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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