

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic structure calculations of the CePt₃Si. ARMANDO REYES-SERRATO, DONALD HOMERO GALVAN, Centro de Ciencias de la Materia Condensada UNAM, Ensenada BC, Mexico — In a recent paper, Bauer *et al.* [1] synthesized CePt₃Si, a heavy fermion material with both transitions magnetic and superconducting, without inversion center in the crystal structure. This compound is very interesting from many points of view. In the present work, we report the analysis of the electronic structure of the CePt₃Si in normal state. The calculation was performed with the program package WIEN2k, which use density functional theory (DFT) based on the full-potential linearized augmented plane-wave (LAPW) plus local orbital (lo) method [2]. We report band structure, total and partial densities of states, 3D density of charge and Fermi surface. We analyze the possible implications of our results in the superconductivity of this material. [1] Phys. Rev. Letter **92**, 027003 (2004). [2] <http://www.wien2k.at>

Armando Reyes-Serrato
Centro de Ciencias de la Materia Condensada UNAM, Ensenada BC, Mexico

Date submitted: 04 Jan 2006

Electronic form version 1.4