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Investigation of the Barriers of Blocking of Magnetization In Strongly Anisotropic SMM By Ab Initio Methods LIVIU CHIBOTARU, LIVIU UNGUR, University of Leuven — A large amount of data concerning the blocking barriers of reversal of magnetization in various complexes with strongly anisotropic metal ions (Ln^{III}, Co^{II}) became recently available. Understanding the mechanisms of formation of these barriers is of primary importance for an efficient design of Ln-based single-molecule magnet (SMM) and represents a challenging task for the theory. Here an ab initio based approach for the investigation of blocking barriers will be presented. The methodology will be applied for the construction of the blocking barriers and the understanding of the variation of SMM properties in the series of mixed 3d-4f trinuclear complexes Co-Ln-Co, Ln=Gd, Tb, Dy. In particular, the reasons for a more pronounced SMM behavior manifested by the gadolinium complex will be elucidated. Another example is a recently synthesized Dy_3 complex, for which the origin of magnetization steps in the hysteresis loops will be explained.

[1] T. Yamaguchi, J.-P. Costes, Y. Kishima, M. Kojima, Y. Sunatsuki, N. Bréfuel, J.-P. Tuchagues, L. Vendier, W. Wernsdorfer *Inorg. Chem.* **2010**, 49, 9125–9135.

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