Huu Trong Phan

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Nangang District, Taipei, Taiwan

Research Experience

08/2024–	Post-doctoral Fellow, Institute of Atomic & Molecular Sciences, (Advisor: Dr. Jer-Lai Kuo)
03-08/2016	Research Assistant, Institute of Atomic & Molecular Sciences, (Advisor: Dr. Jer-Lai Kuo)

Education

2016-2024	**Ph.D.**, Department of Chemistry, National Tsing Hua University, Taiwan
2011-2015	**B.Sc.**, Department of Nuclear Physics, Ho Chi Minh University of Sciences, Vietnam

Work Experience

Institute of Atomic & Molecular Sciences, Academia Sinica

Grid-based Basin Hopping: Developed Basin Hopping search algorithm specialized for grid-based carbohydrate sampling using Neural Network Potentials, enabling efficient identification of low-energy conformers across configurational spaces of 10^6-10^9 possibilities.

Developed efficient Machine Learning Pipeline: Integrating Graph Convolutional Neural Network models for structural search, achieving 100x acceleration compared to traditional *ab-initio* methods while maintaining high accuracy in identifying structurally similar local minima via Neural Network Potentials.

Implemented Target Search tools: Developed XGBoost model to predict low-energy local minima structures with 10 kJ/mol accuracy, eliminating need for excessive geometry optimization calculations.

Classification of carbohydrate structure using CNN: Implemented Convolutional Neural Networks on transformed distance matrices to classify carbohydrate types and predict low-energy conformer likelihood, achieving 0.8 F1 score.

Skills

Programming: Proficient Python, SQL, parallel computing, Bash

Library and Frameworks: Pytorch, Keras, OpenCV, SQLAlchemy

QM Packages: LAMMPS, Gaussian, GAMESS

Data analysis & visualization

Misc: High-performance computing (HPC), experience with PBS, SLURM scheduler.

Language: Fluent English, basic Mandarin, Vietnamese

Presentation Awards

Talks

1. **Phan, H. T.** *A neural network potential assisted first-principles exploration of the structure of monosaccharides* The General Meeting of T2CoMSA and 2023 Student Conference.
   – **Best Oral Presentation Award in English**.

Posters

1. **Phan, H. T.** *Unraveling the low-energy conformers of disaccharides with first-principles accuracy assisted by neural network potentials* The General Meeting of T2CoMSA and 2024 Student Conference.
   – **Excellent Poster Award**.
2. **Phan, H. T.** *Unraveling the low-energy conformers of disaccharides with first-principles accuracy assisted by neural network potentials* The 4th Workshop on Frontier Investigations of Key Species in Atmospheric Chemistry and Astrochemistry.
   – **Outstanding Poster Award**.

Tools & Software

Grid-based Basin Hopping: Grid-based sampling of di- and trisaccharides using on-the-fly Basin Hopping search optimized with Neural Network Potentials.

Publications

G Google Scholar

Journal Articles

1. **Phan, H. T.**, Tsou, P.-K., Dong, C.-H., Hsu, P.-J. & Kuo, J.-L. Unraveling the low-energy conformers of neutral and charged mono- and di-saccharides with first-principles accuracy assisted by neural network potentials. *Phys. Chem. Chem. Phys.* (2025/04 Accepted).
2. Tsou, P.-K., **Phan, H. T.** & Kuo, J.-L. Using Building Block Structures and a Cooperative Approach with Neural Networks and Random Forest to Identify Reactions: A Case Study on the Dissociation of Sodiated Disaccharides. *Phys. Chem. Chem. Phys.* **27,** 4355–4367. ISSN: 1463-9084. doi:10.1039/D4CP04275A (2025).
3. **Phan, H. T.**, Tsou, P.-K., Hsu, P.-J. & Kuo, J.-L. A First-Principles Exploration of the Conformational Space of Sodiated Di-Saccharides Assisted by Semi-Empirical Methods and Neural Network Potentials. *Phys. Chem. Chem. Phys.* **26,** 9556–9567. ISSN: 1463-9084. doi:10.1039/D3CP05362H (2024).

4. **Phan**, **H. T.**, Tsou, P.-K., Hsu, P.-J. & Kuo, J.-L. A First-Principles Exploration of the Conformational Space of Sodiated Pyranose Assisted by Neural Network Potentials. *Physical Chemistry Chemical Physics* **25,** 5817–5826. doi:10.1039/D2CP04411K (2023).

5. Tsou, P.-K., Huynh, H. T., **Phan**, **H. T.** & Kuo, J.-L. A Self-Adapting First-Principles Exploration on the Dissociation Mechanism in Sodiated Aldohexose Pyranoses Assisted with Neural Network Potentials. *Phys. Chem. Chem. Phys.* **25,** 3332–3342. ISSN: 1463-9084. doi:10.1039/D2CP04421H (2023).

6. Jindal, S., Hsu, P.-J., **Phan**, **H. T.**, Tsou, P.-K. & Kuo, J.-L. Capturing the Potential Energy Landscape of Large Size Molecular Clusters from Atomic Interactions up to a 4-Body System Using Deep Learning. *Phys. Chem. Chem. Phys.* **24,** 27263–27276. ISSN: 1463-9084. doi:10.1039/D2CP04441B (2022).

7. Thi Huynh, H., Tsai, S.-T., Hsu, P.-J., Biswas, A., **Phan**, **H. T.**, Kuo, J.-L., Ni, C.-K. & Chiu, C.-c. Collision-Induced Dissociation of Na + -Tagged Ketohexoses: Experimental and Computational Studies on Fructose. *Physical Chemistry Chemical Physics* **24,** 20856–20866. doi:10.1039/D2CP02313J (2022).

8. Chiu, C.-c., Huynh, H. T., Tsai, S.-T., Lin, H.-Y., Hsu, P.-J., **Phan**, **H. T.**, Karumanthra, A., Thompson, H., Lee, Y.-C., Kuo, J.-L. & Ni, C.-K. Toward Closing the Gap between Hexoses and N-Acetlyhexosamines: Experimental and Computational Studies on the Collision-Induced Dissociation of Hexosamines. *J. Phys. Chem. A* **123,** 6683–6700. ISSN: 1089-5639. doi:10.1021/acs.jpca.9b04143 (2019).

9. Chiu, C.-c., Tsai, S.-T., Hsu, P.-J., Huynh, H. T., Chen, J.-L., **Phan**, **H. T.**, Huang, S.-P., Lin, H.-Y., Kuo, J.-L. & Ni, C.-K. Unexpected Dissociation Mechanism of Sodiated N-Acetylglucosamine and N-Acetylgalactosamine. *J. Phys. Chem. A* **123,** 3441–3453. ISSN: 1089-5639. doi:10.1021/acs.jpca.9b00934 (2019).

10. Huynh, H. T., **Phan**, **H. T.**, Hsu, P.-J., Chen, J.-L., Nguan, H. S., Tsai, S.-T., Roongcharoen, T., Liew, C. Y., Ni, C.-K. & Kuo, J.-L. Collision-Induced Dissociation of Sodiated Glucose, Galactose, and Mannose, and the Identification of Anomeric Configurations. *Phys. Chem. Chem. Phys.* **20,** 19614–19624. ISSN: 1463-9084. doi:10.1039/C8CP03753A (2018).

Working papers

1. Ghosh, B., Tsou, P.-K., **Phan**, **H. T.**, Hsu, P.-J. & Kuo, J.-L. Exploration of the conformational space of Glycosaminoglycans forming monomers accelerated by neural network potentials (2025).

Last updated: April 28, 2025