



Iranian Journal of Physics Research, Vol. 11, No. 4, 2012

Electronic properties of antiferromagnetic UBi_2 metal by exact exchange for correlated electrons method

Esmail Ghasemikhah and Saeid Jalali Asadabadi

Department of Physics, Faculty of Science, University of Isfahan, Isfahan
E-mail: sjalali@phys.ui.ac.ir

(Received 13 March 2011 ; in final form 9 November 2011)

Abstract

This study investigated the electronic properties of antiferromagnetic UBi_2 metal by using ab initio calculations based on the density functional theory (DFT), employing the augmented plane waves plus local orbital method. We used the exact exchange for correlated electrons (EECE) method to calculate the exchange-correlation energy under a variety of hybrid functionals. Electric field gradients (EFGs) at the uranium site in UBi_2 compound were calculated and compared with the experiment. The EFGs were predicted experimentally at the U site to be very small in this compound. The EFG calculated by the EECE functional are in agreement with the experiment. The densities of states (DOSs) show that 5f U orbital is hybridized with the other orbitals. The plotted Fermi surfaces show that there are two kinds of charges on Fermi surface of this compound.

Keywords: electric field gradients, UBi_2 , hybridizing, 5f U orbital, fermi surface

For full article, refer to the Persian section