A **DADES DE LA PERSONA SOL·LICITANT(*)**
DATOS DE LA PERSONA SOLICITANTE (*)

COGNOMS / *APELLIDOS*	NOM / *NOMBRE*	DNI / NIF/ NIE / PAS.
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B **MEMÒRIA CIENTIFICOTÈCNICA DEL PROJECTE D'INVESTIGACIÓ**
MEMORIA CIENTÍFICO-TÉCNICA DEL PROYECTO DE INVESTIGACIÓN

Electrical control of probabilistic bits in chiral molecules (ChiralPbit)

Objectives

Molecular electronics -the use of molecules as circuit components, including the study of single-molecule electron transport-[1] offers a unique promise: to employ the rich diversity of molecular chemistry to design and obtain, for each task, a molecule that works better than any generic material, and indeed it has demonstrated substantial advances in the past years, although it still faces open challenges.[2] Within molecular electronics, molecular spintronics -employing the electron's spin degree of freedom in addition to the electron's charge- has reached a series of landmarks, including molecular nanomagnets that keep magnetic memory up to liquid nitrogen temperatures,[3] designing molecular spin qubits that are protected from environmental noise or where a single molecule embodies 3 quantum units of information,[4] or achieving robust spin filters that work at room-temperature and in absence of an external magnetic field, thanks to chirality.[5] At the same time, it also faces unique challenges. We will focus on the following open questions in frontier molecular science:

·understanding and controlling the spontaneous reversal of the magnetization in molecular nanomagnets,

·addressing molecular spin qubits via electric current, to allow for integration into scalable electronic circuits and

·understanding chirality-induced spin selectivity (CISS) to be able to exploit its possibilities.

The dominating role of the barrier for magnetization reversal, once thought to be the key to slow down spin dynamics, is now controversial, with molecular vibrations playing an important part in the process;[6] in any case molecular nanomagnets preserving magnetic memory at room-temperature are still far away. Note however that randomly fluctuating bits (p-bits) are the basis for probabilistic computing,[7] a computing scheme going beyond conventional computing but at the same time much less demanding than quantum computing, and also one of the possible approaches to neuromorphic computing.[8]

At the same time, we are still lacking a clear path for electronic circuit integration of these molecular nanoscale memories, neither for their operation as classical binary (0,1) bits nor as 'probabilistic bits' or p-bits. In the case of their quantum analogues, namely molecular spin qubits, we belong to a European consortium (FATMOLS) that proposes to develop a future emerging technology based on the use of magnetic molecules as components of a quantum processor but which faces difficulties because of the weak coupling with magnetic fields.[9]

Finally, while it is known that molecular chirality, and in particular biomolecular chirality, can add a relevant contribution to spin based technologies,[10] and while there is a tantalizing relation between CISS and quantum sciences,[11] we are still far from having a satisfactory theory that is able to rationalize the often surprising experimental results and allow us to advance towards a rational design of new systems.

The goal of ChiralPbit is to employ molecules to address open questions in spin science and technology.

The 3 main objectives will be pursued in 3 Work Packages and are related with the open questions above:

O1: **explore molecular spin probabilistic bits**, memory units where random fluctuation is a computational resource

O2: **gain electric control over molecular spins with spin-polarized currents** in molecular nanomagnets and spin qubits

O3: **develop a tool for an inexpensive modelling of CISS in biomolecules**

1 D. Xiang et al, *Chem. Rev.*, 2016, 116, 4318
2 F. Evers et al, *Rev. Mod. Phys*., 2020, 92, 035001
3 F. S. Guo et al, *Science*, 2018, 362, 400
4 A. Gaita-Ariño et al, *Nature Chemistry,* 2019, 11, 301
5 R. Naaman et al, *Nature Reviews Chemistry,* 2019, 3, 250
6 L. Escalera-Moreno et al, *Chem. Sci.*, 2018, 9, 3265
7 K. Camsari, Applied Physics Reviews 2019, 6, 011305
8 J. Grollier, Nature Electronics 2020, 3, 360.
9 FAult Tolerant MOLecular Spin processor: http://fatmols.unizar.es/
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11 C. Aiello et al, arXiv:2009.00136, 2020

