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LETTER

Stability of the $MgCO_3$ structures under lower mantle conditions

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ABSTRACT

The presence of carbon in the Earth makes the search for high-pressure carbon-containing phases essential for our understanding of mineral compositions of the Earth's mantle. In a recent study Isshiki et al. (2004) demonstrated that magnesite transforms into a new phase at lower mantle pressures. However, the structure of the emerging phase remained unknown. Here we show, by means of first principles calculations, that $MgCO_3$ magnesite can transform into a pyroxene structure at 113 GPa, which further transforms into a $CaTiO_3$-type structure at about 200 GPa.