligence [Syllabus].
- Spring 2025: Teach CS 663/763 (Master/PhD) – Data Mining [Syllabus].

**Work Experience** **Indiana State University** **(Tenure-Track) Assistant Professor**  
Department of Mathematics and Computer Science August 2023 – July 2024

- Fall 2023: CS 617 – Data Mining [Syllabus]
- Spring 2024: CS 417 – Machine Learning, CS 475/575 – Artificial Intelligence
- Serve in faculty search committees for Departments of Biology and Computer Science.

**Porter Cancer Research Center** **Affiliated Faculty**  
Terre Haute, Indiana February 2024 – July 2024

- Deep Learning for drug discovery & drug repurposing.

**The Center for Genomic Advocacy** **Affiliated Faculty**  
Terre Haute, Indiana February 2024 – July 2024

- Genomic Large Language Models.

**University of California San Diego** **Postdoctoral Fellow & Lecturer**  
Halicioglu Data Science Institute September 2022 – April 2023

- Mentor: Prof. Yusu Wang.
- I taught DSC 40A - Theoretical Foundations of Data Science (Fall 2022) [Course Materials].

**Facebook Inc.**

Ads Machine Learning, Seattle office

**PhD Intern**

June – August 2020

Project:

- Task: Implementation of a transfer learning scheme in distributed system for large-scale sparse neural networks to classify and rank two billion users' advertisements. The framework is built based on Caffe2.
- Programming language: Python.
- Result: The models are implemented, trained and tested on 1 week of Facebook data.

**Google Inc.**

Networking SRE, Sunnyvale office

**Site Reliability Engineer Intern**

June – September 2018, 2019

Project:

- Task: Utilize machine learning and statistical techniques including message passing neural networks to design a methodology for root cause analysis and auto detection of network failures based on network events and topology. The Google's technologies used for this project include Unified Network Model, Borgmon and TensorFlow.
- Programming language: C++ and Python.
- Result: Implementation of several Machine Learning methods on real production data of network topologies and monitoring systems.

**Google Inc.**

Security and Privacy, Chicago office

**Software Engineer Intern**

June 2017 – September 2017

Project:

- Task: Analyze series of Googlers' accesses of sensitive data to detect anomalous behaviors from internal actors. Replace the daily analysis by a real-time analysis to reduce the latency of the current continuous pipeline. Apply Machine Learning and statistical models to evaluate and cluster data access logs in Google distributed systems. The challenge is to integrate with the existing Google's infrastructure, learn and use multiple Google's technologies such as Bigtable and Flume.
- Programming language: Java.
- Result: Successfully tested with artificially generated data that simulates the working pipeline in one year.

**Neural Information Processing Group**

Eötvös Loránd University

**Undergraduate Research Student**

April 2014 – July 2016

- Website: <http://nipg04.inf.elte.hu/>
- Working under the supervision of Prof. Lőrincz András with main focus on facial analysis and sparse coding learning algorithms.

**Conference Proceedings**[Google Scholar]  
[ORCID]

[C15] Khai Le-Duc, David Thulke, Hung-Phong Tran, Long Vo-Dang, Khai-Nguyen Nguyen, **Truong-Son Hy**, and Ralf Schluter, *Medical Spoken Named Entity Recognition*, NAACL 2025. <https://openreview.net/forum?id=TN9bSCtmAz> (abstract)  
<https://arxiv.org/pdf/2406.13337.pdf> (paper)

[C14] Cuong Tran Van, Thanh V. T. Tran, Van Nguyen, and **Truong-Son Hy**<sup>c</sup>, *Effective Context Modeling Framework for Emotion Recognition in Conversations*, ICASSP 2025, DOI 10.1109/ICASSP49660.2025.10888112.

<sup>c</sup>: Corresponding author / PI.<https://ieeexplore.ieee.org/document/10888112>

[C13] Co Tran, Quoc-Bao Tran, **Truong-Son Hy**<sup>c</sup>, and Thang N. Dinh, *Scalable Quantum-Inspired Optimization through Dynamic Qubit Compression*, AAAI 2025 (Oral Presentation).

<sup>c</sup>: co-PI.<https://openreview.net/forum?id=bmMTECo2yj> (abstract)<https://arxiv.org/pdf/2412.18571.pdf> (paper)

[C12] Thanh V. T. Tran, Nhat Khang Ngo, Viet Anh Nguyen, and **Truong-Son Hy**<sup>c</sup>, *GROOT: Effective Design of Biological Sequences with Limited Experimental Data*, KDD 2025, Proceedings of the 31st ACM SIGKDD Conference on Knowledge Discovery and Data Mining V.1., Pages 1385-1396, DOI 10.1145/3690624.3709291. .

<sup>c</sup>: Corresponding author / PI.

<https://dl.acm.org/doi/10.1145/3690624.3709291> (paper)

<https://arxiv.org/pdf/2411.11265.pdf> (preprint)

[C11] Khai Le-Duc, Khai-Nguyen Nguyen, Long Vo-Dang, and **Truong-Son Hy**<sup>c</sup>, *Real-time Speech Summarization for Medical Conversations*, Interspeech 2024, DOI 10.21437/Interspeech.2024-2250.

<sup>c</sup>: Corresponding author / PI.

[https://www.isca-archive.org/interspeech\\_2024/leduc24\\_interspeech.pdf](https://www.isca-archive.org/interspeech_2024/leduc24_interspeech.pdf)

[C10] Zhishang Luo, **Truong-Son Hy**, Puoya Tabaghi, Michael Defferrard, Elah Rezaei, Ryan Carey, Rhett Davis, Rajeev Jain, and Yusu Wang, *DE-HNN: An effective neural model for Circuit Netlist representation*, Proceedings of The 27th International Conference on Artificial Intelligence and Statistics, PMLR 238:4258-4266, 2024.