Projected impact

Thinking in terms of fields of research, ChiralPbit should have a strong impact in molecular magnetism since it will widen the interest of magnetic molecules currently being studied as molecular nanomagnets into the relatively unexplored field of probabilistic computing, as candidates for molecular spin p-bits. Furthermore, in terms of spin devices, ChiralPbit will explore a pathway to overcome a current roadblock of molecules as candidates for quantum devices, namely the difficulty of electric manipulation of spin states. Finally, ChiralPbit will impact the spintronics community by facilitating the inexpensive evaluation of the CISS effect and therefore the rational design of CISS structures.
Thinking in terms of my own research, it will consolidate first my European leadership in the emergent field of molecular quantum computing. Secondly, it will introduce my team in the field of spin p-bits and consolidate my entrance into the field of CISS. More importantly, it will propel me into a position where I can apply for an ERC grant on the field of rational design of biohardware for spintronics; further details on that can be found in the attached document on my work plan to obtain an ERC grant. Let us now examine in further detail the impact of the different work packages:

1. **Opening the field of molecular spin p-bits**

The impact on the Single Molecule Magnet / Single Ion Magnet community of us successfully exploring SMMs and SIMs as p-bits can be expected to be comparable to the impact of these molecules being employed as qubits, a few years ago. If we can judge from that experience, the impact will be immediate and profound. The systems that this community has been studying for decades will suddenly have another potential application. Some new experimental techniques and some theoretical progress will be needed, but essentially most of the existing expertise and infrastructure will find a new utility. A part of this infrastructure are the research networks: I know most of the main actors involved in the chemical synthesis, physical characterization and theoretical modelling in this community, and they know me; this will ensure a rapid spread of new ideas as soon as they have been shown to be fruitful.
The impact on molecular spin qubit community will occur as soon as we can demonstrate the feasibility of employing the same kind of hardware to combine molecular spin qubits and molecular spin p-bits, since this will ease the first practical results of molecules in this field. Indeed, it has been shown that p-bits can mirror a special class of quantum circuits,[12] and the type of efficient optimization performed by quantum annealing can also be realized by networks of p-bits.[13] Like in the case of SIMs, I am integrated in the community of molecular spin qubits, e.g. am part of the FATMOLS network[7]. Any new results from my side will rapidly inspire related experimental and theoretical work on several other European laboratories.

2. **Practical pathway for electric control of spin within devices**

Further impact on molecular spin qubit community will result from this pathway, since a strong electrical coupling to qubits is one of the two remaining obstacles for obtaining scalable qubit devices based on magnetic molecules. Different approaches have been proposed theoretically[14] or attempted experimentally,[15] and in particular we and our collaborators have obtained significant experimental progress in this field lately,[16] but is still remains an open question. As soon as there is a promising way to control molecular spin qubits with voltages, it will be attempted experimentally by our colleagues. Furthermore, an indirect impact will happen in the field of molecular spin p-bits, see previous point. Since electrical communication between p-bits is a requirement for current models of probabilistic computing, this WP will boost the impact of the previous one.

3. **Provide tool for inexpensive evaluation / rational design of CISS biostructures**

