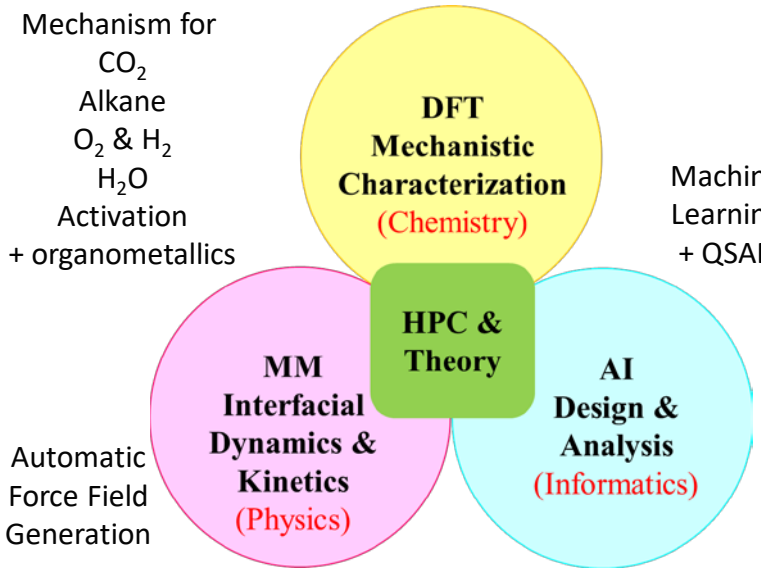
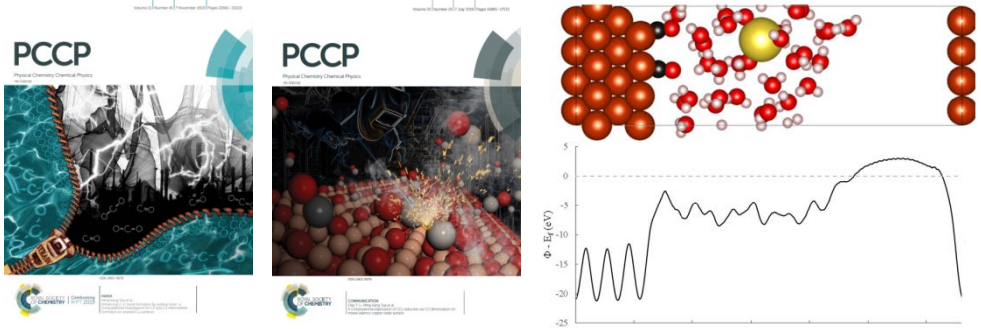
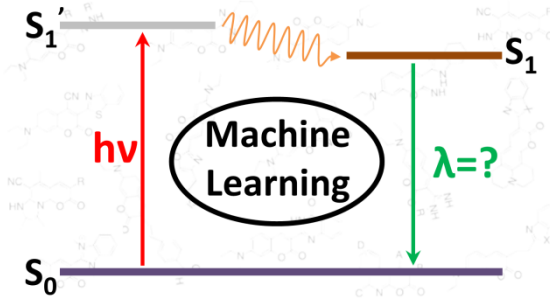
Department of Chemistry

Computational Molecular and Materials Design







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NTU-System & ITRI Taiwan

Publications

- "Operando Time-resolved X-ray Absorption Spectroscopy to Unravel the Chemical Nature: Chemical State-Trapping Strategy Enabling the Highly Selective CO_2 Reduction", *Nat. Commun.* **2020**, 11, 3235
- "Predicting the Emission Wavelength of 10,000-plus Fluorescent Molecules by Clustering and Machine Learning Approaches", *RSC Adv.* **2020**, 10, 23834-23841
- "Enhancing C-C Bond Formation by the Surface Strain: Investigating the C2 and C3 Intermediate Formation on the Strained Cu Surfaces", *Phys. Chem. Chem. Phys.* **2019**, 21, 22704-22710. (cover highlight)
- "A Computational Exploration on CO_2 Reduction via CO Dimerization on Mixed-Valence Copper Oxide Surface", *Phys. Chem. Chem. Phys.* **2018**, 20, 16906-16909. (cover highlight)
- "Interplay between Polarizability and Hydrogen Bond Network of Water: Reparametrizing the Flexible Single-Point-Charge Water Model by the Nonlinear Adaptive Force Matching Approach", *J. Phys. Chem. A* **2018**, 122, 4654-4622.