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Molecular Spins for Quantum Technologies

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Contents

Report Abstract: Please, note that three relevant narratives by the three PIs, (1) S. Hill, (2) M. Affronte and (3) T. Takui, are given in "Report of the Results" below, respectively.
The backgrounds and objectives of this project are as follows:
Among the diverse topics of quantum technologies relevant to quantum computing, near-term quantum technologies applicable to Noisy Intermediate-Scale Quantum devices (NISQ) have been emerging as a realistic approach to long-term scalable quantum computers. Relevant key issues includes to develop methods, theoretical/algorithmic and experimental, for saving qubit resources and executing computation with shallow depth. Molecular spin based quantum technologies give promise for the issues.

(1) We have carried out spectroscopic studies of several potential new molecular spin qubits based on lanthanide atoms. Examples include the Yb(trensal) molecule and various endohedral metallo-fullerenes such as $Gd_2@C_{79}N$. Both of these molecules have been proposed as molecular spin qudits (instead of spin qubits) due to their large electron and nuclear spin multiplicities, which are intrinsic to molecular high spins. The main aim of the investigations is to gain fundamental insights into the mechanisms that cause decoherence in these potential next generation quantum information technologies.

(2) Molecular spins have recently shown quantum features like long coherence time or quantum correlation between spin states that make them suitable for spin memory devices in quantum technologies. The objective is to investigate the intrinsic quantum behavior of spins in magnetic molecules in order to determine viable physical systems and conditions for the realization of quantum memory and sensing devices working in the quantum regime.

(3) Long/near-term scalable quantum computers have the potential to exactly solve Schroedinger Equations. Applications of such quantum computers to practical quantum chemical calculations and quantum simulations are the current focus of the subjects in chemistry, physics and related fields. The objective is to implement efficient quantum algorithms for practical quantum chemical calculations as executable on scalable quantum computers. A key issue of this research field is to implement efficient quantum algorithms which enable us to save qubit resources and execute computations for realistic chemical and physical targets.

The Impacts of the results from this project are as follows:
The results obtained from the part (1) of this project provide direct information on the spin-vibronic coupling in the Yb(trensal) molecule, which represents a major source of spin decoherence, and on the paradigm of why spin qudits, instead of spin qubits, are efficient and enable us to save computational resources necessary for error corrections. The results illustrate chemistry/materials science guidelines and instructions for molecular designing scalable qudits.

The part (2) can contribute to the implementation of quantum memory devices in quantum computing and sensors to detect a vanishingly small number of microwave photons, from both the theoretical and experimental sides.

The part (3) provides efficient quantum algorithms which are completely different from algorithms for classical computers developed so far in terms of the theoretical framework schemes, exemplifying quantum algorithms affording direct calculations of transition energies between different electronic spin states of open shell molecules and atoms. The algorithms, for the first time, render such direct approaches possible, giving quantum chemical calculations with chemical energies of extreme precision. The methods implemented have potentials to be applicable to important problems relevant to energies in other fields.

Report of the Results:

(1) PI, Stephen Hill' achievement made during the period of the project emphasizes as follows:

Outcomes
The project has resulted in three publications in highly regarded journals [1-3], with at least three more manuscripts close to completion [a,b,c]. The PI and members of his group have also

given many presentations describing research carried out under this award. Two graduate students supported on the project received PhDs: Dorsa Komijani, 2018, and Jonathan Marbey, 2020. Both have moved on to excellent positions closely related to the area of quantum information sciences. Dorsa Komijani now works with the company Rigetti, in Berkeley California, which specializes in developing integrated circuits for quantum computing. After a 1-year postdoctoral position during the pandemic in the PIs group at the NHMFL, Jonathan Marbey was recently hired as a postdoctoral scholar in the Laboratory for Physical Sciences at the University of Maryland, a unique university, industry and government collaborative facility specializing in quantum communication, sensing and computing technologies.

The project is expected to have a lasting impact in terms of the development of collaborative relationships involving Florida State University, Osaka City University and the University of Modena and Reggio Emilia. Although set back by the pandemic, which made travel between the institutions impossible, several projects are expected to continue if funding can be secured in order to support future exchanges of personnel. The project will also have a lasting impact in terms of technical developments at the NHMFL, particularly those related to the integration of an Arbitrary Waveform Generator into the pulsed high-field EPR spectrometer, HiPER.