<https://proceedings.mlr.press/v238/luo24a/luo24a.pdf>

[C9] Thuan Trang, Nhat Khang Ngo, Daniel Levy, Thieu N. Vo, Siamak Ravanbakhsh, and **Truong-Son Hy**<sup>c</sup>, *E(3)-Equivariant Mesh Neural Networks*, Proceedings of The 27th International Conference on Artificial Intelligence and Statistics, PMLR 238:748-756, 2024.

<sup>c</sup>: Corresponding author / PI.

<https://proceedings.mlr.press/v238/anh-trang24a/anh-trang24a.pdf>

[C8] Minh H. Nguyen, Nghi D. Q. Bui, **Truong-Son Hy**, Long Tran-Thanh, and Tien N. Nguyen, *HierarchyNet: Learning to Summarize Source Code with Heterogeneous Representations*, EACL 2024.

<https://aclanthology.org/2024.findings-eacl.156.pdf>

[C7] Duc Thien Nguyen\*, Manh Duc Tuan Nguyen\*, **Truong-Son Hy**<sup>\*c</sup>, and Risi Kondor, *Fast Temporal Wavelet Graph Neural Networks*, NeurIPS 2023 (Workshop on Symmetry and Geometry in Neural Representations), Proceedings of Machine Learning Research 228:35-54.

\*: Co-first authors.

<sup>c</sup>: Corresponding author / PI.

<https://proceedings.mlr.press/v228/nguyen24a.html>

<https://openreview.net/pdf?id=Mo5qZaB18v>

[C6] Chen Cai, **Truong-Son Hy**, Rose Yu, and Yusu Wang, *On the Connection Between MPNN and Graph Transformer*, ICML 2023, Proceedings of Machine Learning Research 202:3408-3430.

<https://proceedings.mlr.press/v202/cai23b/cai23b.pdf>

[C5] Cong Dao Tran, Nhut Huy Pham, Anh Nguyen, **Truong-Son Hy**<sup>c</sup>, and Tu Vu, *ViDe-BERTa: A powerful pre-trained language model for Vietnamese*, EACL 2023.

<sup>c</sup>: Corresponding author / PI.

<https://aclanthology.org/2023.findings-eacl.79.pdf>

[C4] **Truong-Son Hy**, Viet Bach Nguyen, Long Tran-Thanh and Risi Kondor, *Temporal Multiresolution Graph Neural Networks For Epidemic Prediction*, ICML 2022 (Workshop on Healthcare AI and COVID-19), Proceedings of Machine Learning Research 184:21-32.

<https://proceedings.mlr.press/v184/hy22a/hy22a.pdf>

[C3] **Truong-Son Hy** and Risi Kondor, *Multiresolution Matrix Factorization and Wavelet Networks on Graphs*, ICML 2022 (Workshop on Topology, Algebra, and Geometry in Machine Learning), Proceedings of Machine Learning Research 196:172-182.

<https://proceedings.mlr.press/v196/hy22a/hy22a.pdf>

<https://arxiv.org/pdf/2111.01940.pdf> (long version)

[C2] Brandon Anderson, [Truong-Son Hy](#) and Risi Kondor. *Cormorant: Covariant molecular neural networks*, NeurIPS 2019.  
<https://dl.acm.org/doi/pdf/10.5555/3454287.3455589>

[C1] Risi Kondor, [Truong-Son Hy](#), Horace Pan, Brandon Anderson and Shubhendu Trivedi, *Covariant compositional networks for learning graphs*, ICLR 2018.  
<https://arxiv.org/pdf/1801.02144.pdf>

Journal  
Publications  
[Google Scholar]  
[ORCID]

[J12] Thanh V. T. Tran, Nhat Khang Ngo, Viet Thanh Duy Nguyen, and [Truong-Son Hy](#)<sup>c</sup>, *LatentDE: Latent-based Directed Evolution for Protein Sequence Design*, Machine Learning: Science and Technology (Q1, Impact Factor = 6.3), Volume 6, Number 1, DOI 10.1088/2632-2153/adc2e2.  
<sup>c</sup>: Corresponding author / PI.  
<https://iopscience.iop.org/article/10.1088/2632-2153/adc2e2/pdf>

[J11] Quang-Dung Dinh, Daniel Kunk, [Truong-Son Hy](#)<sup>c</sup>, Vamsi J. Nalam, and Phuong Dao, *Machine Learning for Automated Electrical Penetration Graph Analysis of Aphid Feeding Behavior: Accelerating Research on Insect-Plant Interactions*, PLOS ONE (Q1, Impact Factor = 2.9, H-index = 435), Volume 20, Number 4, Pages 1-25, DOI 10.1371/journal.pone.0319484.  
<sup>c</sup>: Corresponding author / PI.  
<https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0319484>

[J10] Viet Thanh Duy Nguyen, Nhan Nguyen, and [Truong-Son Hy](#)<sup>c</sup>, *ProteinReDiff: Complex-based ligand-binding proteins redesign by equivariant diffusion-based generative models*, Structural Dynamics (Q1, Impact Factor = 2.8), Volume 11, Issue 6, DOI 10.1063/4.0000271.  
<sup>c</sup>: Corresponding author / PI.  
<https://doi.org/10.1063/4.0000271>

[J9] Khanh-Tung Tran, [Truong-Son Hy](#), Lili Jiang, and Xuan-Son Vu, *MGLEP: Multimodal Graph Learning for Modeling Emerging Pandemics with Big Data*, Scientific Reports (Q1, Impact Factor = 3.8, H-Index = 315), Volume 14, Number 16377, DOI 10.1038/s41598-024-67146-y.  
<https://www.nature.com/articles/s41598-024-67146-y>

[J8] Viet Thanh Duy Nguyen\* and [Truong-Son Hy](#)<sup>\*c</sup>, *Multimodal Pretraining for Unsupervised Protein Representation Learning*, Biology Methods & Protocols (Q1, Impact Factor = 3.6), Volume 9, Issue 1, DOI 10.1093/biomethods/bpae043.  
\*: Co-first authors.  
<sup>c</sup>: Corresponding author / PI.  
<https://doi.org/10.1093/biomethods/bpae043>

