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Pressure-induced phase transformation SnO_2: An ab initio constant pressure study DANIEL YEHDEGO[1], MURAT DURANDURDU[2], University of Texas at El Paso — We study the behavior of SnO_2 under rapid hydrostatic pressures using constant-pressure ab initio simulations. We find that the rutile-type SnO_2 transforms into the $CaCl_2$-type structure. At a high pressure of about 20 GPa, a phase transformation into a cubic fluorite-type structure is observed. The orthorhombic Pnma cotunnite-structured phase is formed above 100 GPa. The transformation mechanisms at the atomistic level are discussed.

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