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Structure of $MgO(MgSiO_3)_n$ in Earth's Lower Mantle: ab initio calculations PATRIC OULEVEY, MOHAMMED SAHNOUN, Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland, SIMONPIETRO DI PIERRO, Laboratoire de Sciences de la Terre, UMR CNRS 5570, Ecole Normale Supérieure de Lyon, France, BERNARD GROBÉTY, Department of Mineralogy, University of Fribourg, CH-1700 Fribourg, Switzerland, CLAUDE DAUL, Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland
— 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_2SiO_4. The goal of the present calculations is to test the stability of this Ruddlesden-Popper phase relative to γ-$(Mg,Fe)_2SiO_4$ and the assemblage $MgSiO_3$-perovskite + MgO magnesiowüstite. We will present our results of this study.

Patric Oulevey
Department of Chemistry, University of Fribourg,
CH-1700 Fribourg, Switzerland

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