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Structures of xenon oxides at high pressures[1] NICHOLAS WORTH, University of Cambridge, CHRIS PICKARD, University College London, RICHARD NEEDS, University of Cambridge, AGNES DEWAELE, PAUL LOUBEYRE, CEA, MOHAMED MEZOUAR, ESRF — For many years, it was believed that noble gases such as xenon were entirely inert. It was only in 1962 that Bartlett first synthesized a compound of xenon. Since then, a number of other xenon compounds, including oxides, have been synthesized. Xenon oxides are unstable under ambient conditions but have been predicted to stabilize under high pressure. Here we present the results of a combined theoretical and experimental study of xenon oxides at pressures of 80-100 GPa. We have synthesized new xenon oxides at these pressures and they have been characterized with X-ray diffraction and Raman spectroscopy. Calculations were performed with a density-functional theory framework. We have used the *ab-initio* random structure searching (AIRSS) method together with a data-mining technique to determine the stable compounds in the xenon-oxygen system in this pressure range. We have calculated structural and optical properties of these phases, and a good match between theoretical and experimental results has been obtained.

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