Abstract Submitted
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Post-stishovite transition in hydrous aluminous SiO_2[1] RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, U of Minnesota, Twin Cities, KOICHIRO UMEMOTO, Department of Earth Sciences, U of Minnesota, Twin Cities, MN, USA and Earth and Life Sciences Institute, Tokyo-Tech, Tokyo, Japan, KATSUYUKI KAWAMURA, Department of Sustainable Resource Science, Okayama University, Okayama, Japan, KEI HIROSE, Earth and Life Sciences Institute, Tokyo-Tech, Tokyo, Japan — Incorporation of aluminum and some water into SiO_2 significantly reduces the post-stishovite transition pressure in SiO_2. This behavior suggests that the ferroelastic post-stishovite transition in subducted Earth's crust could be the source of seismic anomalies with low shear velocities observed in the mid to upper lower mantle. Using ab initio static calculations and molecular dynamics with inter-atomic potentials, we show that hydrogen bonds play a crucial role in lowering the transition pressure. A cooperative redistribution of hydrogen atoms is the main mechanism responsible for the transition pressure reduction in hydrous aluminous stishovite. The effect is enhanced by increasing the water content and suggests a relationship between the depth of these seismic anomalies and degree of hydration of stishovite in the subducted crust.

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