Covalent Functionalization of Transition Metal Phosphide Catalysts with Aryl Groups

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Transition metal phosphides have gained considerable interest as catalysts due to their excellent catalytic properties in the hydrogen evolution reaction (HER) and in the hydrotreating process.[1-3] Covalent surface functionalization of transition metal phosphides offers a promising avenue to modulate catalytic performance and stability by tuning their electronic and structural properties.[4-5] However, covalent surface functionalizations of transition metal phosphides have been barely explored and the relationship between surface ligands and catalytic activity is still not well understood. The development of novel functionalization approaches and fundamental insight into surface ligand effect in catalysis are hence needed to enable rational catalyst design.

Herein, we present a strategy for synthesizing covalently functionalized cobalt phosphide using aryl organohalide and other reagents. The successful surface modification was shown by the characterization of the prepared materials by X-ray photoelectron spectroscopy (XPS). We investigated the catalytic properties of the modified cobalt phosphide in the hydrogenation of an α, β-unsaturated aldehydes as a function of surface ligands with varying electronic properties. This result provides insight into the relationship between catalytic selectivity and the surface chemistry of cobalt phosphide. Our research expands the range of functionalization methods for transition metal phosphide materials and shows that it can serve as a practical approach towards tuning their catalytic properties.

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