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THE SECRET OF THE SUN-RESPONSIVE WINDOW: HOW MISSING ATOMS CHANGE COLOUR

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From the left: Smagul Karazhanov, Inga Pudža, and Aleksejs Kuzmins at the award ceremony of the Achievements in Science 2025 at the Latvian Academy of Sciences, 27 February 2026

Imagine a window that automatically darkens when the sun appears, then turns crystal clear again when the clouds roll in – all without drawing a single watt of electricity. This is the promise of yttrium oxyhydride (YHO), a unique "smart" material that has fascinated scientists for over a decade. Although its colour-changing ability was discovered in 2011 [1], the “why” and “how” behind this magic trick remained a scientific mystery until now. A team of researchers from the Institute of Solid State Physics, University of Latvia (Riga, Latvia), the Institute for Energy Technology (Kjeller, Norway), and the Department of Physics and Astronomy, Ångström Laboratory, Uppsala University (Uppsala, Sweden) has finally cracked the code. They revealed a mechanism that involves "missing" atoms, specifically anion vacancies, and atomic-scale structural relaxations.

A Decade-Long Puzzle

YHO belongs to an emerging class of materials known as mixed-anion systems. Unlike simpler materials such as yttrium hydride (a black metal) or yttrium oxide (a transparent insulator), YHO incorporates both hydride (H^-) and oxide (O^{2-}) anions within a single face-centred cubic (fcc) lattice. This

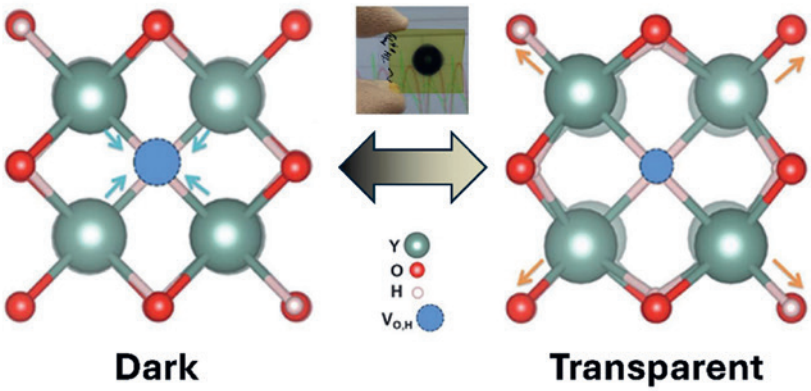


Fig. 1. Calculated local structural arrangements around a vacancy in dark and transparent yttrium oxyhydride thin film

unique combination gives rise to its photochromic properties.

For years, scientists debated what caused YHO to darken under ultraviolet (UV) or blue light. Unlike conventional smart windows that depend on complex multilayer structures and external power sources, YHO achieves photochromism in ambient conditions through internal structural and chemical changes. Some theories suggested that the yttrium atoms changed their chemical state, while others proposed that hydrogen or oxygen atoms were physically moving long distances within the material. However, none of these theories could explain a peculiar phenomenon: why the material's crystal structure contracts when it darkens and expands when it becomes transparent again. To investigate, the research team employed a high-tech "toolbox" that included first-principles calculations and synchrotron-based experiments, carried out at the storage ring, PETRA-III (Hamburg, Germany), which produces extremely bright X-rays [2–4]. By examining the material at the atomic level using X-ray absorption spectroscopy, they found that the answer lay not in the atoms present, but in those that were missing.

The Role of the "Missing" Atoms

YHO is inherently imperfect, featuring numerous anion vacancies – tiny empty pockets in the crystal lattice where a hydrogen or oxygen atom should be. Moreover, yttrium atoms near these vacancies are shifted from their ideal lattice positions. These vacancies are more than structural defects; they drive the colour change. When UV light hits the material, it provides electrons with enough energy to jump into these empty pockets, which changes their electric charge. For example, a positively charged "hydrogen hole" can become negatively charged.

The "Aha!" Moment: Darkening and Shrinking

This change in charge triggers two simultaneous effects that define the photochromic "magic" [2]:

- Tinting (photodarkening): Once these "pockets" are filled with electrons, they start absorbing visible light over a wide energy range (0.5 to 2.6 eV). This results in window shifting from transparent to a dark, brownish-black hue.
- Lattice relaxation (the squeeze): Filling these vacancies alters their electric charge, prompting the surrounding yttrium cations to shift their positions, with yttrium atoms moving inward towards negatively charged vacancies. As a result, the entire crystal lattice contracts, providing the long-sought explanation for the material's "breathing" behaviour.

When the UV light is removed, the electrons slowly escape from these pockets, the yttrium atoms return to their original positions, and the material regains its transparency.

Atomic-Level Evidence: Peering into the Coordination Shells

To verify this mechanism, researchers employed Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy [2, 3]. This method acts as a "microscopic eye" that reveals the average local environment around each yttrium atom in the sample.

The studies revealed a fascinating structural feature: the second coordination shell, corresponding to

the distances between neighbouring yttrium atoms, is divided into two separate subshells. In an ideal cubic crystal, all these distances would be uniform. However, in photochromic YHO, the combination of hydrogen/oxygen mixing and anion vacancies induces a distorted local environment. This splitting persists from temperatures as low as 10 K up to room temperature, demonstrating that it is an intrinsic aspect of the material's photochromic structure.

Importantly, X-ray absorption studies revealed that the oxidation state of most yttrium cations remains stable at approximately +2.5 throughout the entire process. This finding contradicts previous theories suggesting that yttrium itself changed chemical state (from Y^{3+} to Y^{2+}) and supports the idea that the transformation is caused by electron trapping at vacancies.

Towards Smarter Light-Responsive Materials

Understanding the "missing atom" mechanism opens exciting possibilities for defect engineering. Carefully managing the concentration and distribution of anion vacancies during fabrication allows precise tuning of the material's performance.

This breakthrough paves the way for yttrium oxyhydride to be used in high-performance coatings for a range of practical applications, such as energy-efficient buildings, smart goggles, and sun-responsive car roofs. By enabling the material to control incoming sunlight, we could potentially keep buildings cooler and reduce energy consumption – all thanks to the hidden power of anion vacancies.

References

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