The impact on the spintronics community will result from (i) CISS can achieve practically perfect spin filtering, at room temperature and without the need of a magnetic field, (ii) all biomolecules are chiral and thus CISS candidates,[17] and at the same time (iii) our understanding of it is still very inadequate, with a multitude of incomplete and incompatible theories.[11] Initially, we do not aim to provide a new physical model for CISS ourselves, since there are already multiple groups which have been working on this problem for many years. Instead, our goal is to facilitate an effective coarse-grain software package that is versatile and can be adapted to different models. Like the success case of SIMPRE demonstrated,[18] this kind of inexpensive tool can have a great practical effect. Lowering the bar for the calculations by dramatically lowering the processing time means that many systems, which so far have shown to be too complex to be theoretically modeled, will be accessible. In the short term, this will improve the description of these systems; in the mid term it will provide novel insights and allow us to define, in practice, the limits of the model. Our example with SIMPRE demonstrates that it is also possible that this serves to expand the scope of application of very simple models. Our work is already known in the CISS field, and in particular we have been discussing our initial results with experts for some years now, since we are part of European community of Molecular Spintronics. In particular, I am part of the the Core Group of MolSpin, a COST network coordinated by ICMol (Coronado). Additionally, I have started a collaboration with R. Naaman who is the discoverer of the CISS efffect and the scientist that has been at the forefront of this topic worldwide for over 10 years. Finally, the possibility to design CISS biostructures that achieve spin filtering for structural reasons simplifies enormously the obtention of the spintronic devices needed for the two previous objectives, meaning WP3 will further increase the impact of WP1, WP2.

12 K. Camsari et al, *Phys. Rev. Appl.* 2019 12, 034061
13 B. Sutton et al,*Sci. Rep.* 2017, 7, 44370
14 M. Trif et al, *Phys. Rev. Lett.* 2008 101, 217201
15 C. Godfrin et al, *Phys. Rev. Lett.* 2017, 119, 187702
16 J. Liu et al, arXiv:2005.01029, 2020, under review in *Nature Physics*
17 Huizi-Rayo et al, *Nano Lett.* 2020, 20, 12, 8476
18 (a) J.J Baldoví et al, *Dalton Trans.*, 2012, 41, 13705 (b) J.J. Baldoví et al, *J. Comput. Chem.* 2013, 34, 1961

Methodology

Herein is a list of the main theoretical and experimental techniques to be used in ChiralPbit. Further methodological details including which systems the techniques will be applied to are discussed in the Work Plan.

WP1: exploration of **molecular spin probabilistic bits** (p-bits)

· Radial Effective Charge model (as implemented in the SIMPRE software) to inexpensively estimate the CF in lanthanides, [18] and AOM for transition metals,[19] with CASSCF-CASPT2 model (MOLCAS software) as a benchmark method for crucial cases.[20]

· Gaussian for structural calculations for the calculation of spin dynamics following the procedure demonstrated by us.[21]

· SQUID magnetometry (dc and ac) and pulsed EPR to characterize the static and dynamic magnetism of the p-bits in bulk
·structural and physical characterization of thin layers of p-bits: spectroscopical (IR, Raman, XPS, UPS, XAS), microscopical (AFM, STM), magnetical (MOKE, XMCD) ; XAS and XMCD are available in large European centers, the rest are available at the ICMol.

WP2: study the **dynamic control over molecular spins** via Chirality Induced Spin Selectivity (CISS)

· time-dependent exchange Hamiltonian with an auxiliary qubit to effect 1-qubit operations as demonstrated by Loss [22]

· Generalized James' effective Hamiltonian method to extend Loss' method to other cases [23]

· DFT + time-dependent Green's functions to calculate electron transport (TRANSIESTA)[24]

· Monte-Carlo type modelling[25]

· tight binding transport methods[26]

WP3: develop a tool for an **inexpensive estimate of CISS in biomolecules**

·coarse grain methods (ABCLUSTER[27], ESPResSo[28], GFN-xTB[29]) employing the Martini force field[30]

·CISS model by Varela Salazar, Mújica and Medina [31]

·CISS model by Dalum, Hedegård[32]

«In-house» facilities

ICMol has been recognized as a research unit of excellence Maria de Maeztu, with facilities and expertise at the highest level. Our colleagues at the ICMol include 8 ERC grantees that are world experts in molecular spintronics and molecular magnetism and in advanced materials chemistry.

