Electronic and magnetic properties of Mn based double perovskites: Ba_2MnMO_6(M=Mo,Re), $LaBaMnMoO_6$

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Double perovskites(DP) Sr_2FeMO_6(M=Mo,Re) exhibit significant colossal magnetoresistance at room temperature due to the high Curie temperatures. However, Ba_2MnMO_6(M=Mo,Re)and $LaBaMnMoO_6$ which have same valence electrons in Mn 3d atoms, do not show ferromagnetism or the high Curie temperatures. To investigate the electronic and magnetic structure differences between Fe based DP and Mn based DP, we performed first principle calculations[1] for Mn based double perovskites using LSDA and LDA+U methods. Recently, Kanamori and Terakura[2] proposed the ferromagnetic(FM) stabilization mechanism. In $SrFeMoO_6$, a strong hybridization between Fe t_{2g} and Mo t_{2g} orbitals gives the energy gain contributed by the negative spin polarization of Mo t_{2g} bands, and stabilize the strong FM coupling of Fe atoms[3]. In Mn based DP, the calculated results show that all of Mn t_{2g} bands are higer than Fe t_{2g} bands and locate far from the M(M=Mo,Re) 4d or 5d bands. It leads weak hybridization between Fe t_{2g} and M t_{2g} orbitals and small bandwidths of M and Mn t2g bands. The energy gain contributed by Mo t2g bands is smaller than Fe based DP and double exchange is weak in these materials.

References

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