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First-principles phase diagram for Ce-Th system ALEXANDER LANDA, PER SODERLIND, Physics and Advanced Technologies Directorate, Lawrence Livermore National Laboratory, University of California, P.O. Box 808, Livemore, CA 94550, USA, ANDREI RUBAN, LEVENTE VITOS, Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, SE-10044, Stockholm, Sweden, LEONID POUROVSKII, Electronic Structure of Materials, Theoretical Physics Department, University of Nijmegen, 6525ED, Nijmegen, The Netherlands — *Ab initio* total energy calculations based on the exact muffin-tin orbitals (EMTO) theory are used to determine the high pressure and low temperature phase diagram of Ce and Th metals as well as the $Ce_{43}Th_{57}$ disordered alloy. The compositional disorder for the alloy is treated in the framework of the coherent potential approximation (CPA). Equation of state for Ce, Th and $Ce_{43}Th_{57}$ has been calculated up to 1 Mbar in good comparison with experimental data: upon compression the Ce-Th system undergoes crystallographic phase transformation from an fcc to a bct structure and the transition pressure increases with Th content in the alloy. This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract W-7405-Eng-48. A.R. and L.V. are grateful to the Swedish Research Council, the Swedish Foundation for Strategic Research, and the Royal Swedish Academy of Sciences.

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