Molecules as Prototypes for Spin-Based CNOT and SWAP Quantum Gates

Guillem Aromí,[1] Fernando Luis,[2] Olivier Roubeau,[2] David Aguilà,[1] Leoní A. Barrios,[1] Ana Repollés,[2] M. J. Martínez-Pérez,[2] P. J. Alonso,[2]

[1] Universitat de Barcelona, Departament de Química Inorgànica, Diagonal 645, 08028 Barcelona, Spain
[2] Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC–Universidad de Zaragoza, and Departamento de Física de la Materia Condensada, Universidad de Zaragoza, E-50009 Zaragoza, Spain

guillem.aromi@qi.ub.es

The implementation of Quantum Computing relies to a great extent on the capacity to develop the suitable technology for realizing and coherently manipulating quantum bits (qubits) and quatum gates (QGs). Recent proposals suggest that electronic spins would be good candidates to embody the basic quantum information.[1-3] In particular, the states of the total angular momentum of rare earths (RE) have been found to exhibit appropriate coherence times and they could be addressed with local pulses of a magnetic field.[4] In this context, the unlimited versatility of chemical design and synthesis should allow producing suitable molecules as carriers of RE, adapted for the realization of logic operations. The universal gate of quantum computing is the CNOT, which operates on two coupled qubits, by flipping the target qubit depending on the state of the control qubit. By use of a novel asymmetric multidonor ligand (H_3L), we have developed methods for the preparation of coordination complexes of two weakly coupled lanthanides, $[Ln_2X(HL)_2(H_2L)(H_2O)(py)]$ ($X=Cl^-$ or NO_3^-), where each metal lies in a dissimilar coordination environment.[5] This asymmetry provides for a magnetic inequivalence, which, coupled to the strong anisotropy of RE, constitutes a good definition of control and target qubits. The robustness of this chemical synthetic scheme allows for the preparation of analogous molecules of various lanthanide metals. A combination of ac susceptibility, magnetization and heat capacity studies performed in the vicinity of the absolute zero, shows that the member of this family with Tb^{3+} ions meets the ingredients required to implement a CNOT quantum gate.[6] The difference of coordination sites featured in this complexes suggest the possibility of generating analogous complexes containing two different RE ions almost at will, by taking advantage of their different ionic radii. Given the intrinsic difficulty in making heterometallic 4f4f' discrete molecules, such an achievement would be of great importance in lanthanide coordination chemistry. On the other hand, this flexibility would enable a vast choice of quantum gate designs. The success of this designed synthetic strategy will be presented.

References

[1] F. Troiani, M. Affronte, *Chem. Soc. Rev.* **40,** (2011) 3119-3129.
[2] G. A. Timco, T. B. Faust, F. Tuna, R. E. P. Winpenny, *Chem. Soc. Rev.* **40,** (2011) 3067-3075.
[3] G. Aromí, D. Aguilà, P. Gamez, F. Luis, O. Roubeau, *Chem. Soc. Rev.* **41,** (2012) 537–546.
[4] S. Bertaina, S. Gambarelli, A. Tkachuk, I. N. Kurkin, B. Malkin, A. Stepanov, B. Barbara *Nat. Nanotech.* **2** (2007) 39-42.
[5] D Aguilà, L. A. Barrios, F. Luis, A. Repollès, O. Roubeau, S. J. Teat, G. Aromí *Inorg. Chem.* **49** (2010) 6784–6786.
[6] F. Luis, A. Repollés, M. J. Martínez-Pérez, D. Aguilà, O. Roubeau, D. Zueco, P. J. Alonso, M. Evangelisti, A. Camón, J. Sesé, L. A. Barrios, G. Aromí *Phys. Rev. Lett.*, **107**, (2011) 117203.

Figures