

Tuning Catalyst Activity and Selectivity via Coverage Induced Conformational Control

Scientific Achievement

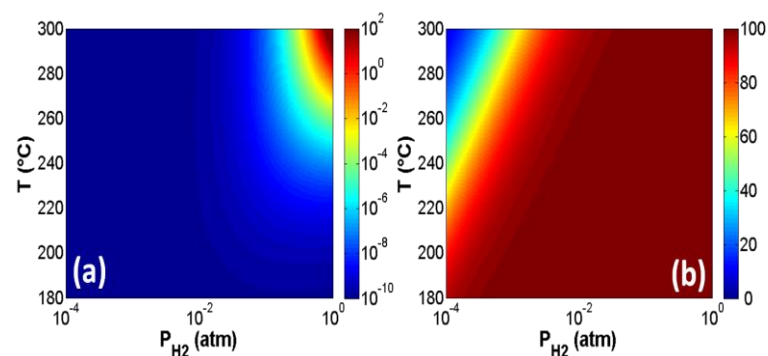
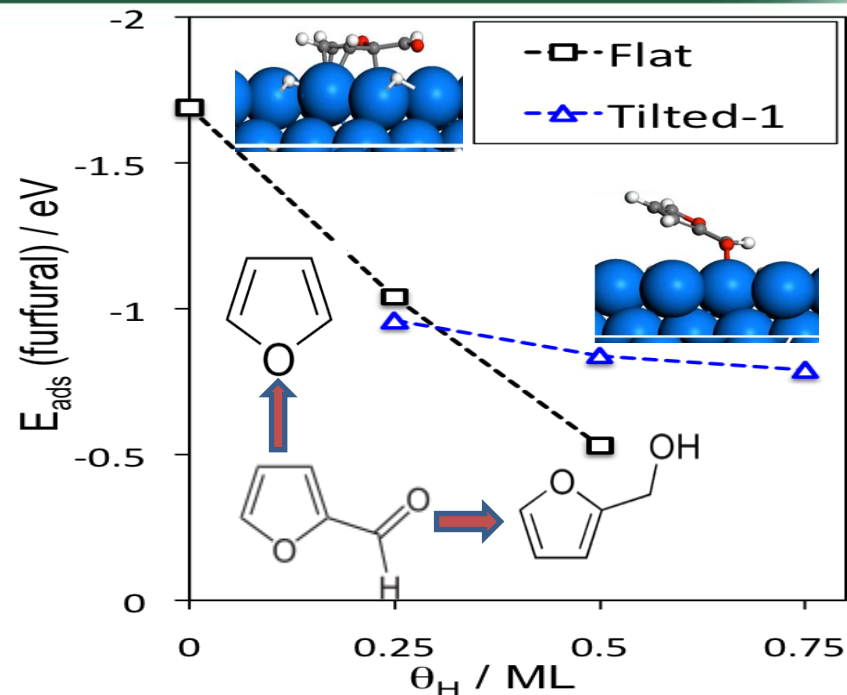
First-principles modeling of furfural hydrodeoxygenation (HDO) including co-reactant effects demonstrates the profound effect of pressure on performance.

Significance and Impact

- HDO is essential for upgrade of biomass.
- Selectivity control is critical.
- Our work is the first DFT demonstration of the effect of co-reactant coverage on selectivity in heterogeneous catalysis.

Research Details

- First-principles density functional theory (DFT) and microkinetic calculations have been performed.
- Co-adsorbed hydrogen tilts the furfural and drastically increases activity and selectivity to furfuryl alcohol.
- Good agreement with experiments for the first time.



Wang, S., Vorotnikov, V. and Vlachos, D.G., *ACS Catal.* **2015**, 5 (1) 104–112.