ORNL finding has materials scientists entering new territory

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Solar cells, light emitting diodes, displays and other electronic devices could get a bump in performance because of a discovery at the Department of Energy's Oak Ridge National Laboratory that establishes new boundaries for controlling band gaps.

While complex transition metal oxides have for years held great promise for a variety of information and energy applications, the challenge has been to devise a method to reduce band gaps of those insulators without compromising the material's useful physical properties.

The band gap is a major factor in determining electrical conductivity in a material and directly determines the upper wavelength limit of light absorption. Thus, achieving wide band gap tunability is highly desirable for developing opto-electronic devices and energy materials.

Using a layer-by-layer growth technique for which Ho Nyung Lee of ORNL earned the Presidential Early Career Award for Scientists and Engineers, Lee and colleagues have achieved a 30 percent reduction in the band gap of complex metal oxides. The findings are outlined in the journal *Nature Communications*.

"Our approach to tuning band gaps is based on atomic-scale growth control of complex oxide materials, yielding novel artificial materials that do not exist in nature," Lee said. "This 'epitaxy' technique can be used to design entirely new materials or to specifically modify the composition of thin-film crystals with sub-nanometer accuracy."

While band gap tuning has been widely successful for more conventional semiconductors, the 30 percent band gap reduction demonstrated with oxides easily surpasses previous accomplishments of 6 percent – or 0.2 electron volt – in this area and opens pathways to new approaches to controlling band gap in complex-oxide materials.

With this discovery, the potential exists for oxides with band gaps to be continuously controlled over 1 electron volt by site-specific alloying developed by the ORNL team. "Therefore," Lee said, "this work represents a major achievement using complex oxides that offer a number of advantages as they are very stable under extreme and severe environments."

ORNL's Michelle Buchanan, associate lab director for the Physical Sciences Directorate, expanded on Lee's sentiment. "This work exemplifies how basic research can provide technical breakthroughs that will result in vastly improved energy technologies," she said.

More information: "Wide band gap tunability in complex transition metal oxides by site-specific substitution,"

Provided by Oak Ridge National Laboratory