[J7] Trong Thanh Tran\* and [Truong-Son Hy](#)<sup>\*c</sup>, *Protein Design by Directed Evolution Guided by Large Language Models*, IEEE Transactions on Evolutionary Computation (Q1, Impact Factor = 14.3), vol. 29, no. 2, pp. 418-428, April 2025, DOI 10.1109/TEVC.2024.3439690.  
\*: Co-first authors.  
<sup>c</sup>: Corresponding author / PI.  
<https://ieeexplore.ieee.org/document/10628050>  
<https://www.biorxiv.org/content/10.1101/2023.11.28.568945v3.full.pdf> (Preprint)

[J6] Nhat Khang Ngo\* and [Truong-Son Hy](#)<sup>\*c</sup>, *Multimodal Protein Representation Learning and Target-aware Variational Auto-encoders for Protein-binding Ligand Generation*, Machine Learning: Science and Technology (Q1, Impact Factor = 6.8), Volume 5, Number 2, DOI 10.1088/2632-2153/ad3ee4.  
\*: Co-first authors.  
<sup>c</sup>: Corresponding author / PI.  
<https://iopscience.iop.org/article/10.1088/2632-2153/ad3ee4>  
<https://openreview.net/pdf?id=4k926QVVM4> (Presented at NeurIPS 2023)

[J5] Thuan Nguyen Anh Trang, Khang Nhat Ngo, Hugo Sonnery, Thieu Vo, Siamak Ravanbakhsh, [Truong-Son Hy](#)<sup>c</sup>, *Scalable Hierarchical Self-Attention with Learnable Hierarchy for Long-Range Interactions*, Transactions on Machine Learning Research (TMLR).  
<sup>c</sup>: Corresponding author / PI.  
<https://openreview.net/pdf?id=qH4YFMyhce>

[J4] Thong Bach, Anh Tong, [Truong-Son Hy](#), Vu Nguyen, and Thanh Nguyen-Tang, *Long-Tailed Visual Recognition with Global Contrastive Learning and Prototype Learning*, Transactions on Machine Learning Research (TMLR).

<https://openreview.net/pdf?id=xWrtiJwJj5>

[J3] Nhat Khang Ngo\*, [Truong-Son Hy](#) <sup>\*c</sup>, and Risi Kondor, *Multiresolution Graph Transformers and Wavelet Positional Encoding for Learning Long-Range and Hierarchical Structures*, The Journal of Chemical Physics (Q1, Impact Factor = 4.4), Volume 159, Issue 3, DOI 10.1063/5.0152833.

\*: Co-first authors.

<sup>c</sup>: Corresponding author / PI.

<https://doi.org/10.1063/5.0152833>

<https://arxiv.org/pdf/2302.08647.pdf> (Spotlight presentation at ICML 2023)

[J2] [Truong-Son Hy](#) and Risi Kondor, *Multiresolution Equivariant Graph Variational Autoencoder*, Machine Learning: Science and Technology (Q1, Impact Factor = 6.8), Volume 4, Number 1, DOI 10.1088/2632-2153/acc0d8.

<https://iopscience.iop.org/article/10.1088/2632-2153/acc0d8>

<https://arxiv.org/pdf/2106.00967.pdf> (Spotlight presentation at ICML 2022, AI for Science Workshop)

[J1] [Truong-Son Hy](#), Shubhendu Trivedi, Horace Pan, Brandon M. Anderson and Risi Kondor, *Predicting molecular properties with covariant compositional networks*, The Journal of Chemical Physics (Q1, Impact Factor = 4.4), Volume 148, Issue 24, DOI 10.1063/1.5024797.

<https://aip.scitation.org/doi/10.1063/1.5024797>

**Workshop Paper  
Presentations**  
[[Google Scholar](#)]  
[[ORCID](#)]

[W9] Tan-Hanh Pham, Bui Trong Duong, Luu Quang Minh, Pham Tan Huong, Chris Ngo, and [Truong-Son Hy](#) <sup>c</sup>, *SilVar-Med: A Speech-Driven Visual Language Model for Explainable Abnormality Detection in Medical Imaging*, CVPR 2025 (Multimodal Algorithmic Reasoning Workshop).

<https://openreview.net/forum?id=4x9nDiilLc> (abstract)

<https://openreview.net/pdf?id=4x9nDiilLc> (paper)

[W8] Viet Anh Nguyen, Nhat Khang Ngo, and [Truong-Son Hy](#) <sup>c</sup>, *Range-aware Positional Encoding via High-order Pretraining: Theory and Practice*, NeurIPS 2024 (Workshop on Symmetry and Geometry in Neural Representations).

<sup>c</sup>: Corresponding author / PI.

<https://openreview.net/pdf?id=tN0n5BuLEI> (extended abstract)

<https://arxiv.org/pdf/2409.19117>

[W7] Thanh V. T. Tran, Nhat Khang Ngo, Viet Thanh Duy Nguyen, and [Truong-Son Hy](#) <sup>c</sup>, *LatentDE: Latent-based Directed Evolution accelerated by Gradient Ascent for Protein Sequence Design*, NeurIPS 2024.

<sup>c</sup>: Corresponding author / PI.

<https://openreview.net/pdf?id=4YkbQGVWGF> (AI for Accelerated Materials Design)

<https://openreview.net/pdf?id=8AmP6pQwyP> (AI for New Drug Modalities)

[W6] Khai-Nguyen Nguyen, Khai Le-Duc, Bach Phan Tat, Le Duy, Jerry Ngo, Long Vo-Dang, Anh Totti Nguyen, and [Truong-Son Hy](#) <sup>c</sup>, *Sentiment Reasoning for Healthcare*, NeurIPS 2024 (Advancements In Medical Foundation Models: Explainability, Robustness, Security, and Beyond).

<sup>c</sup>: Corresponding author / PI.