External collaborations

·F. Luis, in Zaragoza and J. Majer, in Viena, experimental experts in the engineering of electrical circuits for controlling and measuring spin qubits: will collaborate in the magnetic characterization of nano-sized samples

·S. Hill and A. Ardavan experimentalist in Florida and in Oxford respectively, experts in characterizing molecular spin dynamics will perform any EPR experiments which go beyond our in-house expertise

·D. Zueco, quantum theorist, in Zaragoza, will collaborate in the theoretical derivation of models for the control and readout of spins

·K. Franz, a world expert in metallopeptides, germinal developer of the lanthanide binding tags (LBTs) and expert in amino-terminal Cu^{2+}- and Ni^{2+}-binding motifs (ATCUNs): she will consult and provide samples as needed.

·R. Naaman, the discoverer of the Chirality-Induced Spin Selectivity: his team will perform specialized measurements that are currently beyond our expertise

·van der Zant, expert in experimentally characterizing quantum phenomena in electrical nanostructures, including bio-inspired charge transport: he will characterize thin layers as magnetic tunnel junction devices and perform single-molecule experiments

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20 F. Aquilante et al, *J. Comp. Chem.*, 2016, 37, 506.
21 L. Escalera-Moreno et al, *Chem. Sci*., 2020, 11, 1593
22 D. Loss et al, *Phys Rev A* 1998, 57, 120
23 (a) W. Shao et al, *Phys Rev A* 2017, 95, 032124, (b) V. Macri, *Phys Rev A* 2020, 101, 053818
24 J. M. Soler *et al*., *J. Phys. Cond. Matt.* 2012, 14, 2745.
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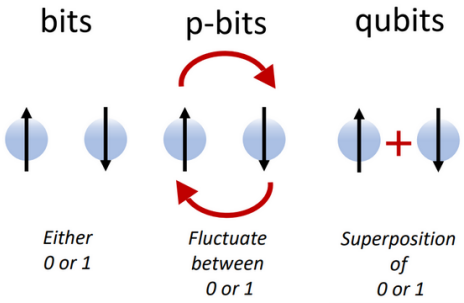
26 A. Tikhonov, *J. Chem. Phys.*, 2002, 116, 10909
27 J. Zhang *et al.*, *Phys. Chem. Chem. Phys.* 2015,17, 24173.
28 F. Weik *et al*., *Eur. Phys. Jour. Spec. Topics,* 2019, 14, 1789.
29 C. Bannwarth *et al*., *J. Chem. Theory Comput.,* 2019, *15***,** 1652.
30 S. J. Marrink, *J. Phys. Chem. B*, 2007, 111, 7812.
31 S. Varela et al., *Phys. Rev. B* 2020 101, 241410(R)
32 S. Dalum et al, *Nano Lett*. 2019, 19, 5253

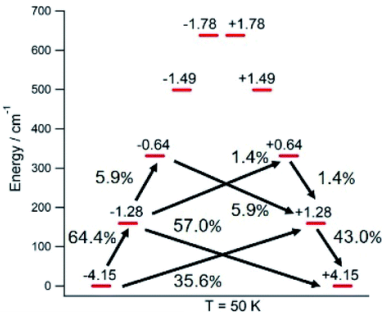
Work plan: work package #1 «Rational design of molecular nanomagnets as p-bits for probabilistic computing»

P-bits fluctuate randomly between 2 values, as depicted in this image from Purdue University's program «An exploration into probabilistic spin logic». In contrast to the long uphill struggle of quantum computers, probabilistic computing has rapidly demonstrated its viability in a practical problem: integer factorization was achieved using stochastic magnetic tunnel junctions.[33] Currently, its main implementation are magnetic tunnel junctions where the soft layer are nanomagnets with a 'low' energy barrier (in the order of k_B·T or below). Here note that «flips per second» have been defined as one key hardware metric,[34] and molecular nanomagnets would be on the low energy barrier limit, for ultra-fast, ultra-small p-bits.



