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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, of the order $-t^2/U$, where t is the transfer parameter and U is the electron promotion energy. At the same time the exchange interaction between single- and double-occupied orbitals, s-d, is always ferromagnetic, of the order $t^2/U \cdot J/U$, where J is the Hund's rule coupling parameter ($J/U \simeq 0.1$). Here we show that the exchange interaction between ground doublet states of lanthanide or actinide ions is characterized by equal in magnitude s-s and s-d kinetic exchange interactions, both scaling as $\sim t^2/U$ [1]. Moreover, the s-d kinetic mechanism prevails in many situations, contributing to antiferromagnetic coupling in the case of collinear magnetic ions. In the non-collinear case the s-d kinetic mechanism can cause an overall ferromagnetic exchange interaction of the order of t^2/U, already for the angle $\sim \pi/4$ between the main magnetic axes on sites, which appears quite counter-intuitive. This new s-d kinetic mechanism is not operative in the case of exchange interaction between strongly anisotropic magnetic doublets and an isotropic spin.

[1] N. Iwahara and L. F. Chibotaru, submitted to Phys. Rev. Lett.

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