

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

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.

Naoya Iwahara
Theory of Nanomaterials Group, Katholieke Universiteit Leuven

Date submitted: 01 Dec 2015

Electronic form version 1.4