Step 2 Evaluation Report

CONFIDENTIAL

Call reference	ERC-CoG-2014
Activity	ERC-COG
Funding scheme	ERC Consolidator Grant
Panel name	PE5-Synthetic Chemistry and Materials
Proposal No.	647301
Acronym	DECRESIM
Applicant Name	Gaita Alejandro
Title	A Chemical Approach to Molecular Spin Qubits: Decoherence and Organisation of Rare Earth Single Ion Magnets

EVALUATION CRITERIA

1. Research Project

Ground-breaking nature and potential impact of the research project

To what extent does the proposed research address important challenges?
To what extent are the objectives ambitious and beyond the state of the art (e.g. novel concepts and approaches or development across disciplines)?
To what extent is the proposed research high risk/high gain?

Scientific Approach

To what extent is the outlined scientific approach feasible (based on the Extended Synopsis)?
To what extent is the proposed research methodology appropriate to achieve the goals of the project (based on the full Scientific Proposal)?
To what extent does the proposal involve the development of novel methodology (based on the full Scientific Proposal)?
To what extent are the proposed timescales and resources necessary and properly justified (based on the full Scientific

2. Principal Investigator

Intellectual capacity, creativity and commitment:

For each of the statements below, reviewers were asked to choose one of the following four responses: Outstanding / Excellent / Very good / Non-competitive

To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?
To what extent does the PI provide evidence of creative independent thinking?
To what extent have the achievements of the PI typically gone beyond the state of the art?
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?

PANEL SCORE AND RANKING RANGE

Final panel score : A (fully meets the ERC's excellence criterion and is recommended for funding if sufficient funds are available)	**Ranking range *:** 1%-65%

* Ranking range of your proposal out of the proposals evaluated by the panel in Step 2, in percent, from 1% for the highest ranked proposals to 100% for the lowest ranked.

PANEL COMMENT

This evaluation report contains the final recommendations and score awarded by the ERC review panel during the second step of the ERC Consolidator Grant review and the ranking range. The panel based its appraisal on prior individual reviews conducted by panel members and external referees and on the interview with the applicant.

The panel closely examined all the individual review reports and, while not necessarily subscribing to each and every opinion expressed, found that they provide a fair overall assessment. The comments of the individual reviewers are included in this report.

The presentation given by the applicant during the interview and the answers to the questions that were addressed greatly contributed to build the panel's view about the proposal's strengths and weaknesses.

Both the individual reviews and the interview were the basis for the discussion and the final recommendation of the panel.

The panel was impressed by the academic excellence of the PI, as well as the progressive construction of the project from WP1-3, with very clear objectives at each stage together with increasingly complex and creative science with high risk/gain potential. The candidate defended questions by the panel with clarity and confidence. The project outcomes will extend significantly beyond the state of the art in chemistry and the related areas of physics and biochemistry, where real networks are already in place.
The panel felt that the budget was not fully justified under all categories and it has been adjusted under travel, post doctoral and technical staff.

The panel therefore recommends the proposal to be retained for funding with a grant not exceeding 1 827 375.00 Euro.

REVIEWER COMMENTS

The following individual reviews have been carried out independently prior to the panel meeting and do not necessarily reflect the panel's final opinion

Reviewer 1

Research Project
Ground-breaking nature and potential impact of the research project: This is an excellent proposal in the area of single molecular studies of magnetic materials. The aim is to investigate and eliminate decoherence in molecular spin qubits, which if successful may lead to increases hysteresis. The objectives are very ambitious and range from theoretic studies to experimental investigations. The results obtained can be ground breaking and would allow for the future high temperature application of such materials in quantum technology. Scientific Approach: The approach taken in this project is original and novel and the project is likely to produce interesting results. The methodology outlined in the proposal is appropriate. The research programme is for a large part based on the development of theoretical concepts using computational studies. In the last tasks experiments are planned but the description of the work planned is somewhat unclear.

