Theoretical Zero-Temperature Isotherm and Structural Stability of Thorium Dioxide

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The static-lattice equation of state (EOS) and structural stability of thorium dioxide (ThO_2) have been investigated, within the generalized gradient approximation to density functional theory, using the relativistic linear combinations of Gaussian-type-orbitals – fitting functions (LCGTO-FF) technique. Two known crystal structures for ThO_2 have been considered here, the ambient fluorite structure and the high-pressure cotunnite structure. The theoretical EOS parameters for the two phases and the calculated transition pressure are consistent with experiment to within the known limitations of the GGA model. The internal lattice parameters calculated for the cotunnite phase of ThO_2 differ substantially from the experimentally determined parameters. The source of this difference will be discussed.

*Work supported by the U.S. Dept. of Energy under contract W-7405-ENG-36.