Identification of post-pyrite transition in SiO\textsubscript{2} by a genetic algorithm\textsuperscript{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\textsubscript{2} beyond the pyrite-type phase. SiO\textsubscript{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\textsubscript{2}. In solar giants and extrasolar planets whose interior pressures are considerably higher than that on Earth, a post-pyrite transition in SiO\textsubscript{2} may occur at \sim 1 TPa as a result of the dissociation of MgSiO\textsubscript{3} post-perovskite into MgO and SiO\textsubscript{2} \textsuperscript{[Umemtoto et al., Science 311, 983 (2006)]. Several dioxides considered to be low-pressure analogs of SiO\textsubscript{2} have a phase with cotunnite-type (PbCl\textsubscript{2}-type) structure as the post-pyrite phase. However, a first-principles structural search using a genetic algorithm shows that SiO\textsubscript{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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