A particularly impactful outcome of this project was the publication of a Perspectives article in Nature Chemistry describing a vision for the deployment of molecular spins in next-generation quantum technologies [1]. Published in 2019, this Perspective has already been cited 190 times (95 citations in 2020 and over 50 at the time of writing this report in 20201). Spins in solids or in molecules possess discrete energy levels, and the associated quantum states can be tuned and coherently manipulated by means of external electromagnetic fields. Spins therefore provide one of the simplest platforms to encode a quantum bit (qubit), the elementary unit of future quantum computers. The Perspective article discusses how chemistry can contribute to the design of robust spin systems based on rare-earth complexes. Using these molecular nanomagnets as key examples, the variety of paths that chemistry has recently opened for quantum technologies is illustrated: from the design of molecular spin qubits with enhanced coherence to their coupling together for implementing quantum logic gates and, finally, to the integration of such molecular quantum units into devices.

Key Findings

Magic angle effects in a trigonal Mn_3^{III} cluster [2]: We have carried out angle-dependent high-frequency EPR studies on a single-crystal of a trigonal Mn_3^{III} cluster with an unusual structure in which the local magnetic easy-axes of the constituent Mn^{III} ions are tilted significantly away from the molecular C_3 axis towards the 'magic-angle' of 54.7 degrees, resulting in an almost complete cancelation of the 2nd-order axial magnetic anisotropy, $D\hat{S}_z^2$, associated with the ferromagnetically coupled total spin $S_T = 6$ ground state. This contrasts the situation in many related Mn_3^{III} single-molecule magnets (SMMs) that have been studied intensively in the past, for which the local Mn^{III} anisotropy tensors are reasonably parallel, resulting in substantial barriers to magnetization relaxation ($U_{eff} \sim 30$-35 cm^{-1}) and magnetization blocking below about 2.5 K. The suppression of the 2nd-order anisotropy [note that the rhombic term, $E(\hat{S}_x^2 - \hat{S}_y^2)$, is also zero on symmetry grounds] in this case results in a situation in which the zero-field splitting (ZFS) of the $S_T = 6$ ground state is dominated by 4th- and higher-order interactions. This provides a unique opportunity to study in depth how molecular geometry influences these interactions that are responsible for quantum tunneling of magnetization in high-symmetry SMMs. Angle-dependent EPR measurements provide a full mapping of the molecular magneto-anisotropy. Meanwhile, irreducible tensor operator (ITO) methods are employed in order to obtain analytic expressions that directly relate molecular anisotropy to the microscopic physics, i.e., the ZFS tensors associated with the individual Mn^{III}

ions, their orientations, and the exchange coupling between the three spins. The ITO methodology improves significantly upon previous numerical methods that have been applied to trigonal SMMs. We find that the magic-angle tilting leads to a massive compression of the $S_T = 6$ ground state energy level diagram (< 3.5 cm^{-1} separate the lowest and highest lying levels in zero-field) and strong mixing between spin projection states. Although these characteristics are antagonistic to SMM behavior, they provide important insights into the physics of polynuclear molecular nanomagnets.

Radical-Lanthanide Interaction in a Tb^{III} Bis-Phthalocyaninato Complex [3]:
Recent studies have highlighted the importance of organic ligands in the field of molecular spintronics, via which delocalized electron spin density can mediate magnetic coupling to otherwise localized 4*f* moments of lanthanide ions, which show tremendous potential for single-molecule device applications. To this end, we employed high-field/high-frequency EPR spectroscopy to study a neutral terbium bis-phthtalocyaninato metalorganic complex, $[TbPc_2]^0$, with the aim of understanding the magnetic interaction between the Ising-like moment of the lanthanide ion and the unpaired spin density on the coordinating organic radical ligand. The measurements were performed on a previously unknown $[TbPc_2]^0$ structural phase crystallizing in the *Pnma* space group. EPR measurements on powder samples of $[TbPc_2]^0$ reveal an anisotropic spectrum, which is attributed to the spin-½ radical coupled weakly to the EPR-silent Tb^{III} ion. Extensive double-axis rotation studies on a single-crystal reveal two independent spin-½ signals with differently oriented (albeit identical) uniaxial *g*-tensors, in complete agreement with x-ray structural studies that indicate two molecular orientations within the unit cell. The easy-axis nature of the radical EPR spectra thus reflects the coupling to the Ising-like Tb^{III} moment. This is corroborated by studies of the isostructural $[YPc_2]^0$ analog (where Y is non-magnetic yttrium), which gives a completely isotropic radical EPR signal. The experimental results for the terbium complex are well explained on the basis of an effective model that introduces a weak ferromagnetic Heisenberg coupling between an isotropic spin-½ and an anisotropic spin-orbital moment, $J = 6$, that mimics the known, strong easy-axis $Tb\cdots Pc_2$ crystal-field interaction.

