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**Predicting Variable Stoichiometric Compounds under High Pressure** QIANG ZHU, ARTEM OGANOV, SUNY-Stony Brook — Materials under pressure often exhibit exotic physical and chemical behaviors. In particular, extremely new stable compounds appear. Here, we studied the variation of stoichiometry under pressure by using the evolutionary search scheme. Two kinds of oxides (Xe-O and Mg-O) have been investigated under megabar pressures. For XeO, we predict the existence of thermodynamically stable Xe-O compounds at high pressures (XeO, XeO<sub>2</sub> and XeO<sub>3</sub> become stable at pressures of 83, 102 and 114 GPa, respectively). For Mg-O, our calculations find that two extraordinary compounds MgO<sub>2</sub> and Mg<sub>3</sub>O<sub>2</sub> become thermodynamically stable at 116 GPa and 500 GPa, respectively. Our calculations indicate large charge transfer in these oxides for both systems, suggesting that large electronegativity difference and pressure are the key factors favoring their formations. We also discuss if these oxides might exist at earth and planetary conditions.

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