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Potential-Dependent Structural Dynamics and Spin Transition of Electrocatalysts

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Abstract: Operando characterization techniques are essential for resolving the dynamic electronic and structural evolution of molecular catalysts under working conditions. Here, we demonstrate the application of operando synchrotron-based X-ray absorption spectroscopy (XAS) and X-ray emission spectroscopy (XES) as a versatile platform for probing electronic structure, oxidation-state variation, and spin-state dynamics in metal–molecular electrocatalytic systems. Using a spin crossover-driven diiron molecular catalyst as a model system, we establish a comprehensive operando measurement strategy capable of correlating electrochemical stimuli with real-time spectroscopic responses. XAS provides quantitative insight into metal oxidation-state modulation and coordination-environment rearrangement, while XES directly probes the evolution of metal 3d electronic configurations and spin states during catalytic turnover. The combined spectroscopic approach enables differentiation between charge redistribution, ligand-field effects, and spin-state transitions—parameters that are often convoluted in conventional *ex situ* measurements. Importantly, the operando cell design and synchrotron spectroscopic methodology presented here are broadly applicable to a wide range of transition-metal molecular and heterogeneous catalytic systems. This work underscores the power of integrating complementary hard X-ray spectroscopies to capture transient electronic structures and establishes a general framework for investigating functional materials under realistic working conditions.

Keywords: *Ammonia and Hydrogen production, synchrotron-based spectroscopy*