Studies of radical-lanthanide exchange coupling in $Dy(Pc)_2$:
Lanthanide complexes bearing radical organic ligands display a unique magnetic coupling mechanism involving delocalized spin density on the ligand and the localized 4f moment of the lanthanide ion. This mechanism can be used to mediate magnetic coupling to normally isolated lanthanide ions, a highly desired property for spintronics applications and quantum information technologies. We have employed high-field/high-frequency EPR techniques to investigate a dysprosium bis-phthalocyaninato metalorganic complex, $Dy(Pc)_2$ [a], which is closely related to the $Tb(Pc)_2$ compound described above, yet it displays distinct magnetic behavior. Of particular interest is the intermolecular coupling between Dy^{III} ions, via the organic ligand framework, which could not be detected for $Tb(Pc)_2$. Double-axis rotation measurements on a single crystal reveal the existence of two molecular orientations in the unit cell, the easy-axis nature of the Dy^{III} moment, and enable measurement of the strength of the intermolecular exchange coupling.

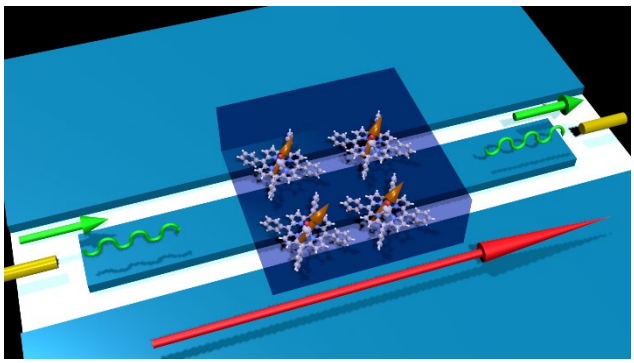
Lanthanide Triple-Decker Compounds as Two-Qubit Gates:
Molecular spin qubits have proven to be promising for implementation of quantum information processing. Scalability is perhaps one of the most attractive properties of molecular magnets since arrays of identical qubits can be synthesized with controllable interactions between them. While earlier research has mainly focused on single qubit operations, recent studies have targeted quantum gates involving two or more qubits. We have carried out extensive

continuous-wave electron paramagnetic resonance studies of symmetric and asymmetric lanthanide triple-decker compounds [b]. This work has focused on the effect of point group symmetry on the magnetic properties of lanthanide ion in sandwich-type ligand systems. It is shown that two inequivalent sites in a dinuclear lanthanide compound can be achieved by engineering the ligand such that the local symmetry of the ion is lowered in one of the two sites. The lower point group symmetry at the lanthanide site also allows for observation of formally forbidden EPR transitions. These findings highlight the potential use of lanthanide dinuclear complexes for two-qubit gate operations.

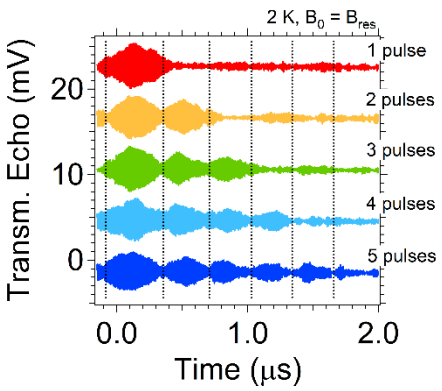
Arbitrary waveform control of molecular spins:
Recent advances in high-power microwave electronics have allowed for the integration of an Arbitrary Waveform Generators (AWG) into a high-frequency (94 GHz) spectrometer, providing a high level of control over the phase, frequency and amplitude of the excitation pulses over a bandwidth of up to 1 GHz. This makes fast/efficient EPR experiments feasible in the time domain, with dramatic improvements in sensitivity and resolution, providing access to microscopic information that is not accessible via previously existing methods. We have obtained preliminary results on a model organic radical system and a Gd^{III} complex to demonstrate the added benefits of pulse shaping afforded by the AWG [c]. This work involved the use of rapid passage pulses for single-shot Fourier-transform EPR detection, enabling CHEESY-detected hole burning (CHEESY = Chirped Echo Spectroscopy) and ELDOR-detected NMR (ELDOR = Electron Electron Double Resonance). We have also demonstrated a population enhancement effect using rapid passage pulses, which can be implemented as a means of initializing molecular spin qudits.

(2) PI, Marco Affronte's achievement made during the period of the project emphasizes as follows:

Outcomes



Within the quest for solid state quantum systems to be used for fundamental as well applied research, molecular spins have recently emerged as a versatile platform with interesting performances in terms of quantum coherence and correlation. Molecular units provides well defined environment to electron spins and they represent elementary bricks for complex nano-architectures and nano-devices. The final goal is to select and control these spin systems in order to encode quantum bits or use them as quantum sensors. In the past three years we have devised special experiments to test this idea.



