Exchange interactions in iron pnictides: beyond long wave approximation

VLADIMIR ANTROPOV, Ames Laboratory, IA, LIQIN KE, MARK VAN SCHILFGAARDE, Arizona State University, AZ — The character of magnetism in the recently discovered iron pnictides is unusual. In particular, the exchange coupling parameters have attracted a lot of attention. However, calculation of these parameters have been based on methods or approximations suitable only for localized magnetic moment systems. Such approximations greatly underestimate the amount of possible itinerant magnetic excitations and can result not only in large quantitative errors, but they often create a wrong picture of magnetic interactions in systems with itinerant magnetic electrons. We present new calculations of the exchange coupling parameters, going beyond the widely accepted long-wave approximation with application for most popular iron pnictide systems. We compare it with earlier calculations and the experimental neutron analysis. The criteria of applicability of long wave approximations have been estimated for a wide range of magnetic systems.