ABSTRACT:

The Fast and Functional: AI-Driven Discovery of High-Entropy Ceramics

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High-entropy oxides (HEOs) are a novel class of materials comprising five or more metal cations uniformly distributed within a single-phase crystal lattice, stabilized by high configurational entropy. This entropy-driven stabilization imparts exceptional structural and thermal stability, resistance to phase segregation, and tunable electronic and ionic properties. Such characteristics make HEOs highly attractive for use in energy technologies, including battery cathodes and bifunctional electrocatalysts. Their compositional flexibility enables the substitution of expensive or critical elements with earth-abundant alternatives without compromising performance. Moreover, the discovery and optimization of HEOs can be greatly accelerated through AI-driven materials design and high-throughput computational screening, facilitating the identification of optimal elemental combinations and synthesis routes. By coupling high configurational entropy with data-driven materials discovery, HEOs represent a powerful platform for developing stable, efficient, and sustainable next-generation energy materials.

The Clean Materials Technology Laboratory at UCL has developed high-throughput, bottom-up synthetic routes to energy materials, [1-4] sometimes containing more than five metal components. These approaches connect nano precursors[1-4] made from flow reactors and automation, AI-informed high-throughput synthesis, and rapid testing to enable accelerated discovery of high-performance materials with reduced elemental content. Examples of this strategy will be presented for high-power and high-energy lithium-ion HEO cathode materials, bifunctional OER/ORR HEO electrocatalysts, and HEO-based solid-state electrolytes derived from LLZO frameworks.

References

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