Principal Investigator	
To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?	Excellent
To what extent does the PI provide evidence of creative independent thinking?	Excellent
To what extent have the achievements of the PI typically gone beyond the state of the art?	Very good
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?	Excellent

Comments (Optional for reviewers)
No comments received

Reviewer 2

Research Project
Ground-breaking nature and potential impact of the research project: The goal of the project is to model decoherence in molecular spin systems of various nuclearities based on lanthanoid complexes. It is not clear that his project really goes beyond the state of the art. It rather appears as the development of the interesting research that the PI and the group he belongs started to develop some years ago. Scientific Approach: The research program is divided in well-developed working packages. This research is in the PI's field of expertise and will start with the development of the software package SIMPRE, originaly evolved in his team. There is no doubt that the group has the skills to develop the proposed research. The budget is mainly focused on personnel as the PI plans to hire a large team of people. Thus the cost for personnel is high. This high number of researchers probably also justify the high amount of money asked for travel. On the contrary the cost for equipment is quite modest and consists only in the purchase of a Q-band extension for the pulsed EPR. The PI justifies his high demand for personnel by the austerity cuts in Spain.

Principal Investigator	
To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?	Very good
To what extent does the PI provide evidence of creative independent thinking?	Very good
To what extent have the achievements of the PI typically gone beyond the state of the art?	Very good
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?	Very good

Comments (Optional for reviewers)
The PI defended his PhD in 2004 in Valencia where he has been since the beginning of his research career with the exception of a two-year period spent in UBC (Vancouver, Canada). The PI has prepared his PhD under the supervision of Professor E. Coronado and he is still working in his group. At the moment he is funded by a "Ramon y Cajal Fellowship". He has published papers in high-impact international journals, but these papers are always published with his PhD supervisor (with two exceptions). He has supervised PhD students. His research is supported by many grants, most of them managed by E. Coronado. The PI is probably a talented researcher but now he has to establish his own independent

reputation.

Reviewer 3

Research Project

Ground-breaking nature and potential impact of the research project:
This is an excellent, highly interdisciplinary proposal dealing with the understanding and preparation of lanthanoid based single-ion magnets to be used in the field of quantum decoherence processes. The work involves the development of new theoretical tools to predict the behaviour of magnetic systems and decoherence phenomena. This part is clearly the most convincing one as it is in the mainstream of the PI activity. The proposed work also includes synthetic aspects and manipulation of quantum states by Electron Paramagnetic Resonance. The synthetic part is much less developed and implies an higher risk which is honestly recognized by the PI. Particularly challenging appears to be WP3, organization of spin qubits via biopolymers. From the proposal it is unclear how this task will be accomplished, probably making use of the excellent competence existing in the Institute where the PI is presently working. The proposal is very well written and structured and the level of risk very well identified. In summary, it is a complex, ambitious, and innovative proposal. The idea to use biological structures seems even too ambitious, but this part of the proposal may not be essential to reach the main goals.

Scientific Approach:
The scientific approach is based on very diverse, yet complementary methods. In order to be successful, the PI should master these diverse approaches and transfer the results from one kind of study to the next level of investigation. Most of the activities are theoretical and new software is going to be produced to screen the possible interesting molecular structures. Should this new software based on a simplified approach fail, more rigorous quantum-mechanical approaches will be used, but this is going to slow down the advancement of the project. The PI seems to master very well the complex physics beyond decoherence in molecular spin qubits. The production of MOF ordered structures or organized biopolymers is clearly relevant to translate the theoretical advances in practical results. However, it is unclear how this can be coordinated by a PI with limited experience in these fields. I think that if this aspect would have been developed into collaboration with some more experienced researcher the possibility of success could have been higher.

There are 10 post-doc or PhD students involved in this work, a very large number that can create problems of coordination and overlap. The entire requests go beyond the maximum allowed but there is no motivation given. In my view the budget can be reduced without damaging the project.

Principal Investigator	
To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?	Excellent
To what extent does the PI provide evidence of creative independent thinking?	Excellent
To what extent have the achievements of the PI typically gone beyond the state of the art?	Excellent
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?	Outstanding

Comments (Optional for reviewers)
The PI's CV shows a growing trend both in terms of quality and quantity. The PI has already a very good track record of publications and a good international experience. He has no major awards and the level of independence is good. Overall, an excellent CV.

