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Structural stability of FeO₂ in the pressure range of lower mantle

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Abstract: Recently the finding of a new iron oxide pyrite-type FeO₂ is reported to involve in the oxygen cycles occurred in Earth's mantle. Understanding of the stability of FeO₂ at high pressures will be critical to model the cyclical process of oxygen in the lower mantle. Here we report the possible pressure-driven phase transition of FeO₂ in the pressure range of lower mantle by combining particle swarm optimization method and different density functional theory (DFT) techniques. We find a possible pressure-driven phase transition from PNNM symmetry phase to PA-3 symmetry (Pyrite-type) phase in the pressure range of lower mantle. Nevertheless, the stability of the PNNM symmetry phase is highly affected by temperature change. The possible pressure-driven phase transition is disappeared when the temperature exceeded 800 K. It is also found that the PNNM symmetry phase is mechanically unstable when temperature is beyond 800 K. Finally, the reactions Gibbs free energies of two possible decomposition reactions of FeO₂ are calculated from different DFT techniques. It is found that the pyrite-type FeO₂ decomposes to Fe₂O₃ and O₂ is the more likely scenario in the relative low-pressure and high-temperature region. However, more detailed calculations, where the phase transitions and the different spin state of iron oxides are also taken into account, are needed to clarify this decomposition reaction.

Keywords: pyrite-type FeO₂, elastic constants, structural stability, high pressure

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