

## Interfacial Properties in Promoting Levulinic Acid Hydrogenation to Gamma-valerolactone and Ammonia Borane Methanolysis

Gamma-valerolactone (GVL), the product of levulinic acid (LA) hydrogenation, has been listed among the top 10 most promising platform chemicals by the US Department of Energy.<sup>[1]</sup> The traditional Ru catalyst<sup>[2]</sup> suffers high metal loading and poor stability against oxidation. To improve it, hexadecyl(2-hydroxyethyl) dimethylammonium dihydrogen phosphate (HHDMA) ligand decorated Ru nanoparticle has been prepared.<sup>[2]</sup> Test results show that the HHDMA-Ru displays higher activity and stability than traditional catalyst. Density Functional Theory (DFT) results demonstrate that the intrinsic acidic properties at the ligand–metal interface under reaction conditions inhibits the O–H bond breaking from carboxylic group, thus stabilize the surface intact carboxylic species from which the less energy demanding path is followed. Moreover, the interfacial acidity increases the robustness of the material against ruthenium oxide formation.

Ammonia-Borane (AB) is regarded as a competitive candidate for chemical hydrogen storage with the advantages of a low molecular weight but high hydrogen content, long-term stability under ambient temperature, and non-toxicity.<sup>[3]</sup> In the second topic, a feasible *in situ* method has been employed to synthesize the noble-metal-free Cu/Co(OH)<sub>2</sub> nanohybrid catalyst. Benefitting from the electronic interaction between Cu nanoparticles (NPs) and Co(OH)<sub>2</sub>, copper is positively charged and the degree of charge transfer can be modulated by varying the metal/support ratio. DFT calculations show that electrostatic interactions play a major role in stabilizing the adsorption of AB while reducing the SN2 barrier<sup>[4]</sup> for the OH<sup>-</sup> attack that initiates the reaction and is the rate determining step.

[1] *Green Chem.* **2010**, *12*, 539–554.

[2] *ChemSusChem* 2012, *5*, 1657–1667.

[2] *Green Chem.* **2017**, *19*, 2361–2370.

[3] *J. Am. Chem. Soc.* **2011**, *133*, 19638–19642.

[4] *Energy Environ. Sci.* **2017**, *10*, 1770–1776.