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Large volume change across OI –> OII phase transition in transition-metal dioxides TiO_2, ZrO_2, and HfO_2 as determined by experiment and theory YAHYA AL-KHATATBEH, New Mexico State University, KANANI K.M. LEE, Yale University, BORIS KIEFER, New Mexico State University — The nature of bonding in transition-metal dioxides TiO_2, ZrO_2, and HfO_2 is of interest as they are potential superhard materials with many industrial applications. Using high-resolution synchrotron x-ray powder diffraction for TiO_2 and ZrO_2, and complementary *ab-initio* computations of these dioxides, we have determined the equation of state of the orthorhombic I (OI) and orthorhombic II (OII) phases. Our measurements are in agreement with the computationally predicted phase sequence of these oxides. The measured volume change across OI –> OII transition is 8.3% for TiO_2 and 10% for ZrO_2 in good agreement with our density-functional theory (DFT) calculations that predict a large volume change for all of these dioxides across the OI –> OII phase transition. For TiO_2, this volume collapse is significantly higher than previously measured (2.6%), but consistent with the volume decreases observed in both ZrO_2 and HfO_2 across this transition. Furthermore, the OII phase was observed to be the most stable phase of TiO_2 and ZrO_2 at high pressure (56 GPa) after heating to high temperatures (above ∼1800 K) and no post-OII phase was observed under these conditions.

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