OAK RIDGE NATIONAL LABORATORY
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Band Gap Tuning in Transition Metal Oxides by Site-Specific Substitution

Disclosure Number

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Technology Summary

Large modulation of the band gap is critically important, but often elusive in designing and tuning certain material systems. For example, in complex transition metal oxides, such large band gap change without compromising the intriguing physical properties arising from the strong correlation has been a long-standing challenge. The present invention employs the layered ferroelectric Bi4Ti3O12 and reports that its band gap can be narrowed as much as one electron volt by site-specific substitution with a specific correlated insulator, while maintaining strong ferroelectricity. When a specific site in Bi4Ti3O12 is preferentially substituted, a split-off state responsible for the band gap reduction is created just below the conduction band, greatly reducing the band gap. The demonstrated band gap tuning in polar oxides paves a new route to controlling the band gap in complex transition metal oxides desired for emerging oxide optoelectronics and energy applications.

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