Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Development of noncollinear-spin DFT+U method with spin-orbit interaction EUNJUNG KO, HYUNGJUN LEE, HYUNGJU OH, Department of Physics and IPAP,Yonsei University. Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University., SE YOUNG PARK, Department of Physics and IPAP,Yonsei University. Department of Physics, Columbia University., HYOUNG JOON CHOI, Department of Physics and IPAP,Yonsei University. Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University. — We developed a DFT+U+SOI method by incorporating spin-orbit interaction (SOI) into a noncollinear-spin generalization of the density functional theory (DFT) plus Coulomb interaction among d electrons, parameterized by U and J. The Coulomb interaction, which is based on the rotationally invariant form, is generalized for noncollinear-spin configuration, and the fully localized limit is adopted for the double-counting term. The spin-orbit interaction is treated in the l-dependent fully separable nonlocal form using additional Kleinman-Bylander projectors generated by relativistic calculations of atoms. We implemented our DFT+U+SOI method into the SIESTA code and performed test calculations for the $4d$ or $5d$ transition metal oxides, the all-in-all-out noncollinear magnetic insulator $Cd_2Os_2O_7$, the canted antiferromagnetic order insulator Sr_2IrO_4, and the paramagnetic insulator Ca_2RuO_4. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2012-C3-046).

Hyoung Joon Choi
Yonsei Univ

Date submitted: 15 Nov 2013 Electronic form version 1.4