Fluorite to Cotunnite Structural Phase Transition in Actinide Oxides

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The light-actinide oxides ThO_2 and UO_2 are known to undergo a pressure induced structural phase transition from the ambient (cubic) fluorite structure to a high-pressure (orthorhombic) cotunnite structure at low temperatures. In this investigation, the relativistic Linear Combinations of Gaussian Type Orbitals – Fitting Function (LCGTO-FF) method has been used to calculate the static-lattice zero-temperature isotherm for both of these oxides for pressures ranging from ambient to well above their respective transition pressures. The cotunnite cell parameters also have been determined for both of these oxides, near the transition. Comparisons are made with experimental data and other calculations.

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