



國立清華大學

NATIONAL TSING HUA UNIVERSITY

Colloquium

Department of Engineering and System Science,
Institute of Nuclear Engineering and Science,
National Tsing Hua University

Employing Computational Models for the Identification and Screening of Single-Atom Metal Nanosheets for Their Potential in Electrochemical Catalysis of Cyanide Reduction Reactions

In this talk, the following content will be presented:

As a catalytic center, the 4N-coordinated post-transition metal (PM) confined within phthalocyanine (Pc) shows promise for the environmentally-friendly synthesis of CH_4 and NH_3 . A range of M–Pc catalysts (where M represents transition-metal based and transition-metal free) is methodically evaluated through DFT mechanistic analysis and electrochemical exploration to determine their stability, activity, and selectivity. Our comparative analysis reveals that the orientational specificity of initial cyanide adsorption would play a crucial role in cyanide electroreduction reaction (CNRR) pathways within diverse M–Pc nanosheets. Specifically, the NC^* model typically requires higher supplies of Gibbs free energy for CNRR, preponderantly resulting in CH_3NH_2 . Conversely, the counterpart of the CN^* model necessitates lower energetic demands, leading to a broader diversity of products including methane and ammonia. From a comprehensive screening of the studied results, we have determined that some specific M–Pc nanosheets (triggered by CN^* model) are the exceptionally proficient electrocatalysts, specifically in producing only CH_4 and NH_3 via the CNRR process, as indicated by our final compiled findings. Among the evaluated nanosheets, the models associated with Ti–Pc, Cr–Pc, Fe–Pc, and Al–Pc stand out, demonstrating significantly higher selectivity and CNRR activity compared to their counterparts. This study advances the understanding of the unique superior characteristics of SACs, subsequently providing innovative perspectives that could directly guide their discovery for CNRR applications.

15:30-17:00, Wednesday, March 20th, 2024

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Selected Publications:

- Shiuan-Yau Wu, Kuang-Yen Chiu, Chen-Hao Fan, and **Hui-Lung Chen,*** “Electrocatalytic carbon dioxide reduction on graphene-supported Ni cluster and its hydride: Insight from first-principles calculations.” *Appl. Surf. Sci.* **2023**, 629, 157418.
- Chen-Hao Fan, Kuang-Yen Chiu, Chih-Wei Hsu and **Hui-Lung Chen,*** “Computational design and screening of single-atom phthalocyanine-coordinated transition metal catalysts for the electrochemical cyanide reduction reaction.” *Appl. Surf. Sci.* **2024**, 643, 158625.
- Kuang-Yen Chiu, Chen-Hao Fan, Chih-Wei Hsu and **Hui-Lung Chen,*** “First-Principles Insight into the Mechanistic Study of Electrochemical Cyanide Reduction Reaction on Post-Transition Metal Based Single-Atom Catalysts Anchored by Phthalocyanine Nanosheets” *ACS Appl. Nano Mater.* **2024**, Accepted.