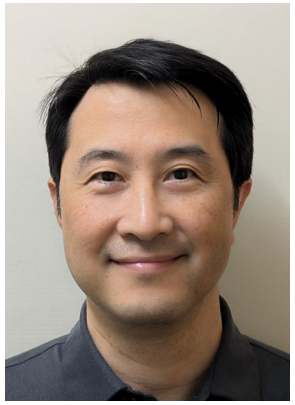
化生研 講演会/ CLS Seminar

Institute of SCIENCE TOKYO

Linking Potential Energy Surfaces with Experimental Observables



Lecturer: Prof. Jer-Lai Kuo

Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

Time & Date: 15:30-17:00, Wednesday 12 March 2025

Place: The 3rd Seminar Room, R1 bldg. Suzukakedai campus (R1棟2F 第三会議室)

Abstract: first-principles calculations are often used to explain experimental data. However, to accurately search the stable structures of molecular systems has always been a challenge. Our research team integrate Deep-Learning Neural Network Potential with first-principles methods to develop "*ab initio* structure search" to boost the speed of structural search of complex sugars and peptides without losing accuracy. Furthermore, PES does not link to experimental observable. We developed "*ab initio* anharmonic algorithm" to extract simple physical pictures to link the structure and experimental vibrational spectra without relying on parameters fitted to experimental data. These new advances can open up new possibilities to engage state-of-the art of AI.

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