We first focused our efforts on their efficient integration in circuits quantum electrodynamics and, more specifically, in reaching their coherent coupling with microwave photons in planar resonators. To monitor molecular spin performances over a wide temperature and magnetic field range we have first developed microwave planar resonators made of high Tc superconductors, obtaining excellent performances up to liquid nitrogen temperature and magnetic fields up to 7 Tesla. Ensembles

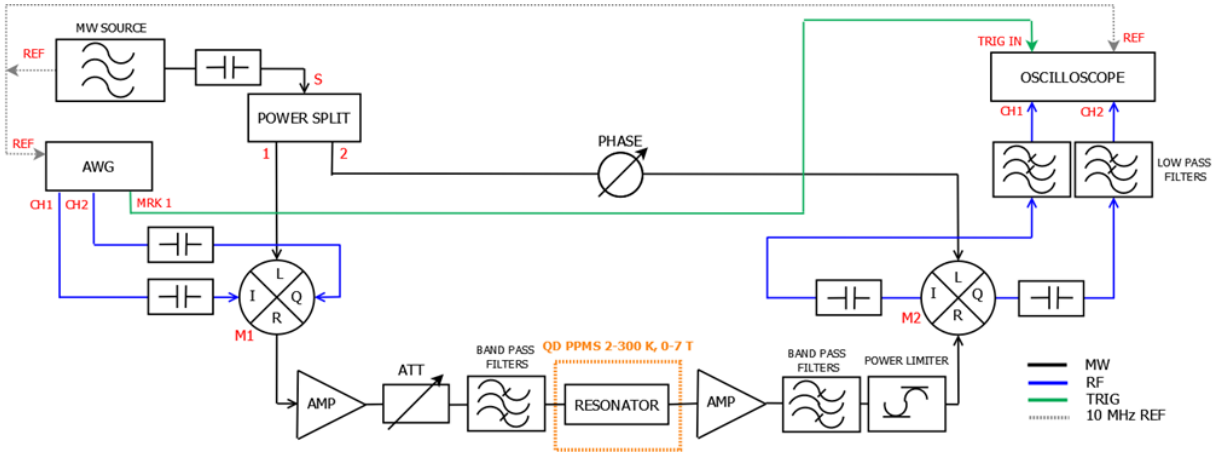
of several different molecular spins systems have been then systematically tested. The regime of high spin-photon cooperativity is achieved with molecular spins diluted in non-magnetic matrix at 0.5 K, while the strong coupling regime is observed with concentrated samples of organic radicals up to 50 K. Metal (vanadium) centers, radicals (DPNO) as well as (CrNi-prussian blue) nanoparticles have been systematically tested also in collaboration with our partners. The possibility to create coherent states among distinct spin ensembles is further explored in similar spectroscopic experiments. This first set of results demonstrated that molecular spins can be efficiently integrated in quantum devices.

We have then developed a setup for pulsed microwaved experiments. With this, we tested diluted oxovanadium tetraphenyl porphyrin (VO(TPP)) as a prototypical molecular spin system for the Storage/Retrieval of microwave pulses when embedded into planar superconducting microwave resonators. We first investigated the efficiency of several pulse sequences in addressing the spins. The Carr-Purcell and the Uhrig Dynamical Decoupling enhance the memory time up to three times with three π pulses. We then successfully store and retrieve trains of up to 5 small pulses by using a single recovery pulse. These results demonstrate the memory capabilities of molecular spin ensembles when embedded into quantum circuits.

Recently, in collaboration with Prof. Takui's group we have tested a new techniques on organic radicals: the readout in the dispersive regime that was originally developed -and it is now largely exploited- for non-demolitive measurement of super- and semi-conducting qubits. The extension of this regime to the semiclassical limit has been only marginally investigated although it holds for a wide class of problems, including advanced magnetic resonance techniques. In our recent work we have investigated the coupling between a coplanar microwave resonator and a diluted crystal of Diphenyl-Nitroxide (DPNO) organic radical in a semi-classical dispersive regime of excitations for the microwave fields. Two-tone transmission spectroscopy experiments show the possibility to reconstruct the spectrum of the spin system by adjusting probe and drive power independently with little loss of sensitivity. Likewise, pulse sequences of detuned microwave frequency allow to measure characteristic relaxation times (e.g., T_1). These results suggests that the Electron Spin Dispersive spectroscopy can be used as complementary tool to investigate the spin response far from resonant cavity signal.

Instrumental

We have realized a heterodyne set up allowed us to encode microwave pulse sequences in our superconducting devices. As planned at the beginning of this AOARD project, in 2018 we acquired an Arbitrary wave Function Generator (*Active Technologies* Arb Rider AWG4022) that constitutes the heart of our instrumentation and allowed us to perform most of studies recently published by our group.