<https://openreview.net/pdf?id=WYn6YIjR41>

[W5] Quang Pham Phuoc Minh, Tiet Nguyen Khoi Nguyen, Lan Chi Ngo, Tho Truong Do, and [Truong-Son Hy](#) <sup>c</sup>, *ESGNN: Towards Equivariant Scene Graph Neural Network for 3D Scene Understanding*, 2024 33rd IEEE International Conference on Robot and Human Interactive Communication.

<sup>c</sup>: Corresponding author / PI.

<https://arxiv.org/pdf/2407.00609.pdf>



[W4] Hugo Sonnerly, Thuan Trang, Thieu N. Vo, Siamak Ravanbakhsh, and **Truong-Son Hy**<sup>c</sup>, *Sequoia: Hierarchical Self-Attention Layer with Sparse Updates for Point Clouds and Long Sequences*, ICLR 2023 (Workshop on Sparsity in Neural Networks).

<sup>c</sup>: Corresponding author / PI.

[https://hytruongson.github.io/HySonLab/Sequoia\\_ICLR\\_2023.pdf](https://hytruongson.github.io/HySonLab/Sequoia_ICLR_2023.pdf)

[W3] Viet Bach Nguyen\*, **Truong-Son Hy**<sup>\*c</sup>, Long Tran-Thanh, and Nhung Nghiem, *Predicting COVID-19 pandemic by spatio-temporal graph neural networks: A New Zealand's study*, NeurIPS 2023 (Temporal Graph Learning Workshop).

\*: Co-first authors.

<sup>c</sup>: Corresponding author / PI.

<https://openreview.net/pdf?id=tkjGiKs2g6>

<https://arxiv.org/pdf/2305.07731.pdf> (long version)

[W2] Nhat Khang Ngo\*, **Truong-Son Hy**<sup>\*c</sup>, and Risi Kondor, *Predicting Drug-Drug Interactions using Deep Generative Models on Graphs*, NeurIPS 2022 (AI for Science Workshop).

\*: Co-first authors.

<sup>c</sup>: Corresponding author / PI.

<https://arxiv.org/pdf/2209.09941.pdf>

[W1] Yanan Long, Horace Pan, Chao Zhang, **Truong-Son Hy**, Risi Kondor, and Andrey Rzhetsky, *Molecular Fingerprints Are a Simple Yet Effective Solution to the Drug-Drug Interaction Problem*, ICML 2022 (Workshop on Computational Biology).

[https://icml-compbio.github.io/2022/papers/WCBICML2022\\_paper\\_72.pdf](https://icml-compbio.github.io/2022/papers/WCBICML2022_paper_72.pdf)

**Preprints &  
Under Review**  
[Google Scholar]  
[ORCID]

[P22] Viet Thanh Duy Nguyen, and **Truong-Son Hy**<sup>c</sup>, *Advances in Protein Representation Learning: Methods, Applications, and Future Directions*, 2025.

<sup>c</sup>: Corresponding author / PI.

<https://arxiv.org/pdf/2503.16659.pdf>

[P21] Tuan-Anh Yang, **Truong-Son Hy**<sup>c</sup>, and Phuong D. Dao, *MOB-GCN: A Novel Multiscale Object-Based Graph Neural Network for Hyperspectral Image Classification*, 2025.

<sup>c</sup>: Corresponding author / PI.

<https://arxiv.org/pdf/2502.16289.pdf>

[P20] Khai Le-Duc, Phuc Phan, Tan-Hanh Pham, Bach Phan Tat, Minh-Huong Ngo, and **Truong-Son Hy**<sup>c</sup>, *MultiMed: Multilingual Medical Speech Recognition via Attention Encoder Decoder*, 2025.

<sup>c</sup>: Corresponding author / PI.

<https://arxiv.org/pdf/2409.14074.pdf>

[P19] Cong Nga Ha, Phuc Pham, and **Truong-Son Hy**<sup>c</sup>, *LANTERN: Leveraging Large Language Models and Transformers for Enhanced Molecular Interactions*, DOI 10.1101/2025.02.10.637522.

<sup>c</sup>: Corresponding author / PI.

<https://www.biorxiv.org/content/10.1101/2025.02.10.637522v1.full.pdf>

[P18] Minh Ngoc Nguyen, Khai Le-Duc, Tan-Hanh Pham, Trang Nguyen, Quang Minh Luu, Ba Kien Tran, **Truong-Son Hy**, Viktor Dremine, Sergei Sokolovsky, and Edik Rafailov, *A Wearable Device Dataset for Mental Health Assessment Using Laser Doppler Flowmetry and Fluorescence Spectroscopy Sensors*, 2024.

<https://arxiv.org/pdf/2502.00973.pdf>

[P17] Tien Dang, Viet Thanh Duy Nguyen, Minh Tuan Le, and **Truong-Son Hy**<sup>c</sup>, *Multi-modal Contrastive Representation Learning in Augmented Biomedical Knowledge Graphs*, 2024.

<sup>c</sup>: Corresponding author / PI.

<https://arxiv.org/pdf/2501.01644.pdf>

[P16] Van Quang Nguyen, Quoc Chuong Nguyen, Thu Huong Dang, and **Truong-Son Hy**<sup>c</sup>, *Hybridising Reinforcement Learning and Heuristics for Hierarchical Directed Arc Routing Problems*, 2024.

<sup>c</sup>: Corresponding author / PI.

<https://arxiv.org/pdf/2501.00852.pdf>

[P15] Tan-Hanh Pham, Hoang-Nam Le, Phu-Vinh Nguyen, Chris Ngo, and **Truong-Son Hy**<sup>c</sup>, *SilVar: Speech Driven Multimodal Model for Reasoning Visual Question Answering and Object Localization*, 2024.

c: Corresponding author / PI.

<https://arxiv.org/pdf/2412.16771.pdf>

[P14] Phuc Pham, Viet Thanh Duy Nguyen, Kyu Hong Cho, and **Truong-Son Hy**<sup>c</sup>, *Generative AI-assisted Virtual Screening Pipeline for Generalizable and Efficient Drug Repurposing*, DOI 10.1101/2024.12.07.627340.

c: Corresponding author / PI.

