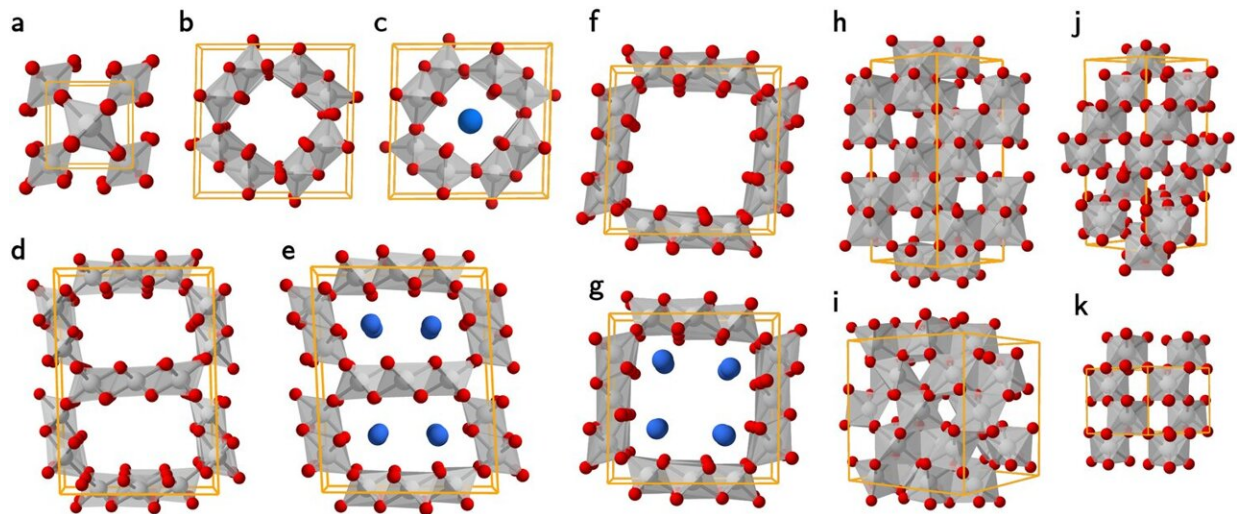


Structure-property relationships in nanoporous and amorphous iridium oxides

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Atomic and crystal structures of the crystalline iridium oxides. a Rutile-type R-IrO₂. b Hollandite-type Ho-IrO₂. c K-intercalated hollandite-type 1K + Ho-IrO₂. d Romanechite-type Ro-IrO₂. e K-intercalated romanechite-type 2K + Ro-IrO₂. f Todorokite-type To-IrO₂. g K-intercalated todorokite-type 4K + To-IrO₂. h Corundum-based C-IrO_{1.5}. i bixbyite-based B-IrO_{1.5}. j R3cR-IrO₃. k P6₃22 P-IrO₃. The iridium, oxygen, and potassium atoms are depicted as gray, red, and blue spheres, respectively, while the octahedra of IrO₆ is shaded in gray. The bulk unit cell is represented by the lines in orange. Credit: *Nature Communications* (2022). DOI: 10.1038/s41467-022-30838-y

South Korean-based researchers have used first-principles quantum mechanical simulations to better understand the structure-property

relationships in various polymorphic phases of iridium oxides to elucidate their outstanding performance in catalyzing the oxygen evolution reaction (OER). The OER is an important half-cell reaction where water is catalytically split to evolve oxygen. However, due to the intrinsic sluggish kinetics of the OER, this leads to an overall poor catalytic performance in general.

The latest findings from computational materials scientist, Professor Aloysius Soon and his team from the Department of Materials Science & Engineering at Yonsei University, demonstrate new physiochemical insights into how nonequivalent connectivity in the amorphous structures strongly enhances the flexibility of the charge states of the [iridium](#) cations, and hence promotes the presence of electrophilic oxygens in them, as compared to their crystalline counterparts. As Professor Soon writes in *Nature Communications*: "A fundamental atomic-scale understanding of high-performance nanopore-containing amorphous oxides of iridium is still very much lacking. And it greatly hinders the establishment of a design rule for further performance improvement."

"This computational study on experimentally reported (but less studied) metastable nanoporous and amorphous iridium oxides provides new physical insight into the structure-property relationship to explain and reconcile the superior OER performance of sub-stoichiometric amorphous iridium oxides. This potentially opens doors for the agile design of iridium-based OER catalysts for modern clean energy technologies," he adds.

Despite the importance of having a firm grasp of complex structure-property relationship in [advanced materials](#), there is still limited understanding of atomic-scale intuitive models for amorphous oxides for clean energy technology.

"To improve the long-term efficacy of the anodic OER, the search for

active, selective, and stable electrocatalysts has been on the rise, and amongst them, oxides (and oxyhydroxides) of iridium and ruthenium are known for their outstanding stability and reactivity in acidic environments," highlights Professor Soon. "A promising way to tune and engineer the structure-property relations of these [oxide](#) catalysts is to control their stoichiometry and polymorphic phase at the atomic-level."

For the first time, systematic density-functional theory calculations have been conducted to examine structure-property relations of nanoporous and amorphous iridium oxides to reconcile the superior [oxygen evolution reaction](#) catalytic performance reported in previous experiments to aid a better design of the next-generation OER catalysts.

"This study potentially opens doors for the agile design of novel iridium-based OER catalysts with [high efficiency](#) for modern clean energy technologies," concludes Professor Soon.

More information: Sangseob Lee et al, Activated chemical bonds in nanoporous and amorphous iridium oxides favor low overpotential for oxygen evolution reaction, *Nature Communications* (2022). [DOI: 10.1038/s41467-022-30838-y](#)

Provided by Yonsei University

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