## Abstract Submitted for the MAR14 Meeting of The American Physical Society

Exchange interaction in lanthanides LIVIU CHIBOTARU, NAOYA IWAHARA, VEACESLAV VIERU, Theory of Nanomaterials Group, KU Leuven, THEORY OF NANOMATERIALS GROUP, KU LEUVEN TEAM — Anderson's superexchange model is applied for analytical derivation of exchange interaction between total magnetic moments  $\mathbf{J}_1$  and  $\mathbf{J}_2$  corresponding to ground atomic multiplets of two exchange-coupled lanthanide ions. Despite the common belief that the exchange interaction is of  $\sim \mathbf{J}_1 \cdot \mathbf{J}_2$  form, we find it corresponding to convolution of tensors  $O_{kq}(\mathbf{J}_1)$  and  $O_{k'q'}(\mathbf{J}_2)$  of ranks  $k, k' \leq 7$ . All contributions are of the same order as the term  $\sim \mathbf{J}_1 \cdot \mathbf{J}_2$  and cannot be neglected. In the case of exchange-coupled lanthanide ion ( $\mathbf{J}$ ) and isotropic magnetic center ( $\mathbf{S}$ ) the exchange interaction is described by convolutions of tensors  $O_{kq}(\mathbf{J}), \ k = 1, 3, 5, 7$  with the spin  $\mathbf{S}$ . Among these contributions  $\sim \mathbf{J} \cdot \mathbf{S}$  is not the dominant term, as was commonly assumed, hence all tensorial components should be taken into account.

Liviu Chibotaru Theory of Nanomaterials Group, KU Leuven

Date submitted: 15 Nov 2013 Electronic form version 1.4