<https://www.biorxiv.org/content/10.1101/2024.12.07.627340v1.full.pdf>

[P13] Quang Dung Dinh, Daniel Kunk, **Truong-Son Hy**<sup>c</sup>, Vamsi J Nalam, and Phuong Dao, *DiscoEPG: A Python package for characterization of insect electrical penetration graph (EPG) signals*, DOI 10.1101/2024.12.05.627099.

c: Corresponding author / PI.

<https://www.biorxiv.org/content/10.1101/2024.12.05.627099v2.full.pdf>

[P12] Quang P. M. Pham, Khoi T. N. Nguyen, Lan C. Ngo, Dezhen Song, Truong Do, and **Truong-Son Hy**<sup>c</sup>, *TESGNN: Temporal Equivariant Scene Graph Neural Networks for Efficient and Robust Multi-View 3D Scene Understanding*, 2024.

c: Corresponding author / PI.

<https://arxiv.org/pdf/2411.10509.pdf>

[P11] Viet Anh Nguyen, Nhat Khang Ngo, and **Truong-Son Hy**<sup>c</sup>, *Range-aware Positional Encoding via High-order Pretraining: Theory and Practice*, 2024.

c: Corresponding author / PI.

<https://arxiv.org/pdf/2409.19117.pdf>

[P10] Viet Tien Pham, Minh Hieu Ha, Bao V. Q. Bui and **Truong-Son Hy**<sup>c</sup>, *LightMed: A Light-weight and Robust FFT-Based Model for Adversarially Resilient Medical Image Segmentation*, DOI 10.1101/2024.09.28.615584, 2024.

c: Corresponding author / PI.

<https://www.biorxiv.org/content/10.1101/2024.09.28.615584v1.full.pdf>

[P9] Tam Trinh, Anh Dao, Hy Thi Hong Nhung, and **Truong-Son Hy**<sup>c</sup>, *VietMedKG: Knowledge Graph and Benchmark for Traditional Vietnamese Medicine*, DOI 10.1101/2024.08.07.606195, 2024.

c: Corresponding author / PI.

<https://www.biorxiv.org/content/10.1101/2024.08.07.606195v3.full.pdf>

[P8] Khai Le-Duc, Quy-Anh Dang, Tan-Hanh Pham, and **Truong-Son Hy**<sup>c</sup>, *wav2graph: A Framework for Supervised Learning Knowledge Graph from Speech*, 2024.

c: Corresponding author / PI.

<https://arxiv.org/pdf/2408.04174.pdf>

[P7] Khai Le-Duc, Khai-Nguyen Nguyen, Bach Phan Tat, Duy Le, Jerry Ngo, Long Vo-Dang, Anh Totti Nguyen, and **Truong-Son Hy**<sup>c</sup>, *Sentiment Reasoning for Healthcare*, 2024.

c: Corresponding author / PI.

<https://arxiv.org/pdf/2407.21054.pdf>

[P6] Khai Le-Duc, Ryan Zhang, Ngoc Son Nguyen, Tan-Hanh Pham, Anh Dao, Ba Hung Ngo, Anh Totti Nguyen, and **Truong-Son Hy**<sup>c</sup>, *LiteGPT: Large Vision-Language Model for Joint Chest X-ray Localization and Classification Task*, 2024.

c: Corresponding author / PI.

<https://arxiv.org/pdf/2407.12064.pdf>

[P5] Cong Dao Tran\*, Thong Bach\*, and **Truong-Son Hy**<sup>\*c</sup>, *Symmetry-preserving graph attention network to solve routing problems at multiple resolutions*, 2023.

\*: Co-first authors.

c: Corresponding author / PI.

<https://arxiv.org/pdf/2310.15543.pdf>

[P4] **Truong-Son Hy** and Cong Dao Tran, *Graph Attention-based Deep Reinforcement Learning for solving the Chinese Postman Problem with Load-dependent costs*, 2023.

<https://arxiv.org/pdf/2310.15516.pdf>

[P3] Ngoc-Dung Do\*, **Truong-Son Hy**\*<sup>c</sup> and Duy Khuong Nguyen, *Sparsity exploitation via discovering graphical models in multi-variate time-series forecasting*, 2023.

\*: Co-first authors.

<sup>c</sup>: Corresponding author / PI.

<https://arxiv.org/pdf/2306.17090.pdf>

[P2] Erik Henning Thiede, **Truong-Son Hy** and Risi Kondor, *The general theory of permutation equivariant neural networks and higher order graph variational encoders*, 2020.

<https://arxiv.org/pdf/2004.03990.pdf>

[P1] **Truong-Son Hy** and Chris Jones, *Graph neural networks with efficient tensor operations in CUDA/GPU and GraphFlow deep learning framework in C++ for quantum chemistry*, 2019.

<https://hytruongson.github.io/HySonLab/CCN-GraphFlow.pdf>

**PhD Students** At University of Alabama at Birmingham, I am grateful to advise talented and hard-working PhD students:

- Viet Thanh Duy Nguyen (from Spring 2025)

**PhD Committee** It is my honor to serve in the PhD committee of:

- Tien Kha Pham, Deakin University, Australia in 2024. His PhD thesis' title is "Memory for Fast Adaptation in Neural Networks".
- Shishir Sarker, Department of Biology, Indiana State University, United States from 2024. His PhD thesis' theme is "Study of regulating the virulence effect by inhibiting SIP binding to RopB".