1st year

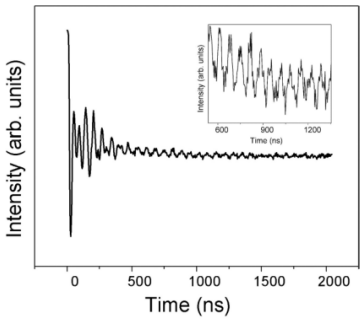
Theoretical study of molecular nanomagnets of two classes:
(a) bis phthalocyaninato lanthanide sandwiches such as $Tb(Pc)_2$ [15] and
(b) lanthanidecene-type sandwiches such as $Dy(Cp)_2$:[3]
Estimate the coupling between spin states and vibrations and the time evolution of the stochastic reversal of magnetization *M(t)*, at different temperatures and with different substituents.The fundamental technique was already demonstrated on an Uranium analogue of $Dy(Cp)_2$ by us (see illustration).[21] In addition we will implement a Monte-Carlo model to simulate *M(t)* and estimate the characteristic parameter «flips per second» of the p-bit.



Standard experimental magnetic characterization of nanomagnets will be performed (SQUID, EPR). Relying on our ongoing studies of a modified $Tb(Pc)_2$[35] and our recent work on substituted $Dy(Cp)_2$,[36] we will obtain magneto-structural correlations: dependence of the spin dynamic behavior with molecular structure.

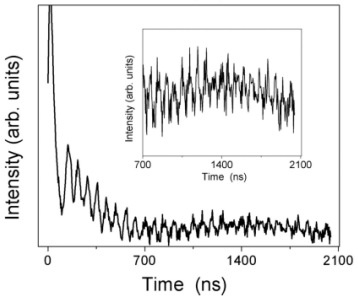
2nd year

Theoretical study of two well-known classes of paramagnetic metallopeptides:
(c) lanthanide-binding tags, (LBT) which we have explored in a related context,[37] and
(d) amino-terminal Cu^{2+}- and Ni^{2+}-binding motif (ATCUN; H2N-X-Y-His where H2N is the N-terminus and X, Y can be any two aminoacids)[38]; see next page for illustration.
Like in the previous systems, we will calculate the time evolution of the stochastic reversal of magnetization, at different temperatures and with different peptidic sequences. Magneto-structural correlations: dependence of the spin dynamic behavior with metal and peptide sequence.



3rd year

Magnetic characterization of the most promising systems. SQUID magnetometry (dc and ac) and EPR (thermal dependence of the spin-lattice relaxation time T1) between 4K and room temperature. We already collected limited data on the pulsed EPR on Gd^{3+} and Nd^{3+}-coordinating LBTs, e.g. see their coherent oscillations in the image.[39] Use the experimental data to refine previous theoretical studies.



4th year

Experimental processing of the chosen system: preparation of self-assembled monolayers and structural characterization, in collaboration with my colleague prof. A. Forment-Aliaga at the ICMol. Characterization of the obtained thin layers as magnetic tunnel junction devices in collaboration with prof. Van der Zant in Delft.

Summary of expected results

M1: simulate the stochastic evolution of the magnetization *M(t)* in SIMs and estimate the p-bit parameter «flips per second»
M2: preparation of SAMs of p-bits for their implementation as devices

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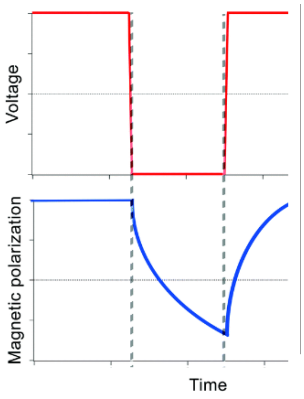
34 B. Sutton et al., IEEE Access 2020, 8, 157238
35 F. Luis et al, work in preparation
36 A. Ullah et al, *J. Phys. Chem. Lett.* 2019, 10, 7678
37 R. Cavanilles et al, *J. Am. Chem. Soc.* 2020, 142, 17572
38 J.T. Rubino et al, *J. Inorg. Biochem.* 2012, 107, 129
39 L.E. Rosaleny et al, *J. Phys. Chem. Lett.* 2018, 9, 4522

