DELIVERABLE 26

Management Committee first progress report

Status of the COST Action

CSO Approval: **30/10/2015**
Start of the Action: **11/04/2016**
End of Action: **10/04/2020**
Total number of COST Countries having accepted the MoU: 24 + 1 NNC (Rep. Moldova).
New COST country Republic of Macedonia.
The budget communicated to the Action for the 2nd GP by the COST Association was 130.000 euros.

The following researchers from International Partner Countries have been invited to participate in our Action:

- Danna Freedman, Department of Chemistry, Northwestern University (USA)
- Steve Hill, National High Magnetic Field Laboratory (USA)
- Enrique del Barco, Department of Physics, University of Central Florida (USA)
- Sally Brooker, Department of Chemistry, University of Otago (NZ)
- Cameron Kepert, School of Chemistry, University of Sydney (AU)
- Andrea Morello, University of Sidney (AU)
- Masahiro Yamashita, Department of Chemistry, Tohoku University (JP)
- Seiji Miyashita, Department of Physics, University of Tokyo (JP)

Description of the Activities

Meetings

1st European Conference on Molecular Spintronics

Bologna (Italy), November 15th-18th, 2016

http://www.ecmols.eu

This conference included a separated workshop for each of the 3 Working Groups and the 2nd Management Committee Meeting.

6th European Conference on Molecular Magnetism

August 27th - 31st 2017

Bucharest, Romania

http://ecmm2017.ro

This conference included a Joint Workshop of WG2 and WG3: Quantum spin science and technologies, and the 3rd Management Committee Meeting.

Dissemination Meetings

ICMM2016 15th International Conference on Molecule-Based Magnets

4 September, 2016 — 8 September, 2016

Japan

12th International Symposium on Crystalline Organic Metals, Superconductors and Magnets (ISCOM2017)

24 September, 2017 — 29 September, 2017

Japan

Intermag 2018 Conference (International Magnetics Conference)

23 April, 2018 — 27 April, 2018

Singapore

Training Schools

9th European School on Molecular Nanoscience (ESMolNa2016), Tordesillas (Spain), May 29th - June 3rd 2016.

10th European School on Molecular Nanoscience (ESMolNa2017), El Escorial (Spain), May 7th - 12th 2017.

Short Training Scientific Missions

56 Short Training Scientific Missions have been accomplished involving the 3 WGs and a wide range of COST countries. The distribution of the grants has also been satisfactory regarding gender (34 males/22 females) and researches categories (28 PhD students/12 ECIs/9 Posdocs/7 Senior Researchers). In relation to Inclusiveness Target Countries there has been a participation of 11 STSMs granted. Near Neighbour Countries have been granted with 2 STSMs.

Dissemination

The Action web page (http://www.icmol.es/molspin/) was created at the beginning of the 1st period and has been since updated regularly. The Action keeps an Updated comprehensive list of all the members which is shown in the above-mentioned web page. The site also contains updated information on events (meetings, training schools), information on STSM calls and acknowledged publications. It also displays a Young Researchers section where ECIs names are listed together with the date of obtention of their PhD, their area of expertise and a link to their CV.

A Mailing list has been created and updated regularly for the dissemination of the Action's activities.

Working Group leaders' reports

WG1 – Leader V.Alek Dediu

The interface engineering in organic/molecular spintronics has unambiguously reached currently the highest scientific level with strong outputs towards the competitiveness of this spintronic branch in applications. MOLSPIN have had a strong role along these achievements by generating a critical networking size able to promote new and radically new ideas and stimulating various project proposals. A joint effort of three MOLSPIN partners (CNR Bologna, Italy - CIC nanoGUNE, San Sebastian, Spain - Univ. Dortmund, Germany) has advanced a new strategy for the molecular and organic spintronics based on quantum Interfacial engineering (T1.1) and Chemical design (T1.2) of functional molecules (Nature Materials 16, 506, 2017). Another joint effort under the guidance of ICMol Valencia and involving CNR and Univ of Dortmund has made a breakthrough in Spin Polarised Organic light emitting diodes (T1.3), demonstrating for the first time the spin polarised injection into HOMO-LUMO electronic molecular levels.

These and other achievements were clearly stimulated by the meetings promoted by COST MOLSPIN and STSMs and more generally by all the networking mechanisms provided by this project.

There is a significant advancement towards the fulfilment of the Milestones 1.1 and 1.2 - in principle, the level expected at the submission of the proposal has been already achieved, but the consortium sees the possibility to go beyond that.

