Mechanisms for High Selectivity in the Hydrodeoxygenation of 5-Hydroxymethylfurfural over PtCo Nanocrystals

Scientific Achievement

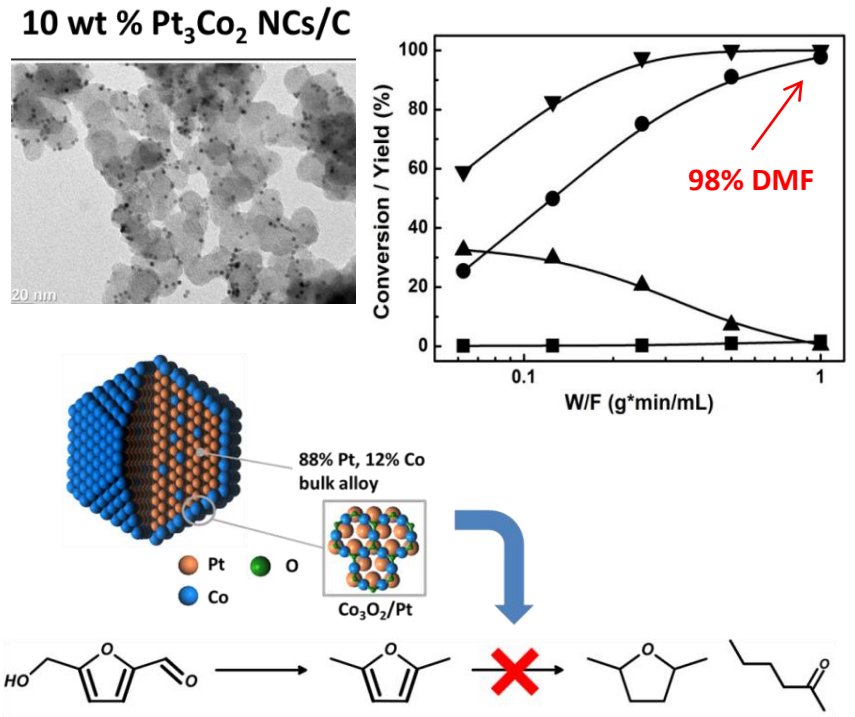
Highly structured Pt-Co nanocrystals (NCs) are synthesized and examined for hydrodeoxygenation (HDO) of 5-hydroxymethylfurfural (HMF). Nearly 100% yield of the desired biofuel product, 2,5-dimethylfuran (DMF), is achieved over the Pt_3Co_2/C NCs catalyst, with remarkable stability lasting more than 14 hours.

Significance and Impact

Although numerous studies have been carried out to control the selectivity of the HDO reaction, the reaction mechanism is still elusive. The present work reports the first ultra-selective and stable Pt-Co catalyst for the HDO of HMF, and proposes a mechanism to explain its high HDO selectivity and stability.

Research Details

- 3~4nm Pt-Co NCs with well controlled size and composition are synthesized via solvothermal method.
- HDO experiments are performed in a continuous flow reactor. Under the optimized space time and reaction temperature, 98% yield of DMF can be achieved over Pt_3Co_2/C catalyst for at least 14 hours' measurement.
- XRD and XAS characterization results indicate that the Pt_3Co_2 NCs consist of a Pt-rich core and a Co oxide surface monolayer.
- DFT calculations reveal that the oxide monolayer interacts weakly with the furan ring to prevent side reactions, providing sites for effective HDO to the desired product.



J. Luo, H. Yun, A. Mironenko, K. Goulas, J. D. Lee, M. Monai, C. Wang, V. Vorotnikov,, C. B. Murray, D. G. Vlachos, P. Fornasiero and R. J. Gorte, *ACS Catalysis*, **2016**, 6, 4095−4104

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