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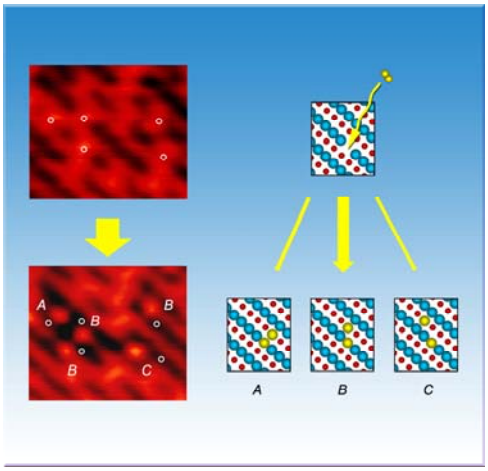
EMSL In Brief
Environmental Molecular Sciences Laboratory

Oxygen Atoms Display Novel Behavior on Common Catalyst

Like waltzing dancers, the two atoms of an oxygen molecule usually behave identically when they separate on the surface of a catalyst. However, new research from the Environmental Molecular Sciences Laboratory reveals that on a particular catalyst, the oxygen atoms act like a couple dancing the tango: one oxygen atom plants itself while the other shimmies away, probably with energy partially stolen from the stationary one.

Scientists from EMSL and Pacific Northwest National Laboratory discovered this unanticipated behavior while studying how oxygen interacts with reduced titanium oxide, a popular catalyst and a model oxide. Their research began with a slice of titanium oxide crystal, oriented so that titanium and oxygen atoms line up on the surface in alternating strips, forming titanium troughs between oxygen rows. By heating the sample, the team created surface imperfections or spots where an oxygen atom vacated its row. Using scanning tunneling microscopy, the researchers found that molecular oxygen only broke apart when it encountered a vacancy.



Migration of "hot" oxygen atoms on the surface of a catalyst was featured on *The Journal of Physical Chemistry C* cover.

The team also expected one of the atoms to make the vacancy its home, and the second to situate itself right next to its former partner. Instead, the scientists found that the mobile oxygen atom, called a "hot" atom, moved one or two crystal lattice spaces away. Among all events the team observed, more than three quarters of the hot atoms hopped one or two spaces away before becoming mired on the surface.

The team postulated that the hot atom may get the energy to move from the rearrangement of the bonds—bonds within the oxygen molecule and between the oxygen atom and titanium surface. The calculated energy from these sources was about two to three times that needed to get an immobilized oxygen unstuck.

"This finding may be important in surface reactivity. We don't know yet," EMSL's Igor Lyubinetsky, lead investigator, says. The chemical event could, for example, be affected by the extra energy the oxygen atom possesses. The effect might also play into whether surface oxygen atoms interfere with the chemistry between the catalyst and other chemicals. In any event, the result will keep chemists tango-ing with new questions for a long time.

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