At University of Alabama at Birmingham, I serve in the PhD committee for junior PhD students:

- Sharif Noor Zisad (from 2024)
- Delower Hossain (from 2024)
- Mengchen Fan (from 2024)
- Sheikh Abujar (from 2024)

**Organizer & Area Chair** I co-organize and serve as a senior meta-reviewer, i.e. area chair, for the following conferences:

- BIODDD 2025 (August 2025) [website]

**Reviewer**

**Journals** (ORCID: <https://orcid.org/0000-0002-5092-3757>)

1. **Nature - Scientific Reports** [Certificate - 01/26/25] [Certificate - 02/24/25]
2. **Computational and Structural Biotechnology Journal** (Elsevier) [Certificate]
3. **Neural Networks** (Elsevier) [Certificate]
4. **BMC Biology** (Springer Nature) [Certificate]
5. **BMC Bioinformatics** (Springer Nature) [Certificate]
6. **Nature - Communications Biology**
7. **Machine Learning** (Springer Nature)
8. **PLOS Computational Biology**
9. **SIAM Journal on Matrix Analysis and Applications**
10. **IEEE Journal of Biomedical and Health Informatics**
11. **IEEE Transactions on Computational Biology and Bioinformatics**
12. **IEEE Transactions on Multimedia**
13. **National Science Review** (Oxford University Press)
14. **Advanced Science** (Wiley)
15. **Journal of Machine Learning Research (JMLR)**



## Conferences

1. **NeurIPS**: 2024, 2023, 2022, 2021
2. **CVPR**: 2025
3. **ICCV**: 2025
4. **ICML**: 2022
5. **ICLR**: 2025, 2024
6. **AISTATS**: 2025, 2024
7. **AAAI**: 2025, 2024, 2023
8. **KDD**: 2025, 2024
9. **Learning on Graphs (LoG)**: 2023, 2022
10. **EMNLP**: 2023
11. **ACL**: 2025, 2024
12. **NAACL**: 2025
13. **IEEE ROMAN**: 2024
14. **ICASSP**: 2025 [Certificate]

## Software

[HySonLab]  
[HyTruongSon]

33. **WaveletPE**: Range-aware Graph Positional Encoding via High-order Pretraining.  
<https://github.com/HySonLab/WaveletPE>
32. **LANTERN**: Leveraging Large Language Models and Transformers for Enhanced Molecular Interactions.  
<https://github.com/HySonLab/LANTERN>
31. **MOB-GCN**: Multiscale Object-Based Graph Neural Network for Hyperspectral Image Segmentation and Classification.  
<https://github.com/HySonLab/MultiscaleHSI>
30. **BioMedKG**: Multimodal Contrastive Representation Learning in Augmented Biomedical Knowledge Graphs.  
<https://github.com/HySonLab/BioMedKG>
29. **ArcRoute**: Hybrid algorithm combining Reinforcement Learning (RL) and heuristics to solve Hierarchical Directed Capacitated Arc Routing Problem (HDCARP).  
<https://github.com/HySonLab/ArcRoute>
28. **DrugPipe**: Generative AI-assisted Drug Repurposing Pipeline.  
<https://github.com/HySonLab/DrugPipe>
27. **TESGNN**: 3D Temporal Equivariant Scene Graph Neural Networks.  
<https://github.com/HySonLab/TESGraph>
26. **LightMed**: A Light-weight and Robust FFT-Based Model for Adversarially Resilient Medical Image Segmentation.  
<https://github.com/HySonLab/LightMed>
25. **EntityKG**: A Framework for Supervised Learning Knowledge Graph from Speech.  
<https://github.com/HySonLab/EntityKG>
24. **VietMedKG**: Knowledge Graph and Benchmark for Traditional Vietnamese Medicine.  
<https://github.com/HySonLab/VietMedKG>
23. **ML4Insects**: A library for EPG signal analysis of pierce-sucking insects.  
<https://github.com/HySonLab/ML4Insects/>
22. **Hierarchical Attention**: Scalable Hierarchical Self-Attention with Learnable Hierarchy for Long-Range Interactions (TMLR).  
<https://github.com/HySonLab/HierAttention>

- 21. EquiMesh:** E(3)-Equivariant Mesh Neural Networks (AISTATS 2024).  
<https://github.com/HySonLab/EquiMesh>
- 20. Protein-Redesign:** Complex-based Ligand-Binding Proteins Redesign by Equivariant Diffusion-based Generative Models.  
[https://github.com/HySonLab/Protein\\_Redesign](https://github.com/HySonLab/Protein_Redesign)
- 19. LatentDE:** Latent-based Directed Evolution for Protein Design.  
<https://github.com/HySonLab/LatentDE>
- 18. Protein-Pretrain:** Multimodal Pretraining for Unsupervised Protein Representation Learning.  
[https://github.com/HySonLab/Protein\\_Pretrain](https://github.com/HySonLab/Protein_Pretrain)
- 17. Protein-Design:** Protein Design by Machine Learning guided Directed Evolution.  
[https://github.com/HySonLab/Directed\\_Evolution](https://github.com/HySonLab/Directed_Evolution)
- 16. Multires-NP-hard:** Symmetry-preserving and multiresolution Reinforcement Learning to solve NP-hard problems in Operations Research including TSP and VRP.  
<https://github.com/HySonLab/Multires-NP-hard>
- 15. CPP-LC:** Implementation in C++ for the Chinese postman problem with load constraints (CPP-LC) with Evolutionary Algorithm, Ant Colony Optimization and many other meta-heuristics.  
[https://github.com/HySonLab/Chinese\\_Postman\\_Problem](https://github.com/HySonLab/Chinese_Postman_Problem)
- 14. Ligand generation:** Target-aware Variational Auto-encoders for Ligand Generation with Multimodal Protein Representation Learning.  
[https://github.com/HySonLab/Ligand\\_Generation](https://github.com/HySonLab/Ligand_Generation)
- 13. GraphLASSO:** Sparsity exploitation via discovering graphical models in multi-variate time-series forecasting.  
<https://github.com/HySonLab/GraphLASSO>
- 12. Machine Learning for Epidemiology:** Predicting COVID-19 pandemic by spatio-temporal graph neural networks.  
[https://github.com/HySonLab/pandemic\\_tgnn](https://github.com/HySonLab/pandemic_tgnn)
- 11. Multiresolution Graph Transformers:** Learning hierarchical structures including proteins, peptides, and polymers by multiresolution graph transformers and wavelet positional encoding.  
<https://github.com/HySonLab/Multires-Graph-Transformer>
- 10. TWGNN:** Fast Temporal Wavelet Graph Neural Networks for learning timeseries with underlying graph structure with applications in traffic prediction and brain networks.  
<https://github.com/HySonLab/TWGNN>
- 9. ViDeBERTa:** A powerful pre-trained language model for Vietnamese (EACL 2023).  
<https://github.com/HySonLab/ViDeBERTa>
- 8. Drugs-Proteins knowledge graph:** Large-scale deep generative models on multi-modal knowledge graph for predicting drug interactions.  
<https://github.com/HySonLab/drug-interactions>
- 7. Spherical CNNs:** PyTorch implementation of Spherical Convolutional Neural Networks with Clebsch–Gordan transform for nonlinearity in the Fourier space.  
<https://github.com/risilab/SphericalNet>
- 6. Learnable MMF:** Learning Multiresolution Matrix Factorization and its Wavelet Networks on Graphs.  
[https://github.com/risilab/Learnable\\_MMF](https://github.com/risilab/Learnable_MMF)

