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Thermal disorder, entropy and the $\alpha - \gamma$ transition in Ce from density-functional theory THOMAS JARLBORG, DPMC, University of Geneva, CH-1211 Geneva 4 — There are many recent theoretical efforts to describe the $\gamma - \alpha$ transition in fcc Cerium. The large volume γ-phase is magnetic, while the low-volume non-magnetic α- phase can be reached at high pressure or low T. It has been recognized that real T-dependent lattice disorder can be important for the electronic structure and properties in some materials with sharp density-of-state variations near E_F. This might also be the case for Ce, because of its narrow f-band at the Fermi level, and its relatively soft lattice. Here are presented results for fcc Ce at different volumes from first principles GGA-DFT band-structure calculations for large supercells with different degrees of T-dependent disorder. Local disorder, local density-of-states and magnetic moments are all connected. It is shown that structural disorder at large temperature has a direct influence on the magnetic γ-phase, and its corresponding entropy. The results corroborate the earlier findings that standard DFT band-theory can describe the T-dependent transition if all entropy contributions are included. In addition, thermal disorder is important for the properties of fcc Ce.

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