Oxides Under Pressure: from Densified Silica to the Rheology of the Earth's Mantle

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The paper will describe recent advances in the atomistic simulation of oxides at extreme conditions of pressure. The simulations are carried out using interatomic force fields optimized by best fit on first-principles (density-functional theory) calculations. The paper will focus on two applications of the method: (a) the mechanisms of permanent densification in silica glass, and (b) the properties of dislocations in MgO, the second most abundant mineral in the Earth's lower mantle.

Keywords: simulation, DFT, high pressure