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二酸化物におけるポストコチュナイト構造転移の理論予測及び実験的観測
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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