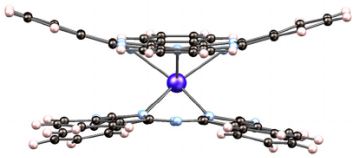
Work plan: work package #2 «Manipulation of a static spin via spin-polarized current»



Manipulation of spin states via an electric circuit has for long been an aspiration in the field of molecular spin qubits, because electric voltages, fields and currents are much easier to control than magnetic fields, both in terms of speed and in terms of spatial confinement. Indeed, I contributed an early proposal to that effort.[40] More recently, we did another proposal in the related context of biomolecular memristors.[41] As illustrated here, when a resident spin is in presence of magnetic exchange with a spin-polarized current, as happens with paramagnetic LBT complexes, [37] a time control over the voltage results in a control of the expectation value at any given time for a single resident spin, or, in the case of a thin layer, over the time dependence of the magnetic polarization. Our goal here is to explore ways to control and measure the quantum state of the resident spin by the time-controlled manipulation of the Hamiltonian, i.e. by choosing when and for how long we switch on the voltage.

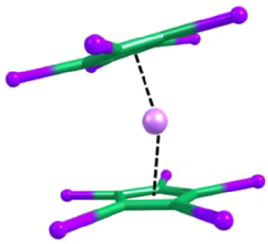
1st year

Starting from the classical work by Loss and DiVincenzo for [22] derive the equations corresponding to our context, initially assuming no barrier for spin reversal in the resident spin and a uniform spin-polarized current (a constant spin 1/2 under the effect of a magnetic field) and a wide window of magnetic exchange J , between 1 and 100 cm^{-1}. The time-dependent Hamiltonian will be a constant magnetic exchange with a radical spin assumed to be polarized by a Zeeman effect but whose presence can be swtiched on or off. To work out the exact equations that apply for our case, we will first find the adequate effective Hamiltonian and then develop a manipulation and readout theory; we will rely on analogous recent work in a related field.[23]



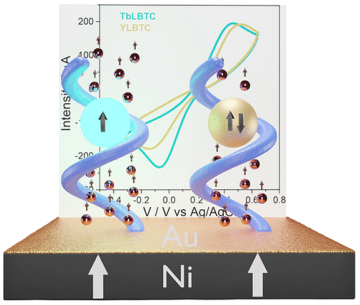
2nd year

Apply the model to experimental systems of types (a) $Tb(Pc)_2$, (b) $Dy(Cp)_2$, (c) LBT and (d) ATCUN (see illustrations in the right column, from top to bottom). In the case of $Tb(Pc)_2$-type systems, we will consider the paralelism to the work of Wernsdorfer, which employs different spin Hamiltonian to manipulate the resident (nuclear) spin.[15] In physical terms, the static Hamiltonian for our molecular spins will be (a) Zeeman, if we need to include an external magnetic field and (b1) nothing else for a S = 1/2, (b2) Zero Field Splitting (D,E), for the case of transition metals or (b3) Ligand Field, for the case of lanthanides.



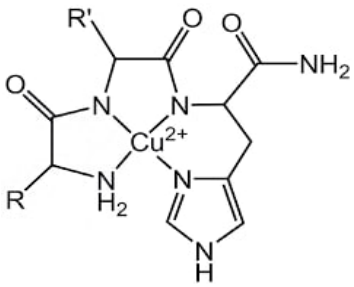
3rd year

Employing the results of WP1, in particular the calculated time evolution of the stochastic reversal of magnetization $M(t)$ of the resident spin for the different systems in absence of an external driving spin, refine the work done so far to consider that the spin-polarized current as a time dependent, stochastic but non-equilibrated mixture of M_s = +1/2 and M_s = -1/2. For this goal, develop a Monte-Carlo type model that is able to re-calculate the «flips per second» of the resident spin in this driven regime, and estimate the control that will be possible in practice, considering state-of-the-art experimental conditions. If the quantum regime seems achievable, model open quantum system dynamics and dissipation.[42]
Determine the most promising systems so far and start the preparation and structural characterization of samples for experimental studies.



