

# The high-pressure phase transitions $\beta$ -tin $\rightarrow$ Imma $\rightarrow$ sh in silicon

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We present an ab-initio study of the high-pressure phase transitions through the structure sequence  $\beta$ -tin $\rightarrow$ Imma $\rightarrow$ sh of silicon. The plane-wave pseudopotential approach to the density-functional theory implemented in VASP is used. A comparison of the results using the local-density approximation and the generalized-gradient approximation is included. We determine the equilibrium properties of each structure and the critical values of the phase transition under hydrostatic pressure. We also investigate in the pressure dependence of the electronic band structure and the corresponding density of states. The order of the phase transitions is discussed taking into account the behavior of the lattice parameters under pressure and the enthalpy barriers which must be crossed during the phase transitions. Finally we show a comparison with experimental results.