The work on Milestones 1.3 and 1.4 is fruitful and positive and we expect to fulfill them in the next period.

WG2 – Leader Herre Van der Zant

WP2 is well underway with the first molecules being synthesized and characterized concerning their basic properties. Transport measurements on selected compounds are now underway. An important aspect of the work is to extend the toolbox of molecules suitable for spintronic applications. An interesting example is the polyoxometalate (POMs) family of molecules, which are expected to have a robust inorganic cage that would preserve the magnetic properties when the molecules are incorporated in solid-state devices. POMs are fabricated in Valencia and e.g. measured in Delft. With the mechanically controlled break junction set-up their suitability to form molecular junctions has been tested. In electromigrated break junction devices detailed low-temperature transport measurements are performed. The measurements show that the high-spin character of the molecule's metallic center is preserved when it is confined in a single-molecule junction and that it can be reversible oxidized by means of a solid-state gate electrode. Several samples display a rich spin structure, including various high-spin multiplets, in which the magnitude and the sign of the spin-exchange couplings can be tuned by both gate voltage and bias voltage. Detailed analysis of the magnetic field dependence of the excitation spectra and the observation of spin-blockaded transitions in the sequential-electron tunneling regime allows us to deduce the precise nature of the high-spin ground states and the low-energy excitations. Concomitantly, we observe Kondo resonances in regimes where high-spin ground states are present, which provide evidence for an underscreened Kondo effect in these junctions. In future measurements we will test whether the single-molecule magnet (SMM) behavior - as seen in bulk crystals of these compounds - is preserved in single-molecule junctions by making quantitative measurements of the zero-field splitting and comparing the results with the known values for crystals. In addition, within the WP theoretical collaborations have been initiated to further study the rich dynamics of these systems.

WG3 – Leader Fernando Luis

T3.1. MOLSPIN collaborations have broadened our catalogue of molecular spin qubits, including simple complexes containing just one lanthanide or a transition metal ion, improving their performance in terms of spin coherence. A goal of the action is to integrate several qubits within a molecular entity. A supramolecular approach, based on linking Cr7Ni qubits via rotaxane molecules, has demonstrated the ability of creating structures hosting up to 7 qubits and to implement two-qubit gates. A step further in complexity might be achieved by linking lanthanide ions to peptide networks. In addition to increasing the number of magnetic centers, another successful approach is to use multiple states from each ion, either arising from its electronic or nuclear spins , to create qudits or multiple qubits. It has enabled the realization of three-qubit gates and of a simple quantum algorithm.

T3.2. Experiments have shown the possibility of extending spin coherence well above liquid Helium temperatures, in some cases showing quantum coherence and Rabi oscillations even up to room temperatura. Coherence is then limited by spin-lattice relaxation, thus its optimization has triggered efforts to measure the spectrum of molecular vibrations and to dis-connect them from the spin relaxation channels. Microscopic theoretical models of spin-phonon coupling have been developed, contributing to improve our understanding of how to create more stable spin states in rigid molecular structures. Finally, progress has been achieved in calculating the phase coherence when, as it happens for isolated molecular spins, it is limited by hyperfine couplings.

T3.3. This task focuses on moving from the study of molecular ensembles to the coherent control and communication of individual molecular spins. MOLSPIN has boosted collaborations between specialists on nano-electronics and molecular magnetism. Outstanding results are the read-out and electrical control of the nuclear spin states of a molecular qudit, which allowed the realization of Grover's algorithm on a single TbPc2 molecule. A method for reading-out an electron spin qubit, based on single molecule electronic transport experiments, has been demonstrated. Micro-wave photons provide a most suitable platform to communicate molecular spin qubits. MOLSPIN collaborations with different approaches to quantum technologies lead to the proposal of a hybrid technology, which combines molecular spin processors with superconducting on chip resonators to coherently wire up the former in a scalable manner. The first successful experiments, showing the possibility of generating hybrid states of light and spin excitations, have been performed on molecular spin ensembles.

M3.1 is complete. Future work must consider how to address multiqubit molecular processors, avoiding problems associated faced by NMR quantum computing, e.g. by a smart combination of tuneable effective couplings and spectroscopic addressing.

MOLSPIN has contributed to the development of methods for organizing and characterizing molecular spin qubits (M3.2). Some proof-of-concept experiments show that it is possible to fabricate and operate quantum devices based on single molecules trapped in between electrodes (milestone M3.3). In order to scale up quantum molecular devices, additional work is necessary to achieve a nanoscopic control in placing suitable individual molecules at given locations of a device (e.g. a superconducting nanoresonator).