Hydrogenation regulation of nitrobenzene in electrocatalytic processes realized

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Graphical abstract. A comprehensive understanding on the selectivity toward electrocatalytic hydrogenation products of nitrobenzene was conducted experimentally and theoretically over a Cu3Pt/C alloying catalyst, revealing the significant role of the applied reduction potential and pH of electrolyte solution in regulating the product selectivity of nitrobenzene hydrogenation. Credit: DOI: 10.1016/j.apcatb.2021.120545

Selective catalytic hydrogenation of nitrobenzene (Ph-NO₂) to high value-added azoxy-, azo- and aminobenzene compounds are considerably important in the organic synthesis industry.

Compared with traditional thermocatalytic processes, the electrocatalysis technique has aroused great research attention, owing to its high hydrogenation efficiency, ambient operating conditions. Unfortunately,
the relevant selective hydrogenation mechanisms are unclear in the reported works.

Recently, researchers led by Prof. Zhang Haimin from the Hefei Institutes of Physical Science (HFIPS) of the Chinese Academy of Sciences (CAS) reported the ultrafine Cu_{x}Pt_{y} alloying nanoparticles anchored on carbon black (Cu_{x}Pt_{y}/C) to achieve potential regulation of electrocatalytic hydrogenation of Ph-NO_{2} and proposed a new hydrogenation mechanism. The result was published on *Applied Catalysis B: Environmental*.

The researchers prepared a series of Cu_{x}Pt_{y} alloying nanoparticles and they found that the Cu_{3}Pt/C can afford almost 100% conversion of Ph-NO_{2} into azoxybenzene with ~99% selectivity at 0.3 V (vs. RHE) and aminobenzene with ~99% selectivity at -0.3 V (vs. RHE) in 1.0 M potassium hydroxide, respectively.

Moreover, the Cu_{3}Pt/C was put into the large-scale electrocatalytic experiment, and the morphology, structure, and activity had no significant change after a long time electrocatalytic test.

Meanwhile, theoretical calculations provided a comprehensive understanding of the selective electrocatalytic hydrogenation mechanisms of Ph-NO_{2} relative to electrolyte pH and applied potential.
