MAR17-2016-020286

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Magnetism, spin-lattice-orbital coupling and exchange-correlation energy in oxide heterostructures: Nickelate, titanate, and ruthenate[1]

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Many interesting physical phenomena and material characteristics in transition-metal oxides (TMO) come out of the intriguing interplay between charge, spin, orbital, and lattice degrees of freedom. In the thin film and/or heterointerface form of TMO, this feature can be controlled and thus be utilized. Simultaneously, however, its detailed characteristic is more difficult to be identified experimentally. For this reason, the first-principles-based approach has been playing an important role in this field of research. In this talk, I will try to give an overview of current status of first-principles methodologies especially for the magnetism in the correlated oxide heterostructures or thin films. Nickelate, titanate, and ruthenate will be taken as representative examples to demonstrate the powerfulness of and the challenges to the current methodologies On the one hand, first-principles calculation provides the useful information, understanding and prediction which can hardly be obtained from other theoretical and experimental techniques. Nickelate-manganite superlattices ($LaNiO_3/LaMnO_3$ and $LaNiO_3/CaMnO_3$) are taken as examples. In this interface, the charge transfer can induce the ferromagnetism and it can be controlled by changing the stacking sequence and number of layers. The exchange-correlation (XC) functional dependence seems to give only quantitatively different answers in this case. On the other hand, for the other issues such as orbital polarization/order coupled with spin order, the limitation of current methodology can be critical. This point will be discussed with the case of tatinate superlattice ($LaTiO_3/LaAlO_3$). For ruthenates ($SrRuO_3$ and Sr_2RuO_4), we found that the probably more fundamental issue could be involved. The unusually strong dependence on the XC functional parametrization is found to give a qualitatively different conclusion for the experimentally relevant parameter regions.

[1]This work was supported by National Research Foundation of Korea (2014R1A1A2057202)