PI, Takeji Takui's achievement made during the period of the project emphasizes as follows:

1. This project has featured in a molecular approach to quantum spin science/quantum information technology, particularly underlying quantum computing and quantum control. From a theoretical viewpoint, rational molecular design/optimization of open shell molecular entities for particular relevant purposes is essential in quest of novel prototypes enabling us to implement targeted quantum spin science/technology. During the period of the project, we have continued to develop reliable molecular theories for spin-orbit couplings in terms of accurate quantum chemical calculations. This helps us predict the magnetic properties, particularly relevant ZFS (Zero-Field Splitting) and **g**-tensors of high spin metallocomplexes in the ground state. ZFS is the most important physical quantity to govern the quantum behavior of molecular spin qudits (instead of qubits), which have the potential benefits to save computational resources in fault-tolerant quantum computing.
2. Beyond molecular systems composed of a few spin qubits, which have their own right for seeking significant physical insights of hidden parameters behind quantum entanglement, the scalable molecular qubits or qutrits (or qudits), as new quantum entities for accelerating quantum computing speed, are emerging, and thus the implementation of practical quantum algorithms for quantum chemical calculations on truly scalable quantum computers has more and more important, although they are long-term. We have shown for the first time that true full-CI (Configuration Interaction) calculations for sizable molecular systems can be executed on quantum computers, implementing quantum algorithms on quantum computers for this purpose. We have reached a significant milestone in implementing such algorithms. During the third year of the period, we have implemented Baysian-phase-estimation (BPE) based quantum algorithms which enable us to directly calculate energy gaps between two electronic spin states having different spin multiplicities without individually inspecting the total energies of the two states.

   Quantum computers can execute full-CI calculations by utilizing the quantum phase estimation (QPE) algorithms including BPE and iterative quantum phase estimation. In these quantum algorithms, the time evolution of wave functions under study is simulated conditionally with an ancillary qubit as the control, which make the implementation of the algorithms to real quantum devices difficult. We note that most of problems in chemistry are relevant to discussing energy differences between two electronic states rather than total energies themselves, and thus it is desirable that the direct evaluations or calculations of energy gaps are implemented for future applications of quantum computers to real chemistry or physics problems. During the period of the project, we have proposed a Bayesian phase difference estimation (BPDE) algorithm, which importantly is a general algorithm to calculate the difference of two eigenphases of any unitary operators. We have shown that the BPDE algorithm is applicable to the direct calculations of energy gaps between two electronic states of real chemical systems on quantum computers. In the BPDE algorithm, the state preparations are made conditional on the ancillary qubit, and the time evolution of the wave functions described in superposition of the two electronic states are executed unconditionally. Numerical quantum circuit simulations for the various energy gaps of the systems including vertical ionization energies, singlet–triplet energy gaps, and vertical excitation energies have revealed that BPDE is capable of computing the energy gap with the accuracy similar to BPE without controlled-time evolution simulations and with the smaller number of iterations during the process of Bayesian optimizations.

   The quantum algorithms implemented in this project utilize the quantum superposition of the two relevant spin states, thus intrinsically affording the same accuracy of the energies

within chemical precision. Notably, only quantum nature intrinsic to quantum algorithms executable on quantum computers renders the direct calculations possible for the first time. It is worth noting that BPDE is a general algorithm enabling to calculate the difference of two eigenphases of any unitary operators, and thus promising to be widely applicable.

3. Quantum control and quantum cybernetics are emerging as essential concepts in the field of quantum information science and quantum technology. Molecular spins are suitable for giving a testing ground for quantum control experiments and associated theoretical considerations, mainly relevant to Lie algebra/group theory. Quantum control experiments on realistic molecular spins have been achieved, illustrating that GRAPE (GRadient Ascent Pulse Engineering) technology, as based on AWG (Arbitrary Wave Generator) microwave setups, is of significant importance in quantum control for molecular spins. Experimentally, we have demonstrated for the first time that the GRAPE technology affords to implement quantum gates in molecular spins, discussing the practicalities of synthetic molecular spins in quantum control.

In Subject 1 above, we have derived further exact analytical expressions for bridging the gap between putative fictitious spin-1/2 Hamiltonian and true full spin Hamiltonian approaches, for the first time. The derived formulas are general and applicable to spin quantum number *S*'s up to $S = 9/2$ in the presence of the static magnetic field. For the year of Option 1, we have generalized the theoretical method for non-collinear cases of the ZFS and g-tensors. For the final year, we have extended our theoretical method to derive the analytical expressions, in which hyperfine tensors are included in both the spin Hamiltonians, and we have revisited some typical examples so far documented, correcting their spin Hamiltonian parameters, which reasonably agree with theoretical ones.

