

## Chenqing (William) Hua

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**OBJECTIVE** I specialize in developing graph neural networks, and their applications for learning representations of molecular and protein data. My current research focuses on encoding protein sequences into geometric representations to predict protein interactions, understanding and simulating the natural protein docking process, and discovering the use of chemical inducers in protein interactions.

**CURRENT OCCUPATION** **McGill University & Mila** Sep, 2022 - May, 2024  
*Master of Science (M.Sc), Fully Funded*  
Specialization: Geometric Deep Learning, Graph Neural Nets, Drug Discovery  
Supervisor: Professor Doina Precup (main) & Professor Guy Wolf

**EDUCATION** **McGill University** Sept, 2018 - May, 2022  
*Honours Computer Science with First-Class Honours, Bachelor of Science (B.Sc)*  
Cumulative GPA: 3.90/4.00  
Thesis: Is Heterophily A Real Nightmare For Graph Neural Networks To Do Node Classification?  
Supervisor: Professor William L. Hamilton

**RESEARCH INTEREST**  
(1) Geometric Deep Learning for Molecules and Proteins  
(2) Deep Generative Models for Molecules and Proteins  
(3) Applications of Graph Representation Learning in Drug Discovery and Health  
(4) Large language Models in Graph Representation Learning for Drug Discovery

**RESEARCH POSITION** **Aureka Biotechnologies** Sept, 2023 - Now  
*Supervisor: Shuangjia Zheng*  
*Effective Protein-Protein Interaction Exploration with PPIretrieval*

**Montreal Institute of Learning Algorithms** May, 2022 - Dec, 2022  
*Supervisor: Yoshua Bengio*  
*GFlowNets for Molecular Conformation Generation*

**Montreal Institute of Learning Algorithms** June, 2021 - Jan, 2022  
*Supervisor: Jian Tang & Guillaume Rabusseau*  
*High-Order Pooling for Graph Neural Networks with Tensor Decomposition*

**Montreal Institute of Learning Algorithms** Dec, 2020 - Apr, 2021  
*Supervisor: William L. Hamilton*  
*Is Heterophily A Real Nightmare For Graph Neural Networks To Do Node Classification?*

**Publication** **MUDiff: Unified Diffusion for Complete Molecule Generation**  
2nd Learning on Graphs Conference  
<https://arxiv.org/abs/2304.14621>  
Hua, C., Luan, S., Xu, M., Ying, R., Fu, J., Ermon, S., Precup, D.

**When Do Graph Neural Networks Help with Node Classification? Investigating the Homophily Principle on Node Distinguishability**  
37th Conference on Neural Information Processing Systems  
<https://arxiv.org/abs/2304.14274>  
Luan, S., Hua, C., Xu, M., Lu, Q., Zhu, J., Chang, XW., Fu, J., Leskovec, J., Precup, D.

**When Do We Need GNN for Node Classification?**  
12th International Conference on Complex Networks and their Applications

<https://arxiv.org/abs/2210.16979>

Luan, S., **Hua, C.**, Lu, Q., Zhu, Jia., Chang, X. W., Precup, D.

**Complete the Missing Half: Augmenting Aggregation Filtering with Diversification for Graph Convolutional Networks**

36th Conference on Neural Information Processing Systems, GLFrontiers (**Oral**)

<https://arxiv.org/abs/2008.08844>

Luan, S.\*, Zhao, M.\*, **Hua, C.\***, Chang, X. W., Precup, D.

**Revisiting Heterophily For Graph Neural Networks**

36th Conference on Neural Information Processing Systems (**Spotlight**)

<https://arxiv.org/abs/2210.07606>

Luan, S., **Hua, C.**, Lu, Q., Zhu, Jia., Zhao, M., Zhang, S., Chang, X. W., Precup, D.

**High-Order Pooling for Graph Neural Networks with Tensor Decomposition**

36th Conference on Neural Information Processing Systems

<https://arxiv.org/abs/2205.11691>

**Hua, C.**, Rabusseau, G., Tang, J.

**PREPRINT**

**Effective Protein-Protein Interaction Exploration with PPIretrieval**

<https://arxiv.org/abs/2402.03675>

**Hua, C.**, Coley, C., Wolf, G., Precup, D., Zheng, S.

**Graph neural networks intersect probabilistic graphical models:**

**A survey**

<https://arxiv.org/abs/2206.06089>

**Hua, C.**, Luan, S., Zhang, Q., Fu, J.

**Is Heterophily A Real Nightmare For Graph Neural Networks To Do Node Classification?**

<https://arxiv.org/abs/2109.05641>

Luan, S.\*, **Hua, C.\***, Chang, X. W., Precup, D.

**AWARD &  
SCHOLARSHIP**

**ICML2023 Travel Award**

July, 2023

**Neurips 2022 Scholar Award**

Nov, 2022-Dec, 2022

**Scholarship of FACS-Acuity Project**

May, 2022-Now

Ministre de l'conomie et de l'Innovation Canada

**Scholarship of CIFAR AI chair program**

May, 2021-Aug, 2021

Canadian Institute for Advanced Research

**Scholarship of Discovery program**

May, 2021-Aug, 2021

Natural Sciences and Engineering Research Council of Canada

**Funding of Calcul Qubec**

May, 2021-Aug, 2021

Calcul Qubec

**Funding of Digital Research Alliance of Canada**

May, 2021-Aug, 2021

Digital Research Alliance of Canada

**Funding of NVIDIA**

May, 2021-Aug, 2021

NVIDIA

**PAST  
PROJECT**

**Title: GFlowNets for Molecular Conformation Generation**

May, 2022 - Dec, 2022

*Topic: Graph Neural Networks, GFlowNet, Molecule Generation*

**Title: TextWorld Neural Algorithmic Reasoning**

Jul, 2021

*Topic: Graph Neural Networks, Algorithmic Reasoner, Reinforcement Learning*

**ACADEMIC  
SERVICE**

**ICML2022, LoG2022, NeurIPS2022 AI4Mat, NeurIPS2022 GLFrontier, ICML2023, NeurIPS2023, KDD2023 PhD Consortium, LoG2023,**

	<b>ICLR2024, ICLR2024 GEM, ICLR2024 AGI, ICML2024</b>	Reviewer
	<b>NeurIPS2023 GLFrontier</b>	Area Chair
	<b>LoG2023 Montreal Meetup</b>	Organizer
<b>EMPLOYMENT</b>	<b>MGSC695 Teaching Assistant</b>	<b>Summer 2022</b>
	MGSC695 Intro to AI & Deep Learning II TA at McGill, Montreal.	
	<b>MGSC673 Teaching Assistant</b>	<b>Winter 2022</b>
	MGSC673 Intro to AI & Deep Learning I TA at McGill, Montreal.	
	<b>MATH340 Grader</b>	<b>Winter 2020</b>
	MATH340 Discrete Mathematics grader at McGill, Montreal.	