may guide the design of more stable perovskite solar cells with improved thermal management, advancing their commercialization. (Reported by Yu-Chun Chuang)

*This report features the work of Jia-Kai Hu, Pai-Chun Wei and their collaborators published in Small **21**, 2408773 (2025).*

TPS 19A High-resolution Powder X-ray Diffraction
ANSTO SIKA – Cold Neutron Triple-axis Spectrometer
NIST SPINS – Spin-polarized Triple-axis Spectrometer

- Inelastic Neutron Scattering
- Hybrid Perovskites, Lattice Dynamics, Thermal Transport, Incommensurate Structures

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Shining X-rays into the Heart of Catalytic Complexity

Seeing through the spinel, element-selected XAS unveils the secret physics that drive high-entropy catalysts.

In the fast-moving field of materials science, researchers are turning chaos into opportunities. A new generation of catalysts, called high-entropy catalysts (HECs), is challenging the traditional notion that simplicity leads to stability. Traditional catalysts typically rely on one or two principal elements, sometimes enhanced by dopants or supports to tailor activity or stability. By contrast, HECs are defined by the deliberate incorporation of multiple principal components—metals, oxides, nitrides, carbides, or sulfides—into a single-phase matrix. The key principle lies in maximizing configurational entropy ($\Delta S_{\text{config}} = R \ln N$), where R is a constant and N is the number of constituent elements. A high ΔS_{config} value can offset the positive enthalpy of mixing, stabilizing otherwise phase-separated systems into uniform crystalline phases. By blending more elements in different proportions, scientists are discovering materials that are not only more robust but also remarkably efficient in driving critical energy reactions. Among these, spinel (AB_2O_4), rock-salt (MO), layered (P2-type), and perovskite (ABO_3) structures are the most widely adopted for HECs as they provide a perfect balance between entropy stabilization and functional versatility. The spinel structure features an entropy-friendly lattice that supports multiple transition metals, high-temperature synthesis, and strong electrochemical stability. Within spinel HECs, this framework enhances thermodynamic stability and improves functional performance, enabling effective charge transfer, reversible redox processes, and extended durability.

Gaining insights into the local environments of spinel structures, including the atomic bonding and oxidation at different sites and electron exchange during reactions, is essential for improving catalyst design. This is where X-ray absorption spectroscopy (XAS) is utilized. Often referred to as a "fingerprint," the XAS technique enables researchers to examine specific elements in complex materials and observe their changes over time. By scanning the energy of X-rays across an element's absorption edge, scientists can identify its oxidation state, coordination geometry, and local bonding environment. This highlights the role of the XAS technique in revealing active sites, oxidation state evolution, and electronic structure modulation. Recent studies conducted this year have demonstrated the effectiveness of using XAS beamlines at the NSRRC. The studies revealed how certain metals can dynamically switch between oxidation states during oxygen evolution reactions,

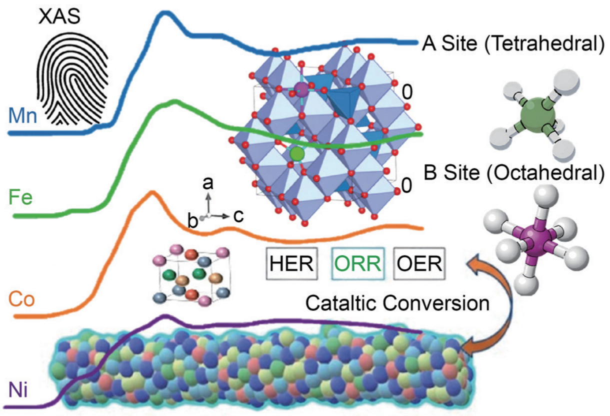

Fig. 1: An in-depth analysis of the AB_2O_4 spinel-type high-entropy catalyst utilizing element-selected XAS techniques reveals significant insights into its catalytic performance and stability.