In Subject 2 above, particularly we also propose a more efficient quantum algorithm which is based on Serber construction of spin eigenfunctions, enabling us to prepare CSFs (Configuration State Functions) on QCs (Quantum Computers) with much less quantum gate operations than our previously proposed one and the constant circuit depth. Also, we have implemented quantum algorithms for theoretically determining electron spin multiplicities of arbitrary electronic wave functions, showing that the algorithms work on quantum computers having a small number of qubits.

In Subject 3, a method is proposed for optimizing the performance of the Adiabatic-Passage Spin Order Conversion technique as quantum control by using AWG technology for molecular spin systems, for the first time.

Archival Publications Published During the Reporting Period:

PI, Stephen Hill's publications:

1. [FSU-3] *Molecular spins for quantum computation*, A. Gaita-Ariño, F. Luis, S. Hill, and E. Coronado, *Perspective in Nat. Chem*. **11**, 301 – 309 (2019); https://doi.org/10.1038/s41557-019-0232-y
2. [FSU-2] *Magic angle effects in a trigonal* Mn_3^{III} *cluster: deconstruction of a single-molecule magnet*, Jonathan Marbey, Pei-Rung Gan, En-Che Yang, and Stephen Hill, *Phys. Rev. B* **98**, 144433 (2018); https://doi.org/10.1103/PhysRevB.98.144433
3. [FSU-1] *Radical-Lanthanide Ferromagnetic Interaction in a* Tb^{III} *Bis-Phthalocyaninato Complex*, Dorsa Komijani, Alberto Ghirri, Claudio Bonizzoni, Svetlana Klyatskaya, Eufemio Moreno-Pineda, Mario Ruben, Alessandro Soncini, Marco Affronte, and Stephen Hill, *Phys. Rev. Mater.* **2**, 024405 [pp. 1 – 9] (2018), Editors Suggestion; https://doi.org/10.1103/PhysRevMaterials.2.024405

Publications in preparation

a. *Studies of radical-lanthanide exchange coupling in the metalorganic complex Dy(Pc)$_2$*, Robert Stewart, Dorsa Komijani, Miguel Gakiya, Michael Shatruk, Alberto Ghirri,Claudio Bonizzoni, Svetlana Klyatskaya, Eufemio Moreno-Pineda, Mario Ruben, Marco Affronte, and Stephen Hill (in preparation).
b. *EPR Studies of Lanthanide Triple-Decker Molecular Complexes: the Effect of Porphyrin in Lanthanide Triple-decker Compounds for Two-Qubit Gate Operation*, Dorsa Komijani, Alberto Ghirri, Claudio Bonizzoni, Svetlana Klyatskaya, Eufemio Moreno-Pineda, Mario Ruben, Alessandro Soncini, Marco Affronte, and Stephen Hill (in preparation).
c. *Arbitrary waveform control in pulsed EPR*, Jonathan Marbey, Krishnendu Kundu, and Stephen Hill (in preparation).

PI, Marco Affronte's publications:

1. [CNR-7] *Transmission Spectroscopy of Molecular Spin Ensembles in the Dispersive Regime*, Claudio Bonizzoni, Alberto Ghirri, Shigeaki Nakazawa, Shinsuke Nishida, Kazunobu Sato, Takeji Takui, and Marco Affronte, *Adv. Quantum Technol*., accepted (2021)
2. [CNR-6] *Microwave Assisted Tunneling in Hard-Wall InAs/InP Nanowire Quantum Dots*, Samuele Cornia, Marco Affronte, Francesco Rossella, Valeria Demontis, Lucia Sorba, and Alberto Ghirri, *Scientific Reports* **9***,* 19523 (2019) https://doi.org/10.1038/s41598-019-56053-2
3. [CNR-5] *Resonant coupling of CsNiCr magnetic nanoparticles with microwave photons*, A. Ghirri, C. Herrero, S. Mazérat, T. Mallah, O. Moze, and M. Affronte, *Adv. Quantum Techno*l. 1900101 (2019); DOI: 10.1002/qute.201900101
4. [CNR-4] *Towards Quantum Sensing with Molecular Spins*, F. Troiani, A. Ghirri, M. G. A. Paris , C. Bonizzoni, and M. Affronte, *Journal of Magnetism and Magnetic Materials* **491**, 165534 (2019); https://doi.org/10.1016/j.jmmm.2019.165534
5. [CNR-3] *Microwave dual-mode resonators for coherent spin-photon coupling*, C. Bonizzoni, F. Troiani, A. Ghirri, and M. Affronte, *Journal of Applied Physics* **124**, 194501 (2018); https://doi.org/10.1063/1.5050869
6. [CNR-2] *Radical-Lanthanide Ferromagnetic Interaction in a Terbium(III) Bis-Phthalocianinato Complex*, Dorsa Komijani, A. Ghirri, C. Bonizzoni, S. Klyatskaya, E. Moreno Pineda, M. Ruben, A. Soncini, M. Affronte, and S. Hill, *Phys Rev, Materials* **2**, 024405 (2018); https://doi.org/10.1103/PhysRevMaterials.2.024405
7. [CNR-1] *Coherent coupling of molecular spins with microwave photons in planar superconducting resonators*, C. Bonizzoni, A. Ghirri, and M. Affronte, *Advances in Physics X* **3**:1, 1435305 (2018); https://doi.org/10.1080/23746149.2018.1435305

