New mechanism of kinetic exchange interaction induced by strong magnetic anisotropy

NAOYA IWAHARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — It is well known that the kinetic exchange interaction between single-occupied magnetic orbitals (s-s) is always antiferromagnetic, while between single- and double-occupied orbitals (s-d) is always ferromagnetic and much weaker. Here we show that the exchange interaction between strongly anisotropic doublets of lanthanides, actinides and transition metal ions with unquenched orbital momentum contains a new s-d kinetic contribution equal in strength with the s-s one [1]. In noncollinear magnetic systems, this s-d kinetic mechanism can cause an overall ferromagnetic exchange interaction which can become very strong for transition metal ions. The importance of the s-d kinetic interaction and the possibility of the ferromagnetic interaction are confirmed in some existing complexes on the basis of the density functional theory calculations. [1] N. Iwahara and L. F. Chibotaru, arXiv:1502.04180.