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Theoretical and experimental evidence on the post-cotunnite phase transition in dioxides

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The cotunnite-type structure is identified as the highest-pressure phase in many dioxides and the post-cotunnite phase was still underdetermined. However, very recently, an *ab initio* work on silica has demonstrated a new possible phase transition to an unexpected hexagonal Fe_2P-type structure at 690 GPa with skipping the cotunnite-type stability at the static temperature (T. Tsuchiya and J. Tsuchiya, Proc. Natl. Acad. Sci. U.S.A. **108**, 1252, 2011). In this study, we systematically examined possibile post-cotunnite phase transitions in several low-pressure analogs of silica, GeO_2, SnO_2, TiO_2, and ZrO_2, with the electronic and crystallographic properties. Based on the theoretical prediction, we have performed in situ LH-DAC experiments and succeeded in experimental synthesis of the Fe_2P-type post-cotunnite phase in TiO_2.

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