4th year

Advance to the final point of the simulation, that also includes realistic transport conditions through the molecule and not just the external control of the voltage. Implement tight-binding calculations of transport through
(a) a single molecule between two contacts and
(b) a single self assembled monolayer of molecules between two planar electrodes,
to translate the previous result into actual experimental voltages. As electrodes, start with the standard Au(111) but also include
Perform an experimental characterization of the best structurally-behaved samples under high-frequency voltage to quantify the actual observed effect. The acquisition and testing of high frequency voltage sources will start early on (1st year) to guarantee sufficient expertise.

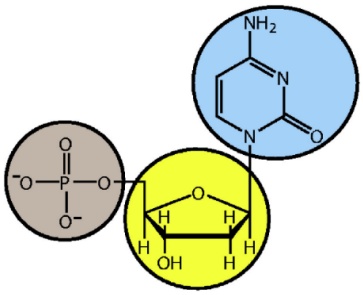


Summary of expected results

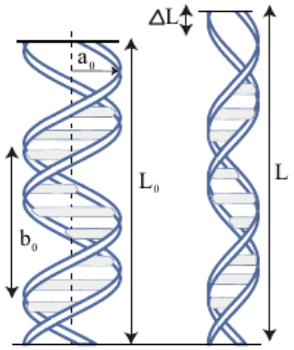
M3: develop a manipulation and readout theory for the control of a resident spin 1/2 via an arbitrary spin-polarized current
M4: theoretically and experimentally estimate the time-dependent magnetization in the driven regime in our systems

40 J. Lehmann et al, *Nature Nanotechnology* 2007, 2, 312
41 S. Cardona-Serra et al, *Phys. Chem. Chem. Phys.*, 2021, DOI: 10.1039/D0CP05236A
42 T. Ramos et al, *Phys. Rev. A* 2016, 93, 062104

Work plan: work package #3 «Versatile modelling of Chirality-Induced Spin Selectivity»

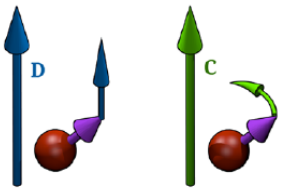


The goal is to develop a versatile model for CISS, that is inexpensive and parametric and uses existing models as a base for fitting its parameters. We will be inspired by the great success of coarse-grained models in biomolecules,[43] illustrated here by an early coarse-grain model for DNA.[44] In ChiralPbit, small parts of the system (such as the ones shown for DNA, or in the case of proteins: peptidic bonds, side residues R, paramagnetic metal ions, substrates) will be parameterized in a coarse-grain fashion, and the parameters of the model will be fitted to reproduce the main structural parameter of existing (and future) 'first principles' models. They key idea here is that while theories of CISS are currently incomplete, complicated and evolving, most of them include one or two parameters that are simple and which are derived from the atomic structure in ways that are either too expensive or excessively simplified.



1st year

Starting from existing coarse-grain models of DNA, develop a coarse-grain procedure to estimate scalar spin-orbit coupling parameter λ_{SO}, a molecular parameter which includes all geometrical overlaps characteristic of a given DNA helix, as defined by Varela, Mújica and Medina.[31] Apply this procedure to double-stranded DNA fragments of length N=2-10, and adjust the model until it is able to reproduce the results of Varela et al on spin-orbit coupling modulation in DNA by mechanical stretching (see figure). In particular, compare our estimated evolution of λ_{SO} with respect length deformation with the results of Bruot et al.[45]



2nd year

Following a similar procedure, but employing as a starting point an existing coarse-grained modelling of CISS in the helicene molecule,[46] we will develop a coarse-grain procedure to estimate vectors C,D as defined by Dalum and Hedegård and illustrated in the image: C is the vector around which the spin passing through the molecule precesses, while, D, instrumental in explaining the CISS effect, defines the direction along a nonpolarized electron spin will be polarized after emerging from the molecule.[32] We will apply this methodology to their collection of helical polyacetylenes as an initial test, then extend it to other analogous hydrocarbons.

