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Phase diagram of Ti metal at high pressure YAHYA AL KHATATBEH, KANANI LEE, BORIS KIEFER, New Mexico State University — Using density-functional theory based ab-initio computations, we have investigated the hexagonal close-packed (hcp) and the hexagonal (ω) structures titanium (Ti), and find good agreement with experiment. The hcp phase yields an equation of state of a zero pressure volume V_0 = 17.37 (0.02) Å^3, an isothermal bulk modulus K_0= 111.9 (0.2) GPa, and its pressure derivative K_0' = 3.60 (0.02). Furthermore, the c/a ratio for both phases increases with increasing pressure. Additionally, the calculated transition pressure from hcp to ω phase compares well with the experimental results with the ω phase more stable than the hcp phase at pressures greater than $\sim$ 5 GPa.

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