PI, Takeji Takui's publications:

1. [OCU-27] *Molecular Optimization for Nuclear Spin State Control via A Single Electron Spin Qubit by Optimal Microwave Pulses: Quantum Control of Molecular Spin Qubits,* Taiki Shibata, Trauki; Yamamoto, Satoru; Nakazawa, Shigeaki; Lapasar, Elham Hosseini; Sugisaki, Kenji; Maruyama, Koji; Toyota, Kazuo; Shiomi, Daisuke; Sato, Kazinobu; Takui, Takeji, *Applied Magnetic Resonance*, **2021**, accepted.
2. [OCU-26] *Transmission Spectroscopy of Molecular Spin Ensembles in the Dispersive*

Regime, Claudio Bonizzoni, Alberto Ghirri, Shigeaki Nakazawa, Shinsuke Nishida, Kazunobu Sato, Takeji Takui, and Marco Affronte, *Adv. Quantum Technol*., **2021**, accepted.

3. [OCU-25] *Structural dynamics of the chromo-shadow domain and chromodomain of HP1 bound to histone H3K9 methylated peptide, as measured by site-directed spin-labeling EPR spectroscopy*, Suetake, I. ; Nakazawa, S. ; Sato, K. ; Mutoh, R. ; Mishima, Y. ; Kawakami, T. ; Takei, T. ; Watanabe, M. ; Sakai, N. ; Fujiwara, T.; Takui, T. ; Miyata, M. ; Shinohara, A. ; Hojo, H. ; Arata, T., *Biochemical And Biophysical Research Communications*, **2021**, 567, 42-48; DOI: 10.1016/j.bbrc.2021.06.010
4. [OCU-24] *Valence tautomerism in a [2 x 2] Co-4 grid complex containing a ditopic arylazo ligand*, Bonanno, N. M. ; Watts, Z. ; Mauws, C. ; Patrick, B. O. ; Wiebe, C. R. ; Shibano, Y. ; Sugisaki, K. ; Matsuoka, H. ; Shiomi, D. ; Sato, K. ; Takui, T. ; Lemaire, M. T., *Chemical Communications*, **2021**; DOI: 10.1039/d1cc01991k
5. [OCU-23] *The Internal Field in a Ferromagnetic Crystal with Chiral Molecular Packing of Achiral Organic Radicals*, Blundell, S. J.; Lancaster, T. ; Baker, P. J. ; Pratt, F. L. ; Shiomi, D. ; Sato, K. ; Takui, T., *Magnetochemistry*, **2021**, 7, Issue: 5, Article Number: 71; DOI: 10.3390/magnetochemistry7050071
6. [OCU-22] *Quantum Algorithm for the Direct Calculations of Vertical Ionization Energies*, Sugisaki, K. ; Toyota, K. ; Sato, K. ; Shiomi, D. ; Takui, T., *Journal of Physical Chemistry Letters*, **2021**, 12, 2880-2885; DOI: 10.1021/acs.jpclett.1c00283
7. [OCU-21] *A quantum algorithm for spin chemistry: a Bayesian exchange coupling parameter calculator with broken-symmetry wave functions*, Sugisaki, K. ; Toyota, K. ; Sato, K. ; Shiomi, D. ; Takui, T., *Chemical Science*, **2021**, 12, 2121-2132; DOI: 10.1039/d0sc04847j
8. [OCU-20] *Syntheses and Properties of (Nitronyl nitroxide)-substituted Tri-phenylamine ortho-Bridged by Two Oxygen and Sulfur Atoms*, Yokoyama, N. ; Tanaka, N. ; Fujimoto, N. ; Tanaka, R. ; Suzuki, S. ; Shiomi, D. ; Sato, K. ; Takui, T. ; Kozaki, M. ; Okada, K., *Chemistry-An Asian Journal*, **2021**, 16, 72-79; DOI: 10.1002/asia.202001227
9. [OCU-19] *A probabilistic spin annihilation method for quantum chemical calculations on quantum computers*, Sugisaki, K. ; Toyota, K. ; Sato, K. ; Shiomi, D. ; Takui, T., *Physical Chemistry Chemical Physic*s, **2020**, 22, 20990-20994; DOI: 10.1039/d0cp03745a
10. [OCU-18] *Magnetic Properties of Metal Clusters Coordinated with (Nitronyl Nitroxide)-Substituted Amidinate Ligands*, Tanimoto, R. ; Suzuki, S.; Kozaki, M. ; Kanzaki, Y. ; Shiomi, D.; Sato, K.; Takui, T.; Tanaka, R. ; Okada, K., *Chemistryselect,* **2020**, 5, 11170-11176; DOI: 10.1002/slct.202002927
11. [OCU-17] *Magnetic Properties of π-Conjugated Hybrid Phenoxyl Nitroxide Radicals with Extended Jr-Spin Delocalization*, Zaytseva, E. ; Shiomi, D. ; Ten, Y. ; Gatilov, Y. V. ; Lomanovich, A. ; Stass, D. ; Bogomyakov, A. ; Yu, AX. ; Sugisaki, K. ; Sato, K. ; Takui, T. ; Bagryanskaya, E. ; Mazhukin, D., *Journal of Physical Chemistry A*, **2020**, 124, 2416-2426; DOI: 10.1021/acs.jpca.9b11856
12. [OCU-16] *Redox-Induced Modulation of Exchange Interaction in a High-Spin Ground-State Diradical/Triradical System*, Nagata, A. ; Hiraoka, S. ; Suzuki, S.; Kozaki, M. ; Shiomi, D. ; Sato, K. ; Takui, T.; Tanaka, R. ; Okada, K., *Chemistry-A European Journal*, **2020**, 26, 3166-3172; DOI: 10.1002/chem.201905465
13. [OCU-15] *Synthesis of Trioxotriangulene Stable Neutral pi-Radicals Having Alkyl Substituent Groups, and Their Effects on Electronic-spin and pi-Stacking Structures*, Murata, T. ; Yokoyama, M. ; Ueda, A. ; Kanzaki, Y. ; Shiomi, D. ; Sato, K. ; Takui, T. ; Morita, Y., *Chemistry letters,* **2020***,* 49, 95-98; DOI: 10.1246/cl.190761
14. [OCU-14] *Trioxotriangulene with carbazole: a donor-acceptor molecule showing strong near-infrared absorption exceeding 1000 nm*, Murata, T. ; Kariyazono, K. ; Ukai, S. ;

