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Discovery of pyrite-structured FeO₂ at high pressure¹ QINGYANG HU, Stanford University, HO-KWANG MAO, Carnegie Institution of Washington, WENDY MAO, Stanford University — We conducted x-ray diffraction experiment and first-principles simulation on the assemblage of ferric iron oxide and oxygen. The sample was compressed up to one megapressure (100 GPa) and heated by a double-sided laser to above 2000 K. We identified a previous predicted but not experimentally observed FeO₂ phase and solve the structure by multigrain single crystal method. Iron peroxide is energetically stable above 75 GPa and holds greater amount of oxygen than any other iron oxides. We further recognized this phase also relates to the decomposition of iron oxy-hydroxide at high pressure. The extreme stability of FeO₂ can result in accumulating high-density iron peroxide at mantle basal and ascending hydrogen to the crust. This work suggests a new paradigm in the research of Fe-O-H ternary system under extreme conditions.

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