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Comparative High-Pressure Study on Rare-Earth Fluorite-Type Oxides with Increasing Configurational Entropy

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Rare-earth fluorite-type oxides provide an ideal platform to investigate the role of configurational entropy on structural stability under extreme conditions. In this talk, I will present a comparative high-pressure study of a series of multicationic rare-earth oxides with increasing configurational entropy, ranging from binary systems ($(CePr)O_2-\delta$) to ternary, quaternary ($(CePrLaNd)O_2-\delta$), and higher-order multicationic compositions.

High-pressure synchrotron X-ray diffraction and Raman spectroscopy experiments up to ˜30 GPa reveal that all compositions retain the cubic fluorite structure over a broad pressure range, despite pronounced lattice disorder and chemical complexity. A reproducible compression anomaly is observed between ˜9 and 16 GPa, characterized by a plateau in the volume–pressure relation and changes in vibrational modes, which is attributed to internal lattice rearrangements and bond-angle distortions rather than a crystallographic phase transition.

With increasing configurational entropy, the fluorite lattice exhibits enhanced resilience against pressure-induced transformations. However, in the intermediate-entropy systems, signatures of pressure-induced amorphization emerge at higher pressures, manifested as reversible broad background contributions in diffraction patterns, highlighting the delicate balance between entropy stabilization and local structural frustration.

By extending the study to quaternary and higher-order compositions, this work provides new insights into how entropy, cation size mismatch, and lattice distortion collectively govern the high-pressure response of fluorite-type rare-earth oxides. These results contribute to a broader understanding of entropy-stabilized oxides under extreme conditions and their potential robustness in high-pressure environments.

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