Surface science goes inorganic

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A collaboration between researchers at Northwestern University's Center for Catalysis and scientists at Oxford University has produced a new approach for understanding surfaces, particularly metal oxide surfaces, widely used in industry as supports for catalysts.

This knowledge of the surface layer of atoms is critical to understanding a material's overall properties. The findings were published online Feb. 14 by the journal *Nature Materials*.

Using a combination of advanced experimental tools coupled with theoretical calculations, the research team has shown how, using methods commonly taught to undergraduate chemistry students, one can understand how atoms are arranged on a material's surface. (These methods date back to the pioneering work of Linus Pauling and others to understand the chemical bond.)

"For a long time we have not understood oxide surfaces," said Laurence Marks, professor of materials science and engineering in the McCormick School of Engineering and Applied Science at Northwestern. "We only have had relatively simple models constructed from crystal planes of the bulk structure, and these have not enabled us to predict where the atoms should be on a surface.

"Now we have something that seems to work," Marks said. "It's the bond-valence-sum method, which has been used for many years to understand bulk materials. The way to understand oxide surfaces turns out to be to look at the bonding patterns and how the atoms are arranged and then to

follow this method."

Marks, together with Kenneth Poeppelmeier, professor of chemistry in Northwestern's Weinberg College of Arts and Sciences, and Martin Castell, university lecturer in the department of materials at Oxford, led the research.

In the study, Northwestern graduate student James Enterkin analyzed electron diffraction patterns from a strontium titanate surface to work out the atomic structure. He combined the patterns with scanning-tunnelling microscopy images obtained by Bruce Russell at Oxford. Enterkin then combined them with density functional calculations and bond-valence sums, showing that those that had bonding similar to that found in bulk oxides were those with the lowest energy.

Writing in a "News and Views" article from the same issue of Nature Materials, Ulrike Diebold from the Institute of Applied Physics in Vienna, Austria, said, "This simple and intuitive, yet powerful concept [the bond-valence-sum method] is widely used to analyze and predict structures in inorganic chemistry. Its successful description of the surface reconstruction of $SrTiO_3$ (110) shows that this approach could be relevant for similar phenomena in other materials."

More information: The *Nature Materials* paper is titled "A homologous series of structures on the surface of SrTiO3 (110)." The authors of the paper are James A. Enterkin (first author), Arun K. Subramanian, Kenneth R. Poeppelmeier and Laurence D. Marks, from Northwestern, and Bruce C. Russell and Martin R. Castell, from Oxford.

Provided by Northwestern University