

Jer-Lai Kuo



Research Fellow

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Education:

- Aug 1995 B.Sc, Department of Physics, National Taiwan University, Taipei, Taiwan
- Aug 1997 M.Sc, Department of Physics, National Taiwan University, Taipei, Taiwan
- Jan 2003 Ph.D, Doctor of Philosophy, Chemical Physics, Ohio State University, U.S.A

Experience:

- Jan 2003 Postdoctoral Fellow, Chemistry, University of Pennsylvania, USA
- Dec 2004 Assistant Professor, SPMS, Nanyang Technological University, Singapore
- April 2009 Associate Research Fellow, IAMS, Academia Sinica, Taipei, Taiwan
- March 2014 Research Fellow, IAMS, Academia Sinica, Taipei, Taiwan

Selective Honors & Awards:

- Sept/2016 Mid-career Award, Asian Consortium on Computational Materials Science, Japan
- Mar/2019 Asia Special Lecture Award in Theoretical Chemistry, Chemical Society of Japan
- Aug/2022 Presidential Scholar Award, Academia Sinica, Taiwan
- Feb/2024 Outstanding Research Award, National Science and Technology Council, Taiwan

Research Areas:

Computational Chemical Physics

Selective Publications:

1. "Conformational Analysis of Protonated N-Acetyl Hexosamines: Unexpected Methylation Effects from First-Principles and Machine Learning", *Phys. Chem. Chem. Phys.* **27**, 20614 (2025)
2. "Unravelling low-energy conformers of neutral and charged mono-/di-saccharides with first-principles accuracy assisted by neural network potentials", *Phys. Chem. Chem. Phys.* **27**, 11780 (2025)
3. "Identifying Low-Barrier Transition States in Disaccharides Using Building Block Structures: A Cooperative Approach with Neural Networks and Random Forests", *Phys. Chem. Chem. Phys.* **27**, 4355 (2025)
4. "A first-principles exploration of the conformational space of neutral and sodiated di-saccharides assisted by semi-empirical methods and neural network potentials", *Phys. Chem. Chem. Phys.* **26**,

