Bifunctional Acid Catalysts Make Furan Derivatives

Scientific Achievement

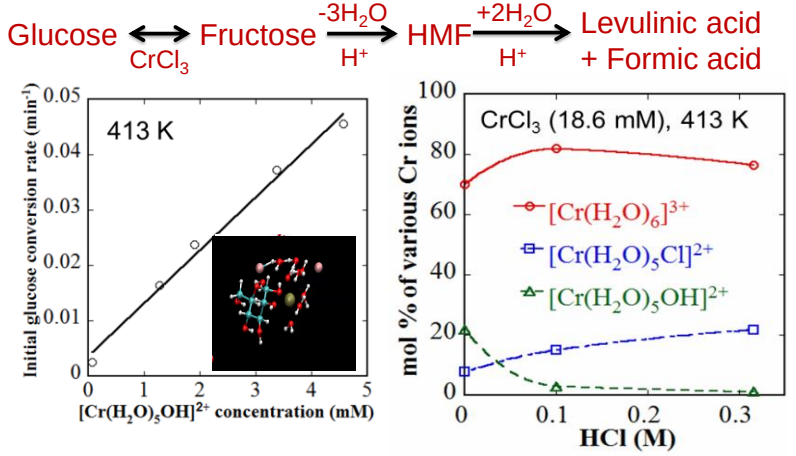
The hydrolyzed metal ions ($[Cr(H_2O)_5OH]^{2+}$, $[Al(H_2O)_5OH]^{2+}$) have been identified as the most active species in metal salt ($CrCl_3$, $AlCl_3$) catalyzed aldose-ketose isomerization in water.

Significance and Impact

- **Identification of the active species in the metal salt catalyzed aldose-ketose isomerization in aqueous media and the first revelation of the interplay of the Lewis and Brønsted acid catalysts in hydroxymethylfurfural (HMF) and furfural production from glucose and xylose, respectively.**
- **Opening up opportunities to optimizing HMF and furfural production and developing heterogeneous catalysts for the aldose-ketose isomerization based on the identification of active catalytic site in homogeneous catalysis.**

Research Details

- Kinetics results combined with metal salt speciation in aqueous media identify for the first time the active metal ions for aldose-ketose isomerization.
- Extended X-ray absorption fine structure spectroscopy and Car–Parrinello molecular dynamics simulations show that glucose displaces water in the first coordination shell of Cr ion to enable isomerization.



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