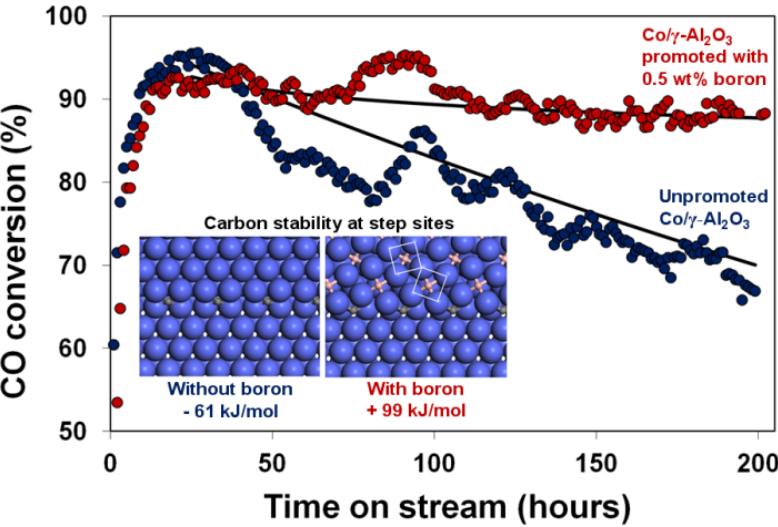


Modeling-guided Catalyst Design. Mark Saeys

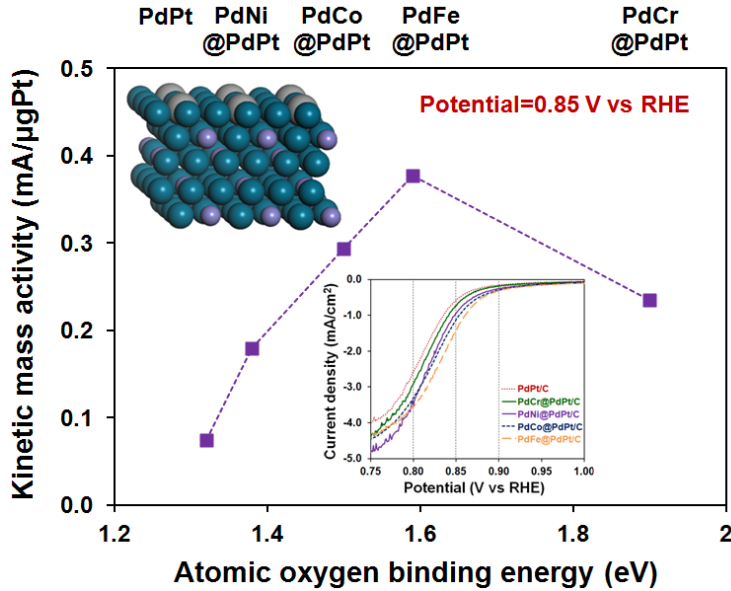


Guided by first principle modeling, boron was discovered to prevent deactivation by carbon deposition for Ni and Co-based catalysts by selectively destabilizing carbon species near step sites. This discovery was experimentally confirmed.

Tan, Chang, Borgna, Saeys, J. Catal. 280, 50 (2011)

Volcano-optimal core-shell PdM@PdPt/C oxygen reduction catalysts were discovered by combining first principle modeling with careful catalyst synthesis and characterization. For the optimal PdFe@PdPt/C catalyst, the current density per Pt atom is 10 times higher than for commercial Pt/C catalysts.

Trinh, Yang, Lee, Saeys, J. Catal. 291, 26 (2012)



Molecular Modeling: a tool for catalyst discovery.