Enchancing Catalyst Discovery Using Single Metal Atoms for Green Chemistry Reactions

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Achieving carbon neutrality requires urgent action to reduce CO_2 emissions and transition to a low-carbon economy. This project addresses three essential reactions for agriculture, environmental sustainability, and clean energy: electrochemical nitrogen reduction (NRR) for green ammonia (NH_3) synthesis, CO_2 reduction (CO_2RR) to produce valuable chemicals, and water splitting for green hydrogen (H_2) production. These processes depend on the development of efficient electrocatalysts, which continue to present a significant scientific challenge. This research employs computational simulations to predict the performance of single-atom catalysts (SACs) supported on low-cost two-dimensional (2D) materials, based on carbon nitrides. The combination of highly active single atoms and the high surface area, tunable electronic properties, and electrochemical stability of selected carbon nitrides makes them ideal candidates for efficient NRR, CO_2RR, and water splitting reactions. The talk will show how calculations can help to unveil the reactivity and structure of single-atom catalysts. I will discuss the advantages of electrocatalytic processes and how to efficiently screen SACs and dual-atom catalysts for NRR and CO_2RR mechanisms, without facing the challenging reaction mechanisms of both reactions.

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