Reviewer 4

Research Project
The proposal addresses a very important question - whether quantum mechanics can be exploited in real, solid-state materials. The applicant proposes detailed theoretical and experimental investigations into new forms of single-molecule magnet (SMM), which are materials that have shown potential for quantum information applications. Currently there are many obstacles to the use of these systems and much important detail regarding the phenomenon of decoherence remains unknown. This is therefore an important and fertile area for future research. Arguably, the most promising SMM, combining a large spin and suitable anisotropy) was the first discovered (Mn12 acetate). However recent work on the lanthanoid complexes has reignited this field and this proposal is, therefore, quite timely. The ability to design and synthesise these systems with desirable properties could be revolutionary! The objectives are ambitious and will move the field beyond the state of the art. A good balance is achieved between objectives that will develop the field as it stands currently (contained in WP1) and objectives that will break substantial new ground (WPs 2 and 3). The theoretical description of these systems in terms of an analysis based on the crystal field Hamiltonian seems an interesting path. The use of a successful theory to directly inform synthesis is, of course, the right way forward. Developing an understanding of the coupling of a small number of spin qubits (WP2) has been attempted in other systems, and represents the logical next step if WP1 is fruitful. Finally, the possibility of making extended structures of these objects using metal-organic frameworks or biological molecules (WP3) would certainly take the field into new and exciting territory. This latter plan would develop the field across disciplines, allowing contact with the large research effort addressing low-dimensional (i.e. 1d and 2d), strongly interacting spin structures. This is a particularly exciting possibility. A particular strength of this proposal is the identification of the risks and gains and the balance achieved to mitigate risks. The work is organised in such a way as to maximise the yield of results from the moderate gain objectives, while allowing progress towards the most ambitious objectives. The bulk of the proposal is concerned with addressing WP1, which provides the solid foundation of the project - developing the theoretical and computational tools and the related synthesis strategy. This is arguably of moderate gain, but will likely be successful. WP2 and WP3 are higher risk, but will clearly

break much new ground if successful.

Scientific Approach:
The project, as outlined, seems highly feasible given the applicant's previous work in this area and the background to the science that is discussed in the proposal. The development of the crystal field theoretical tools is well within the capabilities of the applicant. The master-equation approach is risky, but the proposal makes clear the alternatives that can be utilised if necessary. It remains to be seen whether this will provide the promised 'phenomenology for decoherence' in general terms, but certainly represents an important step that should be taken. The practical aspects involving the chemistry and state manipulation rely on skills and approaches that the applicant has already demonstrated. The feasibility of the higher risk parts of the proposal is more difficult to assess, but a good case is made in the proposal and sensible plans are outlined.

The research methodology is well explained and seems appropriate. I would ask the applicant why the lanthanoid-based systems, in particular, represent the most promising candidates for future application. I agree that they are a logical place to look (particularly given the expertise of the proposer) but I was unsure if they had particular properties that made them special in this context. (The applicant mentions several times that they are a 'hot topic', but I am left unsure quite why.) The theoretical modelling is well justified as being an area of very high potential for gaining key insights into the decoherence problem. The proposal makes clear all of the technical steps what will be made in developing this area. The synthetic and experimental strategy is well justified and highly appropriate, particularly the use of EPR in this context, which has provided important progress in the field in the past.

The main novelty in the methodology that will be developed is in the theoretical part of WP1. A strength of the proposal is that SIMPRE2.0 (the computer package that will result from the theoretical modelling) will allow automated screening of materials in order to identify the building blocks of the systems to be developed. It was slightly less clear from the proposal exactly what would constitute success for WP2 and WP3. Is this simply overcoming the (presumably considerable) difficulties in synthesis and characterisation of the coupled systems, or are there criteria that the applicant has identified which would demonstrate whether these are suitable areas to take forward towards technological applications? This was especially the case for WP2, where the applicant has clearly made a significant contribution already, but where I was unsure exactly how far this area was to be exploited in this project. I would welcome more concrete information here.

The proposed timescales and resources are well justified and seem highly appropriate. The applicant gives a clear description of the current situation for researchers in Spain and has planned the project well within that working environment. Plans for the additional personnel are quite clear and well thought out.

