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Identification of post-pyrite transition in SiO2 by a genetic algorithm[1] SHUNQING WU, Iowa state U and Xiamen U, KOICHIRO UMEMOTO, GEO, U of Minnesota, KAI-MING HO, MIN JI, CAI-ZHUANG WANG, Ames Lab, Iowa state U, RENATA WENTZCOVITCH, MSI and CEMS, U of Minnesota — Here we propose a new phase of SiO_2 beyond the pyrite-type phase. SiO_2 is one of the most important minerals in Earth and planetary sciences. So far, the pyrite-type phase has been identified experimentally as the highest-pressure form of SiO_2. In solar giants and extrasolar planets whose interior pressures are considerably higher than that on Earth, a post-pyrite transition in SiO_2 may occur at $\sim$ 1 TPa as a result of the dissociation of $MgSiO_3$ post-perovskite into MgO and SiO_2 [Umemtoto et al., Science 311, 983 (2006)]. Several dioxides considered to be low-pressure analogs of SiO_2 have a phase with cotunnite-type ($PbCl_2$-type) structure as the post-pyrite phase. However, a first-principles structural search using a genetic algorithm shows that SiO_2 should undergo a post-pyrite transition to a hexagonal phase, not to the cotunnite phase. The hexagonal phase is energetically very competitive with the cotunnite-type one.

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Koichiro Umemoto

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