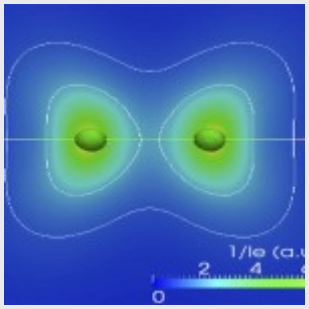
Spin States in Molecules from a Quantum Information Perspective



Title: Spin States in Molecules from a Quantum Information Perspective
When: Thursday, 11 February (2016), 12:00h
Place: Departamento de Física Teórica de la Materia Condensada, Facultad Ciencias, Module 5, Seminar Room (5th Floor).
Speaker: Filippo Troiani, S3 Instituto Nanoscience (CNR), Modena, Italy.

Molecular nanomagnets represent a playground for the controlled generation of highly nonclassical states [1]. In this talk, I will give an overview on the theoretical investigation of such states in terms of quantum-information theoretical quantities. As a representative example, I will discuss the case of spin clusters with dominant exchange interaction. Different forms of entanglement (bi- and multi-partite, between individual and collective spins) are shown to be present in ground state of these systems. These nonclassical features are detectable through experimentally accessible quantities (entanglement witnesses), and partially engineerable by means of available chemical substitutions [2]. Interestingly, spin entanglement can also be investigated in nonmagnetic atoms and molecules, within the framework of density-functional theory. In these systems, spin-pair entanglement decays with a characteristic length scale, which represents a sensitive indicator of the presence of atomic shells and molecular covalent bonds [3]. Time permitting, I will mention additional investigations of spin states in molecules from a quantum-information perspective. These include the quantitative characterization of Schrödinger-cat states [4] and the design of optimal parameter estimation processes within the framework of quantum estimation theory [5].

References

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