

Ming-Kang (Brad) Tsai



Professor

Department of Chemistry

National Taiwan Normal University (NTNU)

No. 88, Sec. 4, Tingchow Rd., Wenshan Dist.,
Taipei 11677, Taiwan

Office: +886-2-77496217

Tel: +886-988008571

Email: mktsai@ntnu.edu.tw

Webpage: <https://sites.google.com/view/ntnu-mkt>

Education:

2000 – 2005 Ph.D. in Computational Chemistry, University of Pittsburgh

1993 – 1997 B.S. in Applied Chemistry, National Chiao Tung University

Experience:

2010 – present Fulltime Faculty, Department of Chemistry, NTNU

2026 – present Joint Professor, Ph.D. Program in Biomedical Artificial Intelligence, National Tsing Hua University

2021 – present Adjunct Professor, Department of Chemistry, Fu Jen Catholic University

2007 – 2010 Postdoctoral Researcher, Brookhaven National Laboratory, NY, USA

2005 – 2007 Postdoctoral Researcher, Pacific Northwest National Laboratory, WA, USA

Selective Honors & Awards:

- Outstanding young investigators of innovation-oriented trilateral collaboration of NTU system (2024).
- Principle investigator of innovation and application of nanoscience thematic program (2020-2022)

Research Areas: Computational Chemistry, Chemical Informatics

Selective Publications:

1. "Modeling Solvatochromic Effect by a Two-Step Machine Learning Approach for Organic Chromophores", Ye, Z.-R., and Tsai, M.-K.* et al. *ACS Eng. Au* **2026**, 6, 159-169.
2. "Feature-Driven Prediction of HOMO-LUMO Gaps in Transition-Metal Complexes Using the SLEET Model: A SMILES-Based Transformer Framework", Hung, S.-H., and Tsai, M.-K.* et al. *J. Chem. Theory Comput.* **2025**, 21, 6410-6420.
3. "Enhanced Predictions for the Experimental Photophysical Data Using the Featurized Schnet-based Approach", Hung, S.-H., and Tsai, M.-K.* et al. *J. Chem. Theory Comput.* **2023**, 19,

4559-4567.