Identification of post-pyrite transition in SiO₂ by a genetic algorithm¹ 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 SiO₂ beyond the pyrite-type phase. SiO₂ 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 SiO₂. In solar giants and extrasolar planets whose interior pressures are considerably higher than that on Earth, a post-pyrite transition in SiO₂ may occur at ~ 1 TPa as a result of the dissociation of MgSiO₃ post-perovskite into MgO and SiO₂ [Umemtoto et al., Science 311, 983 (2006)]. Several dioxides considered to be low-pressure analogs of SiO₂ have a phase with cotunnite-type (PbCl₂-type) structure as the post-pyrite phase. However, a first-principles structural search using a genetic algorithm shows that SiO₂ 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.

¹This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering and NSF under ATM-0428774 (VLab), EAR-0757903, and EAR-1019853.