ABSTRACT CODE

Exchange coupling in Eu chalcogenides

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Eu O and Eu chalcogenides belong to a rare type of magnetic insulators (semi-conductors), which order ferro-magnetically [FM] (EuSe and EuTe only at applied pressure). FM order in insulators open up an interesting possibilities for application in spintronics, particularly as spin filters in tunnel barriers. Despite the simple NaCl crystal structure and $4f^7$ configuration of Eu, which results in simple Heisenberg magnet behavior, the nature of the exchange interactions is still unclear. Several models of exchange coupling have been developed in the past decades, but a quantitative investigation based on ab-initio electronic structure is still missing. We present preliminary results of FLAPW LDA+U calculations. We complement the total energy calculation (which indeed predicts EuO and EuS to be FM) with analysis based on Wannier function formalism. The latter allows for direct calculation of hopping and exchange parameters. Compared to commonly used atomic orbitals and resulting tight binding fits, the Wannier functions contain the information about chemical environment (hybridization) in a physically transparent way.