Targeted electronic structure modification in catalysis: a case study of dual-metal catalyst for CO hydrogenation

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Targeted modification of chemical and electronic structure of hybrid organic-inorganic compounds is a powerful tool for modulating the properties of materials in various applied fields [1], including catalysis, where it can be used to decrease the reaction barriers and alternate its pathways. Mixed-metal strategy has a peculiar place among such approaches [2], since it allows to easily change the reducibility characteristics of a catalytic material [3], including the ionization potentials and the work-function, as well as the electron localization and the adsorption patterns of reaction intermediates [1-4]. This is particularly important for the redox reactions [4-5], such as CO hydrogenation. In this report, the chemical approaches [1-3] for targeted electronic structure modification are outlined and are further illustrated by the case of CoCu dual-metal nitrogen-doped graphene-based (Cu/Co-CN) catalyst for selective formation of ethanol from syngas. The synergistic effect of Co and Cu increases the density-of-states near the Fermi level and facilitates the electron injection towards the adsorbates, that allows reaching a space-time yield toward $C_{2+}OH$ of 851.8 mg/(g·h), ranking this catalyst among the best in this class[5].

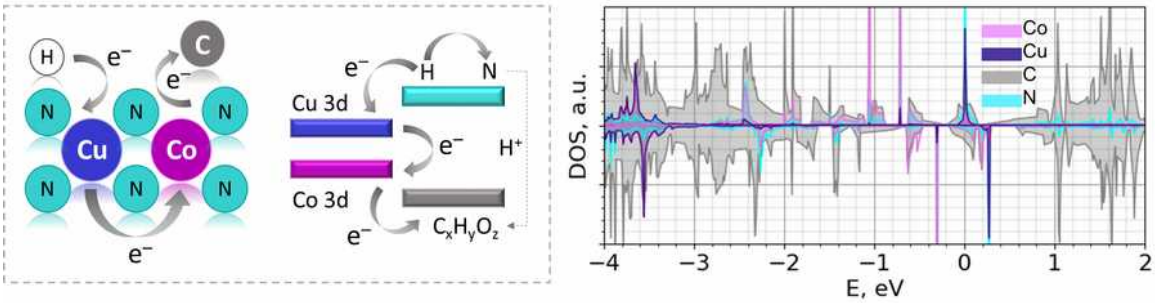

Fig.1 Electronic structure features and working principles of Co/Cu-CN catalyst.

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