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Giant exchange interaction in mixed lanthanides NAOYA IWAHARA, VEACHESLAV VIERU, LIVIU UNGUR, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — Combining strong magnetic anisotropy with strong exchange interaction is a long standing goal in the design of quantum magnets. The lanthanide complexes, while exhibiting a very strong ionic anisotropy, usually display a weak exchange coupling, amounting to only few wavenumbers. Recently, an isostructural series of mixed Ln-R-Ln complexes with R the N_2^{3-} radical have been reported, in which the exchange splitting is estimated to reach hundreds wavenumbers [1,2]. Here we apply a new methodology allowing to establish on the basis of DFT and *ab initio* calculations the microscopic mechanism governing the unusual exchange interaction in these compounds [3]. We find it to be basically kinetic and highly complex, involving non-negligible contributions up to seventh power of total momentum $\hat{\mathbf{J}}$ of each Ln site. The performed analysis also elucidates the origin of magnetization blocking in these compounds. Contrary to general expectations the latter is not always favored by strong exchange interaction. [1] J. D. Rinehart, M. Fang, W. J. Evans, and J. R. Long, Nat. Chem. **3**, 538 (2011). [2] J. D. Rinehart, M. Fang, W. J. Evans, and J. R. Long, J. Am. Chem. Soc. **133**, 14236 (2011). [3] V. Vieru, N. Iwahara, L. Ungur, and L. F. Chibotaru, arXiv:1509.02206.

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