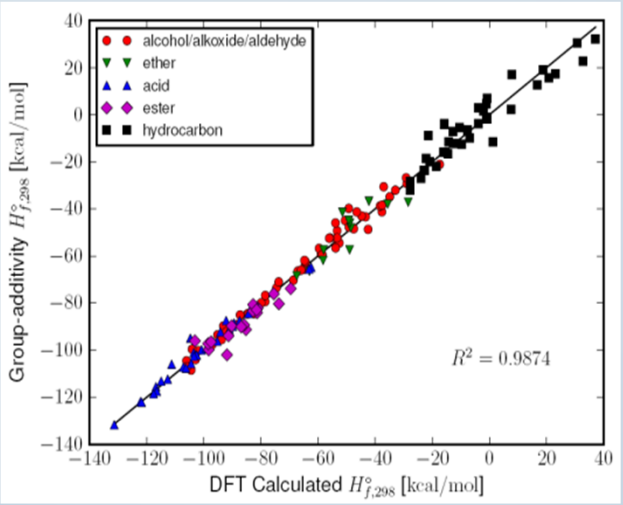
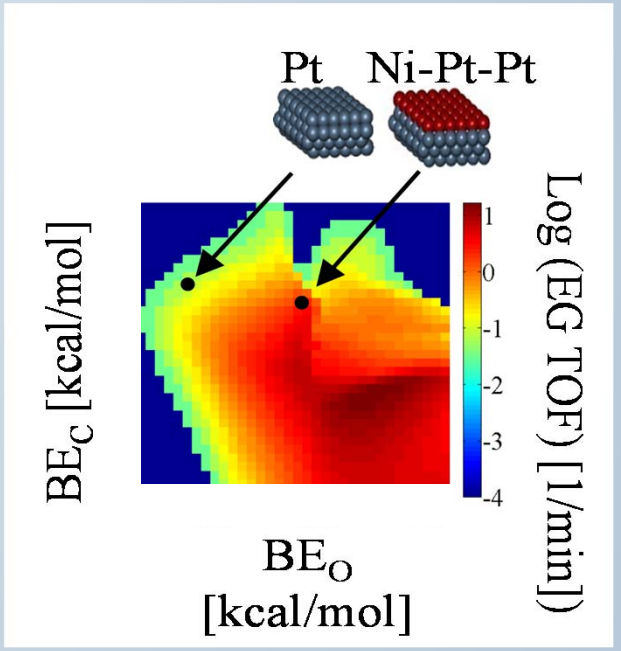
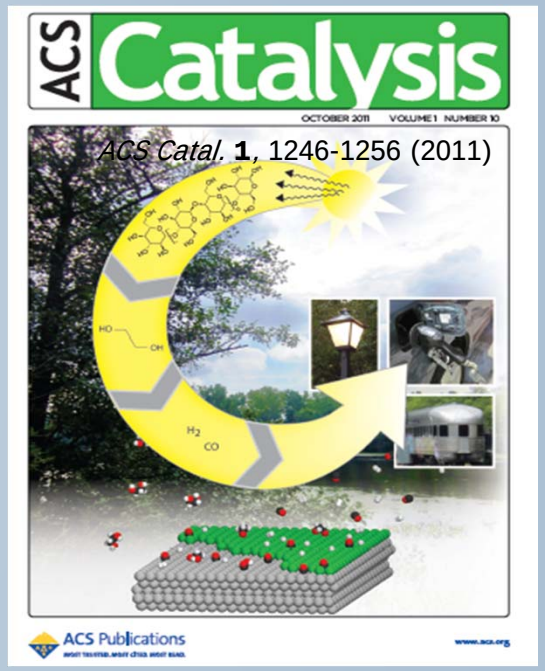
Computational High Throughput Screening of Catalytic Materials







- 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, H_2) (middle graph)