

Controlling the Redox Non-Innocence of Ligands. Implications for Catalysis

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Considerable attention has traditionally focused on the impact of transition metal formal oxidation state (and thus d-orbital count) on catalytic transformations. What has received lesser attention is the control of the formal redox state of the ligand, and its impact on catalytic activity. Ligand redox poise is critical to achieving the long-sought goals of “reverse engineering” precious metal catalysts with Earth-abundant metal replacements; the latter tend to be more redox reluctant than precious metals, which have until now dominated industrial catalysis. This presentation will focus on our efforts to employ computational methods to understand the links between precious and base metal catalysts, and the challenges involved in modeling systems with delicate electronic coupling between the metal and ligands.