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The role of anharmonicity in the ab-initio phase diagram of calcium MARCO DI GENNARO, SRIJAN KUMAR SAHA, MATTHIEU JEAN VERSTRAETE, University of Liege — In the 32-119 GPa pressure range and at room temperature, a simple cubic phase was reported for calcium in many different experiments. Standard linear response theory, both within density functional perturbation theory and frozen phonon calculations, presents dynamical instabilities for simple cubic in the whole pressure range. Many other possible candidate phases, as well as several possible stabilization mechanisms for simple cubic phase, have been proposed as the result of *ab-initio* predictions but the role of temperature on the relative stability of the different phases has not been investigated systematically. We revisit the stability of three candidate phases of calcium for the intermediate pressure range and for various value of temperatures, taking explicitly into account thermal corrections relative to electronic as well as phononic entropy and anharmonic contributions. This corrects the discrepancies among previous theoretical results and experiments, and presents a different picture of the temperature driven phase transition, which results from dynamical anharmonic stabilization of simple cubic and de-stabilization of the tetragonal phase. Transport quantities are calculated in the stabilized phases, to provide additional points of comparison with experiments.

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