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Prediction of crystal structures and motifs in the Fe-Mg-O system at Earth's core pressures

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Fe, Mg, and O are among the most abundant elements in terrestrial planets. While the behavior of the Fe-O, Mg-O, and Fe-Mg binary systems under pressure have been investigated, there are still very few studies of the Fe-Mg-O ternary system at relevant Earth's core and super-Earth's mantle pressures. Here, we use the adaptive genetic algorithm (AGA) to study ternary $Fe_xMg_yO_z$ phases in a wide range of stoichiometries at 200 GPa and 350 GPa. We discovered three dynamically stable phases with stoichiometries $FeMg_2O_4$, Fe_2MgO_4, and $FeMg_3O_4$ with lower enthalpy than any known combination of Fe-Mg-O high-pressure compounds at 350 GPa. With the discovery of these phases, we construct the Fe-Mg-O ternary convex hull. We further clarify the composition- and pressure-dependence of structural motifs with the analysis of the AGA-found stable and metastable structures. Analysis of binary and ternary stable phases suggest that O, Mg, or both could stabilize a BCC iron alloy at inner core pressures.