Structure of MgO(MgSiO$_3$)$_n$ in Earth’s Lower Mantle: ab initio calculations

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— Ruddlesden-Popper (RP) compounds are composed of alternating perovskite-type and rocksalt-type structural elements. MgSiO$_3$ and MgO are found as separate phases in Earth’s lower mantle. Both structural elements occur also in the hypothetical RP-series MgO(MgSiO$_3$)$_n$. It is interesting to explore the high pressure-high temperature stability of such RP-structures. Using the augmented plane wave implementation of Density Functional Theory we investigate the structural stability at lower mantle conditions of the member with $n = 1$ e.g. Mg$_2$SiO$_4$. The goal of the present calculations is to test the stability of this Ruddlesden-Popper phase relative to $\gamma$-(Mg,Fe)$_2$SiO$_4$ and the assemblage MgSiO$_3$-perovskite + MgO magnesiowüstite. We will present our results of this study.

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