Molecular Spin Quantum Manifesto

State of the art
After the first theoretical proposal to use *molecular spins* for qubit encoding (2001), research in this field has achieved important milestones:

- **coherence times** exceeding 10μs at liquid helium temperature have been reported in several ensembles of molecular electron spin systems (2007-to date) with T_2 approaching 1*ms* in nuclear spin free environments. Latest reports (2015-16) show micro-sec coherence time and direct observation Rabi oscillations even at room temperature in diluted molecular electron spin ensembles.

- different strategies **to protect spin states** from decoherence effects have been theoretically proposed and experimentally tested (2016) thanks to fine engineering of molecular states and levels.

- **read out of a single molecular spin** located at a tunnel junction or on a CNT/graphene quantum dot has been demonstrated (2011-12).

- dc and ac hyperfine Stark effect was used **for an electrical manipulation of single nuclear spin within a molecule** with individual relaxation time (T_1) exceeding 10sec. (2012). **Rabi and Ramsey experiments** performed on a single nuclear spin in a molecule (2014) compare well with similar experiments performed with P or Bi defects in Si. Ramsey T_2 times are 300μs. with $\pi/2$ pulse-lengths of 100ns.

- pump & probe techniques based on scanning probe microscopy have been used to detect the quantum coherence of a single magnetic atom on a surface (2015); extension to magnetic molecules appears feasible and it is in progress.

- molecular engineering allows to **control the g-factor** of the spins by changing the surrounding ligands. Moreover, thanks to the molecular engineering of crystal field, molecular spins are excellent test beds to check methods **to manipulate spins by electric fields**.

- **spin entanglement** between and within molecules was shown by different techniques (since 2009): molecular spin clusters/arrays offer an incredible variety of spin topologies to test entanglement at the molecular scale.

- in the last few years, research has focused on experimental tests of universal **two-qubit logic gates** with molecular spin units. Schemes and compounds for switchable effective qubit-qubit interactions in presence of permanent exchange couplings are now available.

- thanks to the flexibility in designing molecular architectures, theoretical proposals for the use of molecular spins as **quantum simulators** (2011) or **quantum cellular automata** have been put forward. Theoretical schemes to implement quantum error correction codes in molecules with multiple spin degrees of freedom have also been developed.

- thanks to the synthetic approach that guarantees (cheap) production of identical molecular units, the **hardware scalability** is offered by the bottom up fabrication process. More in general, chemical synthesis virtually offers continuous tuning of properties to suit a particular application.

- **strong coupling regime** between molecular electron spin ensembles and microwave resonators (2015) has been achieved also at finite (T=50K) temperatures. The possibility of achieving the strong coupling with single molecules has been put forward and experiments are in progress. This opens the door to develop scalable architectures using molecular spins coupled to quantum circuits.

Perspectives

The results achieved in the last ten years in this field show that molecular spins represent an excellent playground to test novel ideas and protocols. Achievements obtained in only one decade demonstrate that these systems have performances -at least- comparable to those of other solid state qubits while specific features make molecular spins complementary to other quantum systems.

Contribution of Molecular Spins to Quantum Technologies:

- **Quantum computing and hardware**

✓ Quantum properties of magnetic molecules are robust and can stand transfer from frozen solutions or diamagnetic crystalline matrices to different environments, thus allowing their application as elementary quantum units in any hybrid solid state architectures.

✓ Flexibility of bottom up fabrication processes, including low cost self-assembly processes, allows realization of ordered 1D, 2D, or 3D arrays of molecular spins with atomic precision and offer complementary nanotechnology tools for the realization of a quantum hardware.

✓ Alternative methods to address single molecules (for instance by electronic junctions/circuits, or by scanning tips or by superconducting resonators) offer the possibility to explore novel approaches to read out and manipulate electron and nuclear spins at single molecule scale, also exploiting spin-orbit coupling or antisymmetric exchange or **combining different degrees of freedom (spin, charge, photons…)**

✓ The remarkable versatility and capability of the chemical design to engineer molecular levels and states provides great potential for scaling up quantum computation, the implementation of **quantum error correction codes**, and the development of **efficient algorithms within individual molecules**.

- **Quantum simulation and software**

✓ Supramolecular assemblies allow to design and implement several architectures suitable for quantum simulation.

✓ Molecular spin clusters are described by simple Hamiltonians with an outstanding degree of accuracy. Hence, they are ideal systems to test quantum simulators implemented with different kinds of qubits, like transmons, cold atoms or ion traps.

- **Quantum sensing**

✓ Molecular engineering allows to dress spins with an infinite variety of functional organic ligands which can be used to decorate surfaces or to selectively interface spins with organic or biological systems.

✓ Entangled spin molecular states show quantum enhanced sensitivity to external magnetic fields.

Societal Impact.

Europe has a leading role in Molecular Magnetism. Genuine quantum effects in molecular electron spin systems have been discovered and intensively studied in the last twenty years by an interdisciplinary community including experimental and theoretical chemists and physicists. Europe has invested on the study of quantum effects in molecular magnetic clusters through MC ITN and individual fellowships, NMP networks of excellence, FET, ERC and COST projects. Most of the achievements and proposals for the exploitation of molecular spin for quantum technologies came from European researchers and this community is well structured by FP6 and FP7 EU programs and achievements are internationally recognized (f.i. EuroPhysics Prize, 2002).

Molecular magnetism and related quantum effects represent an ideal and interdisciplinary playground to train new generation of young researchers as demonstrated in the recent past. Excellent experience in setting Training network and Advanced Schools are within the track record of this community.

There is a long tradition in collaborating with different industries including those working on Spin Resonance, Magnetometry, Spintronics, Scanning Probe Techniques and, more in general, on nanotechnologies: their potentiality to enter in the field of Quantum Technology is high and they may disclose completely new applications in fields which are still unexplored. Support is needed in this direction to fill the gap between basic research and new technologies.