Developed a first-principles based thermochemistry and kinetics toolbox for metal catalyzed heterogeneous reactions

Predicted region for optimal catalyst activity via high throughput computing

Captured experimental trends in activity and selectivity: Pt < Ni-Pt-Pt

Proposed higher activity (subject to kinetics and thermodynamic constraints) for catalytic pyrolysis of ethylene glycol to syngas (CO, H₂) (middle graph)

Salciccioli and Vlachos, *ACS Catal.* 1, 1246 (2011)