화학과 세미나

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Developing Electronic Structure Method for Transition-Metal Chemistry

Transition metals have functioned as key mediators of electron transfer across a wide range of cutting-edge applications, including artificial metalloenzymes, photosensitizers, organic light-emitting diodes, supported metal electrocatalysts, and battery cathodes. More recently, they have attracted growing interest as promising qubits capable of storing quantum information. The physicochemical properties of transition-metal containing systems are remarkably tunable, with subtle changes in coordination geometry, ligand field, or local environment. While this tunability highlights their exceptional potential, it also introduces significant challenges in accurately predicting and optimizing their properties.

This presentation will introduce the development of quantum chemistry methods aimed at better addressing these challenges. Our group is developing three parallel methodologies to build an unified theoretical framework for predicting the physicochemical properties of real world transition metal complexes. The first part is the development of electronic structure methods to efficiently obtain charge-transfer, metal-centered, and multiplet states, in order to accurately describe the processes involving these states.[1] The second part covers nonadiabatic dynamics simulations, based on the newly developed electronic structure methods. We will present preliminary results of ultrafast spin-crossover dynamics simulations in a photosensitizer system. The last part focuses on the development of new modeling strategies for complex real-world environments. In particular, we will introduce a new strategy modeling extended environments with a single embedded transition-metal defect.

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