**5. MGVAE:** Multiresolution Equivariant Graph Variational Autoencoder (MGVAE) and Multiresolution Graph Networks (MGN) for supervised molecular properties prediction, unsupervised molecular representation learning, graph generation, citation link prediction and graph-based image generation.

<https://github.com/HyTruongSon/MGVAE>

**4. LibCCNs:** Covariant Compositional Networks Library is an easy-to-use and efficient implementation of Covariant Compositional Networks (CCNs) with TensorFlow and PyTorch's APIs based on a shared common C++ core.

<https://github.com/HyTruongSon/LibCCNs>

**3. Invariant Graph Networks:** A PyTorch implementation of the Invariant and Equivariant Graph Networks.

<https://github.com/HyTruongSon/InvariantGraphNetworks-PyTorch>

**2. GraphFlow:** Deep Learning framework built from scratch in C++/CUDA that supports symbolic/automatic differentiation, dynamic computation graphs, tensor/matrix operations accelerated by GPU and implementations of various state-of-the-art graph neural networks and other Machine Learning models.

<https://github.com/HyTruongSon/GraphFlow>

**1. Fourier Transform Library:** 1D/2D FFT, DFT and DCT; JPEG image compression.

<https://github.com/HyTruongSon/Fourier-Transform-Library>

## Awards

**Data Science Postdoctoral Fellowship**

September 2022 – July 2024

Awarded by the Halicioglu Data Science Institute at University of California San Diego.

**Postdoctoral Fellowship (Declined)**

September 2022 – July 2024

Awarded by the Vector Institute (Canada).

**University Unrestricted (UU) PhD Fellowship**

Spring quarter 2022

Awarded by the graduate committee at University of Chicago.

**University Unrestricted (UU) PhD Fellowship**

Autumn quarter 2017

Awarded by the graduate committee at University of Chicago.

**First-class Graduation Honor**

Class of 2016

Awarded by the highest GPA achiever by Faculty of Informatics at Eötvös Loránd University.

**The title of Excellent Student of the Faculty**

Academic year 2014 - 2015

Awarded to 2 out of 4,000 BSc. students (0.05%) of the Faculty of Informatics with outstanding academic performance and scientific activity at Eötvös Loránd University.

**Stipendium Hungaricum Full Scholarship**

September 2013 – July 2016

Awarded by the Government of Hungary that covers tuition fee and living expenses.

**First position at National Conference of Students' Scientific Association** April 2015

Thesis: *Semi-supervised Adaptive Facial Tracking Method*.

**Morgan Stanley Scholarship**

2015

Amount: 75,000 HUF.

**1st place at Hungarian ACM Programming Contest**

October 2015

Team ELTE-Sparrows solved 9/10 problems, ranked 1 out of 35 teams nationwide.

**The 2015 ACM ICPC Central Europe Regional Contest**

November 2015

Team ELTE-1 achieved Honorable Mention in Zagreb, Croatia.

**2nd place at Hungarian ACM Programming Contest**

October 2014

Team ELTE-UFGM-UFPB solved 5/10 problems, ranked 2 out of 33 teams nationwide.

**The 2014 ACM ICPC Central Europe Regional Contest**

November 2014

Team ELTE-2 achieved Honorable Mention in Krakow, Poland.

- 7th place at ACM ICPC Asia Regional Programming Contest** November 2012  
Team DiscreteMath achieved Consolidation prize, ranked 7 out of 59 teams from Asia.
- Special prize at the NAPROCK 4th International Programming Contest** 2012  
Location: Omuta, Japan.
- Silver Cup at the Vietnam Olympic of University Students in Informatics** 2012  
Location: Hanoi, Vietnam.
- Runner-up prize at the National Excellent Student Contest in Informatics** 2011  
Location: Hanoi, Vietnam.

## Media

- The newspaper of Vietnam Ministry of Science & Technology wrote an article about my lab's research in AI for Protein Design: [\[link\]](#)
- UAB wrote an article about my lab's research in AI for Drug Discovery: [\[link\]](#)
- Article about myself at Thanh Nien Newspaper, one of the major newspapers in Vietnam: [\[Vietnamese\]](#) [\[English\]](#)
- Article about my advices for younger generation at Thanh Nien Newspaper: [\[Vietnamese\]](#)
- At my middle school in 2024: [\[link\]](#)
- At UChicago in 2020: [\[link\]](#)
- At ELTE in 2016: [\[link\]](#)

