First principles calculation of high pressure phase of AlOOH (delta-phase)

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Using the first principles calculation method, we investigate the crystal structure of high-pressure phase of AlOOH (delta-AlOOH). It is important as a substance in subducting sediment rocks and as a possible water reserver in the Earth's lower mantle. Three types of stable structure are obtained relating to the hydrogen position. Two have an asymmetric hydrogen bond and other a symmetric one. We find that the asymmetric hydrogen bond of low-pressure phase transforms to symmetrized phase under high pressure of 28 GPa. The symmetrized phase has remarkably larger bulk modulus than those of the asymmetrized phases. Our results indicate that the subtle change of hydrogen position causes the significant effect on hydrogen bonding nature and elastic property of delta-AlOOH.