Inductive Effects in Cobalt-Doped Nickel Hydroxide Electronic Structure Facilitating Urea Electrooxidation

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Electrochemical oxidation of urea provides an approach to prevent excess urea emissions into the environment while generating value by capturing chemical energy from an abundant waste product of industrial and agricultural processes. Presently, the source of high catalytic activity in state-of-the-art doped nickel catalysts for urea oxidation reaction (UOR) activity is poorly understood, which hinders the rational design of new catalyst materials. In particular, cobalt-doped $Ni(OH)_2$ catalysts remain one of the most widely studied multimetal experimental systems for UOR, yet the exact role of cobalt as a dopant in $Ni(OH)_2$ to maximize the intrinsic activity towards UOR remains unclear. This talk highlights how tuning the Ni:Co ratio in $Ni_{1-x}Co_x(OH)_2$ catalysts alters both structural and electronic states, both properties were experimentally demonstrated to influence the number and intrinsic activity of redox-active surface sites. Density functional theory calculations allow us to further probe how the electronic states of $Ni(OH)_2$ are influenced by the presence of Co as a dopant in the surface layer. We show that the introduction of Co alters the Ni 3d electronic state density distribution to lower the minimum energy required to oxidize Ni and can potentially influence surface-adsorbate interactions.