Principal Investigator	
To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?	Outstanding
To what extent does the PI provide evidence of creative independent thinking?	Excellent
To what extent have the achievements of the PI typically gone beyond the state of the art?	Excellent
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?	Outstanding

Comments (Optional for reviewers)
The applicant is clearly a creative and productive scientist who I hope the ERC will support. He has demonstrated the ability to lead theoretical and experimental projects and has published results in high quality journals that have earned many citations. Much of his work has been in this field, but he has expertise and experience outside molecular magnetism, which is crucial to the work proposed here. He has worked on many funded projects, been awarded a large number of short fellowships and made contributions to conferences and academia as would be expected for a candidate at this level. I was also impressed by the applicant's commitment to outreach, which is very laudable and encouraging, as is the applicant's commitment to free software and open dissemination of the results from the project. The applicant also has a good record in forging international collaborations with leading theoreticians and experimentalists, which does inspire some confidence for the future of this work beyond this project.

Reviewer 5

Research Project
Ground-breaking nature and potential impact of the research project: This proposal aims at developing theoretical models in order to describe or predict the quantum coherence of spin-based qubits for quantum computing (QC), embodied in lanthanide ions. A method already provided by the authors to consider the crystal field based on point charges will be developed in order to incorporate covalency and spin-orbit coupling. It is also proposed to bring into the model the various factors influencing decoherence, namely coupling with the lattice, coupling with nuclear spins and coupling with neighbouring electronic spins. The time dependent evolution of the quantum phase and amplitude of any such system is expected to be described after this lengthy investigation. The challenge is of paramount importance since quantum coherence is one of the main issues of concern regarding the search for a suitable technology for QC. Currently, this property has been explored for some real Ln systems showing great promise. This precise description will be a true breakthrough in the area and shall guide experimental research towards the preparation of more suitable physical systems towards the goal of implementing QC. Further working packages (WPs) aim at studying theoretically and experimentally multiqubit systems, which represents an additional, more challenging milestone, which will necessarily have to be overcome in the phenomenal goal of realizing quantum information processing (QIP) with spin-qubits. The proposed research thus addresses a fundamental problem in nanoscience. The proposals WPs are of increasing ambition. The best developed WP (WP1) is proposed with gradual gain of complexity and aims to bring the predictive capacity of the area significantly beyond the state of the art, although beginning from well established (in part by the PI) basis. The goals of WP2 and WP3 are for the most part significantly ground breaking. However, some important aspects are currently being studied and developed in very similar terms (specifically, using and studying real Ln molecules as realizations of qugates). As stated by the PI, the main part of the project (WP1) is a continuation of his specialty (modelling the crystal field around Ln ions) drastically expanded in order to reach the ambitious goal of describing or predicting the quantum coherence of Ln spin-based qubits. This goal is clearly high gain since this would constitute a very significant step forward in this very relevant context. Given the previous knowledge and experience of the PI, a large part of this WP does not seem to entail exceedingly high risk, as pointed out by the PI. The other WPs are of very high gain. In there, it is proposed to investigate, theoretically, but also experimentally, multiqubit systems and the possibility to realize quantum gates (qugates), perform more complex algorithms or implement fault tolerant error quantum correction codes. However, these have been put forward in far less precise terms, which necessarily confer these, at least in appearance, with significantly higher risk. The same can be said about the proposal of WP3; it is mentioned that higher dimensionality in the organization of Ln-based qubits should allow to implement complex coding (such as Lloyd’s scheme). However, there is very little precision and concretion about how to do it.

Scientific Approach:
The PI has demonstrated the capacity to develop (in pioneering ways) theoretical models for describing the crystal field of lanthanides, and the ensuing properties of magnetic relaxation and quantum tunelling. The propositions to improve these models and incorporate the prediction of decoherence (by including the coupling to phonons) appears thus feasible. The selection or preparation of MOFs of lanthanides as infinite qubit arrays is feasible (as mentioned by the PI, many such MOFs are available in the literature). Identify ideal conditions, using theoretical models, to minimize decoherence within these systems may be achieved. It is not clear how this will be probed experimentally. The implementation of complex algorithms with these higher dimensionality materials is not quite well explained.

