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Post-stishovite transition in AlOOH-incorporated SiO₂¹ KAT-SUYUKI KAWAMURA, Tokyo Institute of Technology, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, University of Minnesota, KEI HIROSE, Tokyo Institute of Technology — In 2007, Lakshtanov et al. [Proc. Nat. Acad. Sci. 104, 13588 (2007)] showed that the incorporation of AlOOH into SiO₂ significantly reduces the transition pressure between stishovite and CaCl₂-type phases. In the present paper, we investigate theoretically the effect of hydrogen and aluminum on this transition. First-principles calculations show that aluminum has no effect on the transition pressure. However, hydrogen bonds play a crucial role, suggesting that a cooperative redistribution of hydrogens aids the post-stishovite transition. Large-scale molecular dynamics simulations using model potentials confirm this effect and reveal the nature of the hydrogen motion. This effect produces a strong temperature dependence on the transition pressure and should make the latter sensitive to hydrogen content in the material.

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Koichiro Umemoto

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