

# Restructuring Catalyst Surfaces

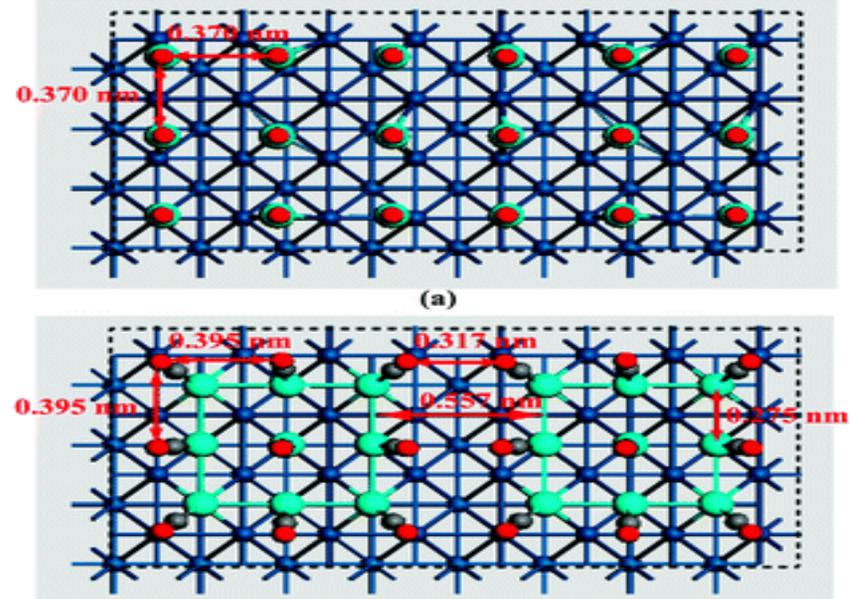
**Objective:** Use simulation to understand the ability of surfaces to restructure under the influence of gaseous adsorbates.

**Implications:** Revealing the arrangement of metal atoms that form at active sites will yield increased understanding of heterogeneous catalysis mechanisms.

**Accomplishments:** DFT studies at NERSC show that CO molecules bind to small Pt nanoclusters on the catalyst surface.

- The nanoclusters seem to maximize bonding of more CO molecules.
- VASP reveals the stabilization energy gained by cluster formation and suggests the atomic arrangement.
- Formation of small metallic clusters opens a new avenue for understanding catalytic activity under high pressures.

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(top) Starting geometry of CO and Pt atoms. (bottom) After relaxation to minimize energy in the DFT calculation, two (3 × 3) clusters form. Dark blue circles represent Pt atoms in the slab layers; light blue circles represent Pt atoms at the surface. Red and gray circles represent oxygen and carbon atoms, respectively.