The theoretical section of the project is proposed in a well-structured manner and the methodology put forward for achieving the various goals is appropriate. It is planned to increase the degree of complexity, while the know-how of the PI in the various areas should lead to attain the goals, which, as mentioned before will push forward the current state of the art.
Parts of the methodology suggested for WP2 and WP3 are appropriate. However, the implementation of complex algorithms is not clearly explained.
The task of WP3 dealing with inclusion of qubits within biopolymers is much more delicate. It appears as a very good solution for sequencing various connected qubits in a desired manner, however, the goal seems too ambitious for constituting a somewhat marginal part of the project, considering the fact that the PI does not seem to have experience in this type of chemistry.

In general, the proposal is original in implementing novel methodology; incorporate the coupling to phonons to the Hamiltonian of the Ln spin in order to model decoherence and then predict its time evolution. The use of pulsed EPR techniques to study and characterize the decoherence is becoming common practice. The authors however propose to build on recent experiments performed by them, showing that playing with the experimental parameters it is possible to significantly improve the quantum coherence.
The authors do not seem to propose (or give sufficient details about) significantly new methodologies in chemistry for the production of suitable systems relevant to WP1 and WP2, as well as the first part of WP3. However, the method for preparing multiqubit systems based on biopolymers appears as radically original.

The timescales are adequate and justified for most part of the project except for task 3.2, which would justify almost an entire grant, and a much higher degree of detail. Thus I would cut the cost related to this last part of the project (i.e. one postdoc). The PI should have justified the need of 100.000EUR for travelling.

Principal Investigator	
To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?	Excellent
To what extent does the PI provide evidence of creative independent thinking?	Outstanding
To what extent have the achievements of the PI typically gone beyond the state of the art?	Excellent
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?	Outstanding

Comments (Optional for reviewers)
The PI exhibits a good track record of publications, many of very high impact, of which one needs to highlight especially these that are pioneering in the field of the proposal. He has been successful at his different stages of his career, particularly during his postdoctoral stays. The PI has shown the capacity to direct top research and to succeed in the training of young scientists. This is good proof that the PI should be capable to lead this ambitious project, most especially as it regards the theoretical developments and spectroscopic analysis of real systems. In terms of the chemical synthesis of new and ground breaking objects of study, this quality is less evident, most especially on systems Evidence of the PI for independent and creative thinking is already this research proposal. He has shown this capacity also with his current research, which constitute landmarks in the field. This has been also manifested in the talks and presentations he has been invited to give, which clearly show that he is opening research lines fully independently of current and past “supervisors”. The key publications by the PI suggest that he has the capacity to overcome the state of the art. He is not corresponding author in some of them but his achievements as independent researcher show that his input was fundamental in them. As a young researcher he has demonstrated already that he is one of the few experts in this challenging field, and that he is able to put forward and develop very original ideas to bring it forward. Level of commitment. The level of commitment (85%) is above the average. Very appropriate in the current circumstances of the PI, which shall be to the best benefit of the project, in particular since it does not scale with the PI’s salary cost (assumed by the local institutions).

Reviewer 6

Research Project
Ground-breaking nature and potential impact of the research project: The proposal contains some goals that are really appealing and despite the challenge, it is reasonable to think that the applicant could reach these goals. It is worth to take into account the multidisciplinary nature of the proposal that includes synthesis and characterization of compounds as well as theoretical studies of such systems. The high gain tasks are those that will result in the achievement of new systems with multi-qubit properties. The applicant gives high importance (gain) to some tasks devoted to the theoretical study of such systems that are just to give some insights for the possible synthetic targets. Really, the high gain task must be the task where it is experimentally shown that the desired physical properties are fulfilled. Hence, basically the high gain tasks, taking into account the state of the art in this research field, are those involved in the work package 3 as well as the last tasks in work packages 1 and 2. These research goals can be considered as being beyond the state of the art and they address important challenges. Scientific Approach: The analysis of the three work packages shows an increase of difficulty, and consequently a bigger challenge. Thus, for instance the goals of the first work package are relatively close to the actual state of the art in the field and consequently feasible without major risks. The high risk/high gain tasks are those, mentioned in the previous paragraph, that would lead to new systems with desired physical properties (work package 3). The research methodology involving crystal field (CF) parameters (including the computer code developed from the applicant) is quite risky, because it is based on fitting of some experimental data in order to extract many CF parameters (with the overparametrization problem) and the results could not be clear. The timeline is appropriate for the project.