## Invited Talks

- 13. UAB Department of Mechanical and Materials Engineering** January 24, 2025  
Talk: *Geometric Deep Learning for Protein Science and Drug Discovery*.  
Host: Prof. Mark Banaszak Holl.
- 12. University of Alabama at Birmingham** May 15, 2024  
Talk: *Geometric Deep Learning for Protein Science and Drug Discovery*.  
Host: Prof. Ragib Hasan.
- 11. University of Massachusetts Boston** April 11, 2024  
Talk: *Geometric Deep Learning for Protein Science and Drug Discovery*.  
Host: Prof. Albert Kao.
- 10. VinUniversity** December 28, 2023  
Talk: *Graph representation learning and Deep generative models on graphs*.  
Host: Prof. Le Duy Dung (Andrew).
- 9. Indiana State University** February 1, 2023  
Talk: *Graph representation learning and Deep generative models on graphs*.  
Host: Prof. Arash Rafiey.
- 8. Virginia Commonwealth University** September 30, 2022  
Talk: *Graph representation learning and Deep generative models on graphs*.  
Host: Prof. Thang Dinh.
- 7. Le Quy Don Technical University (Military Technical Academy)** September 8, 2022  
Talk: *Graph representation learning and Deep generative models on graphs*.  
Host: Faculty of Information Technology.
- 6. FPT Software** June 2, 2022  
Talk: *Graph representation learning and Deep generative models on graphs*.  
Host: FPT AI Center.
- 5. Vector Institute for Artificial Intelligence** April 6, 2022  
Talk: *Graph representation learning and Deep generative models on graphs*.  
Host: Prof. Pascal Poupart.

#### 4. University of California San Diego

February 24, 2022

Talk: *Graph representation learning and Multiresolution machine learning.*

Host: Prof. Rose Yu, Prof. Yusu Wang.

#### 3. California Institute of Technology

February 3, 2022

Talk: *Graph representation learning, deep generative models on graphs and multiresolution machine learning.*

Host: Prof. Anima Anandkumar.

#### 2. University of Illinois Chicago

January 26, 2022

Talk: *Graph representation learning and Deep generative models on graphs.*

Host: Department of Mathematics, Statistics, and Computer Science.

#### 1. Argonne National Laboratory

January 5, 2022

Talk: *Graph representation learning, deep generative models on graphs and multiresolution machine learning.*

Host: Dr. Stefan Wild, Dr. Emil Constantinescu.

#### Senior Collaborators

- Prof. Risi Kondor, University of Chicago [website]
- Prof. Yusu Wang, University of California San Diego [website]
- Prof. Andrey Rzhetsky, University of Chicago [website]
- Prof. Siamak Ravanbakhsh, McGill University / MILA (Canada) [website]
- Prof. Long Tran-Thanh, University of Warwick (United Kingdom) [website]
- Prof. Huong Dang, Lancaster University (United Kingdom) [website]
- Prof. Erik Thiede, Cornell University [website]
- Prof. Arash Rafiey, Indiana State University [website]
- Prof. Takuya Akiyama, Indiana State University [website]
- Prof. Kyu Hong Cho, Indiana State University [website]
- Prof. Thang N. Dinh, Virginia Commonwealth University [website]
- Prof. Phuong Dao, Colorado State University [website]
- Prof. Vamsi Nalam, Colorado State University [website]
- Prof. Rhett Davis, North Carolina State University [website]
- Prof. Nhung Nghiem, Australian National University (Australia) [website]
- Dr. Thieu N. Vo, Ton Duc Thang University (Vietnam) [website]
- Dr. Nghi D. Q. Bui, FPT Software AI Center (Vietnam) [website]
- Dr. Dao Huu Hung, FPT Software AI Center (Vietnam) [website]
- Dr. Van Nguyen, FPT Software AI Center (Vietnam) [website]
- Dr. Rajeev Jain, Qualcomm [website]
- Dr. Michael Defferrard, Qualcomm [website]
- Prof. Matthew Might, University of Alabama at Birmingham [website]

#### Teaching Assistant (UChicago)

#### 9. CAPP 30271 - Mathematics for Computer Science and Data Analysis

Winter 2022

Instructor: Prof. Amitabh Chaudhary

#### 8. MPCS 53112 - Advanced Data Analytics

Autumn 2021

Instructor: Prof. Amitabh Chaudhary

#### 7. CMSC 25025 - Machine Learning & Large-Scale Data Analysis

Spring 2021

Instructor: Prof. Yali Amit

#### 6. CMSC 35400 - Machine Learning

Winter 2021

Instructor: Prof. Yuxin Chen

Website: <https://sites.google.com/uchicago.edu/stat-37710-cmsc-35400-w21/>

- 5. CMSC 25025 - Machine Learning & Large-Scale Data Analysis** Spring 2019  
Instructor: Prof. Yali Amit
- 4. CMSC 15100 - Introduction to Computer Science I** Autumn 2018  
Instructor: Adam Shaw & Matthew Wachs  
Website: <http://people.cs.uchicago.edu/~adamshaw/cmssc15100-2018/index.html>
- 3. MPCS 53111 - Machine Learning** Spring 2017  
Instructor: Prof. Amitabh Chaudhary  
Website: <https://mpcs-courses.cs.uchicago.edu/2015-16/spring/courses/53111>
- 2. CMSC 25400 - Machine Learning** Winter 2017  
Instructor: Prof. Risi Kondor  
Website: <http://people.cs.uchicago.edu/~risi/cmssc25400.html>
- 1. CMSC 22600 - Compilers for Computer Languages** Autumn 2016  
Instructor: Prof. John Reppy  
Website: <https://www.classes.cs.uchicago.edu/archive/2016/fall/22600-1/>

## Professional Memberships

- Institute of Electrical and Electronics Engineers (IEEE): Since 2024
- Association for Computing Machinery (ACM): Since 2024

## Qualifications

*Programming Languages:* C/C++, Java, Python, Matlab, Haskell, Ada, Pascal, SQL, HTML/CSS.  
*Libraries:* TensorFlow, PyTorch, STL, OpenGL,  $\text{\LaTeX}$ .  
*Tools:* Vim, Netbeans, Eclipse, Codeblocks, Dev-C++, Microsoft Visual Studio & Office.