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Pressure-induced ferroelastic phase transition in SnO_2 from density functional theory[1] LEI YANG, WEILIU FAN, YANLU LI, LEI WEI, XIAN ZHAO, Shandong University — We studied the high-pressure ferroelastic transition of rutile- to $CaCl_2$-type SnO_2 within density functional theory and Landau free energy theory. Softening mechanism of B_{1g} mode (order parameter Q) and the coupling mechanism between the soft B_{1g} mode and the soft transverse acoustic (TA) mode (strain ε) are clarified by calculating Landau energy map around the ground state. It is found that the Sn-O-Sn bending induced soft B_{1g} mode effectively reduces the excess energy increase caused by bond stretching, which however always leads to SnO_6 octahedral distortion. The octahedral distortion is subsequently minimized by lattice distortion strain ε, which interacts with the soft B_{1g} mode to further increase the stability of system.

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