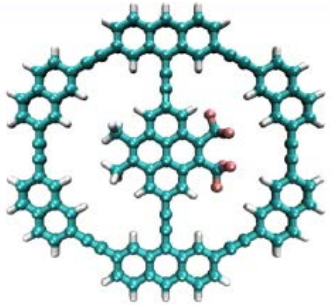
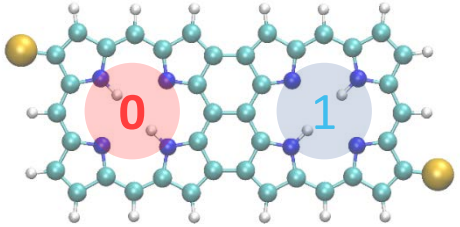
Department of Chemistry

Computational Design of Nano and Energy Materials

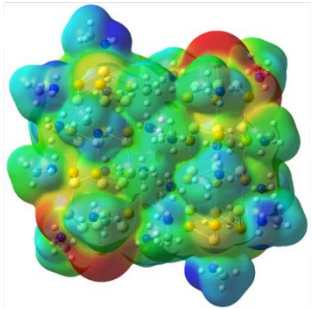
We focus on theoretical simulation, characterization and prediction of material systems with novel electronic properties. We applied computational chemistry to understand the catalytic chemical and electrochemical reaction mechanisms with an aim to help modify, optimize, and design new energy systems. We have carried out DFT investigations on fuel cells, CO2 recycling, and energy storage systems. We are also interested in applying first-principles studies to investigate the structural, electronic, and luminescence properties of small molecular systems in general. We have developed intimate collaborations with experimental groups in an aim to achieve a more profound understanding from a microscopic perspective.

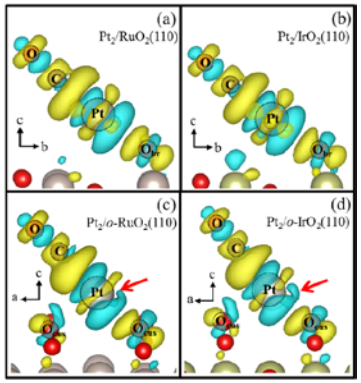


Single molecular electronics



Catalytic and Mechanistic Studies for Chemical Reactions





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National Taiwan Normal University

Publications

- C.-Y. Liu and E. Y. Li*, "Termination Effects of Pt/v-$Ti_{n+1}C_nT_2$ MXene Surfaces for Oxygen Reduction Reaction Catalysis", ACS Appl. Mater. Interfaces, 2019, 11(1), 1638-1644
- E. Y. Li*, "Systematic and efficient band tracing for chiral CNTs via natural helical crystal lattice model", Carbon, 110, 336-342 (2016)
- T.-E. Hsieh†, T.-W. Yang†, C.-Y. Hsieh, S.-J. Huang, Y.-Q. Yeh, C.-H. Chen, E. Y. Li*, and Y.-H. Liu*, "Unraveling the Structure of Magic-Size $(CdSe)_{13}$ Cluster Pairs", Chem. Mater. 2018, 30(15), 5468-5477