Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Sorting Category: 10.1.6 (C)

Density-functional electronic structure and the origin of the Dzyaloshinskii-Moriya spin interaction in MnSi K.V. SHANAVAS, S. SATPATHY, Department of Physics & Astronomy, University of Missouri — The metallic helimagnet MnSi has been found to exhibit skyrmionic spin textures when subjected to magnetic fields at low temperatures. The Dzyaloshinskii-Moriya (DM) interaction plays a key role in stabilizing the skyrmions, which arises from the anisotropic part of the super-exchange coupling and is of the form $\vec{D} \cdot (\vec{S}_i \times \vec{S}_j)$. The constant $\vec{D}$ depends on the strength of spin-orbit interaction of Mn d states and the orbital mixing induced by the distortion of $MnSi_6$ octahedra from the centrosymmetric rock salt phase. Using density functional theory based electronic structure calculations and symmetry analysis, we study the nature of the electronic ground state and the origin of the DM interaction in the B20 phase of MnSi. The ground state in the undistorted phase corresponds to d^6 configuration at Mn and p^2 at Si sites. The distortion reduces bandwidths and intermixes the ground state with the excited states, leading to a significant DM spin-orbit interaction.

S. Satpathy
satpathys@missouri.edu
Department of Physics & Astronomy, University of Missouri

[X] Prefer Oral Session
[ ] Prefer Poster Session

Date submitted: 13 Dec 2011 Electronic form version 1.4