Revealing Catalyst Structure under in-situ Conditions

Scientific Achievement

Atomistic analysis of in-situ EXAFS data to determine the structure of bimetallic catalysts during aqueous phase reforming (APR) of ethylene glycol.

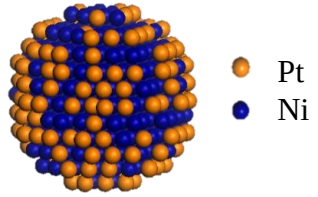
Significance and Impact

These results clearly indicate that bimetallic catalysts undergo structural transformation under reaction conditions, demonstrating the importance of in-situ techniques.

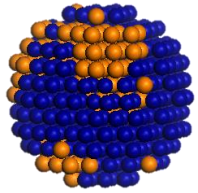
Research Details

- In-situ EXAFS reactor studies were performed for APR of ethylene glycol over supported NiPt bimetallic catalysts.
- An atomistic simulator was built to reconstruct atomistic detail of nanoparticles from EXAFS data.
- Under reaction conditions, Ni atoms segregate to produce Ni-terminated bimetallic particles.
- These results verify our previous DFT and UHV predictions of high activity Ni-terminated bimetallics.

Coordination Number	***10% H_2 at 225 °C—NiPt/C***	
	Experimental	Simulation
Pt-Pt	2.0 ± 0.7	2.74 ± 0.02
Pt-Ni	3.8 ± 0.3	4.39 ± 0.02



Coordination Number	***APR at 225 °C—NiPt/C***	
	Experimental	Simulation
Pt-Pt	6.0 ± 1.4	6.2 ± 0.1
Pt-Ni	1.9 ± 0.8	3.64 ± 0.04



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