Principal Investigator	
To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?	Excellent
To what extent does the PI provide evidence of creative independent thinking?	Outstanding
To what extent have the achievements of the PI typically gone beyond the state of the art?	Excellent
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?	Outstanding

Comments (Optional for reviewers)
The candidate has a good background with a solid expertise in quantum chemistry computations. The PI is the appropriate person to integrate physics (quantum mechanical theory) and chemistry (synthesis and characterization of compounds) in order to achieve the goals of the proposal.

Reviewer 7

Research Project
Ground-breaking nature and potential impact of the research project: The proposal seeks to develop methods for understanding decoherence in molecular qubits based on lanthanide complexes, moving on to polynuclear lanthanide complexes and finally organization of qubits. This is clearly an important and ambitious research challenge. The program SIMPRE 2.0 will be useful for the wider scientific community, if properly distributed and supported. The risk is spread across the three WPs. Only the final part on 'programmable biopolymers' is high risk and I would have liked to have seen more on this and exactly how this will work. Scientific Approach: The PI discusses decoherence mechanisms for SMMs, which can be reduced in some cases for a high tunnel splitting, but in others for a low tunnel splitting. So, it is not sure how reducing the docherence from all the different mechanisms can be reconciled? Perhaps this is the reason to undertake the project. Overall the methodology is logical, moving from WP1-3. It will develop some novel methodology & should achieve some of the goals. Resources seem generally justified, travel at 100k Euros seems high though.

Principal Investigator	
To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?	Excellent
To what extent does the PI provide evidence of creative independent thinking?	Excellent
To what extent have the achievements of the PI typically gone beyond the state of the art?	Excellent
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?	Very good

Comments (Optional for reviewers)
In places there is some over-selling e.g. 'a field shaped by seminal contributions of the PI' when in Ln-based SIMs the seminal work was by Ishikawa. The PI is already employed 100% on a Ramon y Cajal fellowship, but will spend 85% of his time working on the ERC grant, if awarded? I don't see how this will work in practice and this needs to be explained.

Reviewer 8

Research Project
Ground-breaking nature and potential impact of the research project: This is a very exciting proposal based on the synthesis of SMM - formed by specific lanthanoid complexes, to study their spin systems when these are single spin qubits, or when they comprise coupled two or more spin qubits, with the aim of modelling decoherence in molecular spin systems. Ultimately the PI plans to extrapolate to infinite systems formed by the complex organisation of spin qubits. The work will impact on the wider field of quantum computing as well as going some way to understand the fundamental nature of qubits and qugates. The project is both highly theoretical and yet relies on chemical synthesis at the outset of WP1. The early WP discusses the expansion of their software SIMPRE- developed by the PI- in order to consider carefully the best targets for directed synthesis. Finally the PI considers how, and what examples in biology, eg biopolymers - can be regarded as ordered arrays of molecular spin cubits. This latter part of the project seems rather removed from the remainder and very challenging for the 5 year project. The PI has carefully annotated the risks and potential high gain from the various stages of the proposal and yes there are risks, but with a cutting edge proposal in a novel area, this is not surprising. Scientific Approach: The project is certainly feasible to the point where current experience and knowledge runs out, but the PI is well equipped to create new knowledge and continue to take this field forward combining chemical synthesis with theory and new computational methods. New computational tools will emerge from the project as well as new versions of SIMPRE. The description of staff numbers/years is not easily extracted for the costs section, but the PI charges little for himself, to concentrate on more co-workers supported by the grant. The need for the Q band pulsed EPR instrument is made well enough, although the last sentence above the Table is very terse.

Principal Investigator	
To what extent has the PI demonstrated the ability to propose and conduct ground-breaking research?	Excellent
To what extent does the PI provide evidence of creative independent thinking?	Excellent
To what extent have the achievements of the PI typically gone beyond the state of the art?	Excellent
To what extent does the PI demonstrate the level of commitment to the project necessary for its execution and the willingness to devote a significant amount of time to the project (min 50% of the total working time on it and min 50% in an EU Member State or Associated Country) (based on the full Scientific Proposal)?	Excellent

Comments (Optional for reviewers)
No comments received