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Crushing Elemental Calcium into a High Temperature Superconductor. ZHIPING YIN, Department of Physics, UC Davis, FRANCOIS GYGI, Dept. of Applied Science, UC Davis, WARREN PICKETT, Department of Physics, UC Davis — The high temperature superconductivity (up to 25 K) observed in elemental Ca at high pressure extends across several phase boundaries, making understanding the crystal structures of Ca under high pressure of great importance. Above 100 GPa, both experiment and theory indicate three possible structures, having space groups $P4_32_12$, Cmca and Pnma. The reported room temperature structure, primitive simple cubic in the 32-109 GPa range, is dynamically unstable at T=0 throughout this range, according to linnear response calculations of the phonon spectrum. Structure optimization and constant pressure enthalpy calculations using density functional theory reveal that several structures (the structures mentioned above, an I-43m structure, and simple cubic)are quasi-degenerate, and hence are competing, in the pressure ranges 40-80 GPa and 100-130 GPa. Volume collapse transitions of the Cmca and Pnma structure will also be described. We discuss the implications of these findings for the observed room temperature "simple cubic" phase. Linear response calculations give $T_c \sim 20$ K for several of the phases at high pressure. Predictions of electron-phonon coupling in the 120-220 GPa regime will also be discussed.

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