3rd year

Choose the best CISS physical model at the time that is usable on polypeptides (default to Dalum, Hedegård) and develop a coarse-grain procedure working on peptides to estimate its key structural parameter, employing the «fragment orbital based description of charge transfer including backbone orbitals» formulation.[47] If possible, we will include the hybridization with the substrate into the modelling, as it has been repeatedly shown to be crucial.[48] If the best theory is based on vibrations, as some recent advances indicate,[49] employ our expertise in coupling vibrations to different kinds of molecular excitations to generate a coarse-grain model that parameterizes the local contributions to molecular vibrations. Apply the resulting procedure to the same test systems employed by the work that develop the model; default to a short series of well-characterized peptides:

4th year

Apply the latest model to the systems we will be studying experimentally by then: paramagnetic complexes based on LBTs and/or ATCUN. Extend to variations of the complexes we have, namely:

a) single-aminoacid substitutions that do not significantly alter the coordination to the metal

b) extension, after the coordinating sequence, by means of a poly-alanine segment which will tend to form a long α-helix.

Time permitting, extend to other options would be more desirable to optimize the CISS effect.

Summary of expected results

M5 Inexpensive modelling of CISS in DNA, hydrocarbons and proteins.

M6 Rationalization of our experimental results.

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Budget considerations

The majority of the work will be theoretical, allowing for the largest part of the budget to be devoted to salaries. In principle, this will be 3 predocs involved in this project, although we expect to be able to cover two of these positions via independent funding, e.g. the FPI program associated with the Maria de Maeztu and via our European collaborations such as FATMOLS, and in this case we will also be able to hire a technician for the duration of the project. All in all, we expect ChiralPbit to cover 2 salaries on average (<50k€/year). The personnel cost will be reduced in the first year.

The experimental tasks which will have substantial associated costs: characterization of spin and magnetization dynamics in molecular spin qubits and nanomagnets, characterization of p-bit behavior with high-frequency voltage sources, characterization of CISS effect. Equipment and consumables will be acquired as needed to allow for these tasks to be carried out. At the same time, I am currently starting to acquire a cluster for intensive calculations to accelerate all of my theoretical research, and the since the current project is heavily theoretical it will also be crucial for that goal. Most of the equipment cost will be concentrated on the first year (60k€). There will be an additional cost of minor equipment (2k€/year) and consumables (~20k€/year), and external characterization plus delivery services (~20k€/year).

Furthermore, we plan substantial research stays for all predoctoral members of the team (~10k€/year), meaning the external collaborations will not just consist on shipping samples or exchanging emails but in significant intensification of the present cooperation level and additional expertise and valuable research experience for the PhDs. This will be complemented by diffusion of results by participation in scientific meetings and conferences. The last year we will organise a workshop (~3k€). We estimate a cost of ~5k€ in open access fees, starting in the second year.

	Year 1	Year 2	Year 3	Year 4
PhD	5548.20	22192.80	22192.80	22192.80
Technician	9945.00	19890.00	19890.00	19890.00
Indirect costs	1752.28	4759.56	4759.56	4759.56
Equipment	60000.00	2000.00	2000.00	2000.00
Consumables	16000.00	20000.00	20000.00	16700.00
External characterization	0.00	18000.00	18000.00	18000.00
Delivery services	0.00	2000.00	2000.00	2000.00
Travel	2554.52	6157.64	6157.64	6157.64
Open access	3000.00	5000.00	5000.00	5000.00
Workshop	0.00	0.00	0.00	3300.00
Web	1200.00	0.00	0.00	0.00
Total	**100000.00**	**100000.00**	**100000.00**	**100000.00**

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