

Computational Catalyst Screening for Low Temperature Diesel Engine Emission Treatment

Research Themes

Discovery of catalytic activity trends for CO, NO and propylene oxidation reactions under low temperature diesel engine emission conditions. Design of metal alloy catalysts with better oxidation performance for diesel engine emission treatment.

Build a reactor model with metal concentration gradients along the reactor to reduce the use of precious metals.

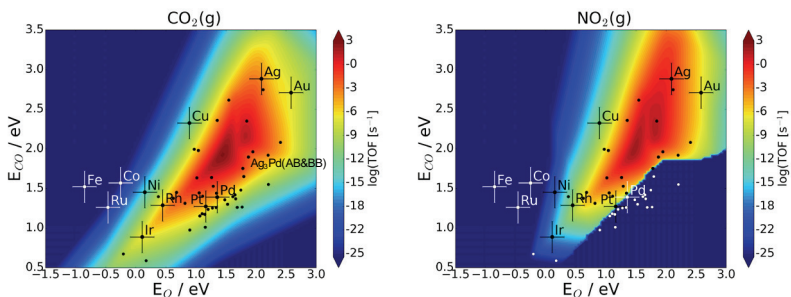
Recent Accomplishments

Two reactivity descriptors were identified to reliably assess catalytic activity trends. A series of noble metal alloys with superior low temperature oxidation performance was predicted by computational screening.

Received Colt Refining Student Award from the International Precious Metals Institute for work with precious metals.

Issues

Low temperature combustion (LTC) diesel engines improve fuel efficiency, but the commonly used diesel oxidation catalysts, which are based on Pt and Pd alloys, have insufficient activity at the reduced exhaust temperature of LTC engines. Therefore, an improved diesel oxidation catalyst with suitable low temperature activity is needed to fully capitalize on the advances in engine technology.



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