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Uncover the nature of cubic-rhombohedral transition in Fe1-xO QINGYANG HU, George Mason University, YANG DING, HPSynC, Carnegie Institute Washington, HONGWEI SHENG, George Mason University — Transition metal monoxide Fe1-xO is an archetypal Mott insulator and an important geological compound. Despite considerable study during the past few decades, the origin of the high-pressure cubic-rhombohedral transition in this fundamental material is still not fully understood. Combining high-pressure nanoscale x-ray diffraction imaging techniques, we conducted density-functional theory (DFT) based first-principles calculations to reveal the nature of the transition. Our theoretical calculations confirm the conclusions drawn from our imaging experiments that the pressure-induced rhombohedral distortion of Fe1-xO is associated with <111> stacking defects cluster and is ferroelectric in nature.

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