Ueda, A. ; Kanzaki, Y. ; Shiomi, D. ; Sato, K. ; Takui, T. ; Morita, Y., *Organic Chemistry Frontiers*, **2019**, 6 (17), 3107-3115; DOI: 10.1039/c9qo00663j

15. [OCU-13] *Trityl-Aryl-Nitroxide-Based Genuinely g-Engineered Biradicals, As Studied by Dynamic Nuclear Polarization Multifrequency ESR/ENDOR, Arbitrary Wave Generator Pulse Microwave Waveform Spectroscopy, and Quantum Chemical Calculations,* Kazunobu, S.; Hirao, R.; Timofeev, I.; Krumkacheva, O.; Zaytseva, E.; Rogozhnikova, O.; Tormyshev, V.M.; Trukhin, D.; Bagryanskaya, E.; Gutmann, T.; Klimavicius, V.; Buntkowsky, G.; Sugisaki, K.; Nakazawa, S.; Matsuoka, H.; Toyota, K.; Shiomi, D.; Takui, T., *Journal of Physical Chemistry A*, **2019**, 123, 7507-7517; http://dx.doi.org/10.1021/acs.jpca.9b07169
16. [OCU-12] *EPR and DEER Characterization of New Mixed Weakly Coupled Nitroxide Triradicals for Molecular Three-Spin Qubits,* Zaytseva, E.; Timofeev, I.; Krumkacheva, O.; Parkhomenko, D.; Mazhukin, D.; Sato, K.; Matsuoka, H.; Takui, T.; Bagryanskay, E., *Applied Magnetic Resonance*, **2019**, 50, 967 – 975; https://doi.org/10.1007/s00723-019-01125-9
17. [OCU-11] *Quantum Chemistry on Quantum Computers: Quantum Simulations of the Time Evolution of Wave Functions under the S^2 Operator and Determination of the Spin Quantum Number S.* Sugisaki. K.; Nakazawa, S.; Toyota, K.; Sato, K.; Shiomi, D.; Takui, T., *Phys. Chem. Chem. Phys*., **2019,** 19, 30128 – 30138; DOI: 10.1039/c9cp02546d
18. [OCU-10] *Quantum Chemistry on Quantum Computers: A Method for Preparation of Multiconfigurational Wave Functions on Quantum Computers without Performing Post-Hartree–Fock Calculations,* Sugisaki, K.; Nakazawa, S.; Toyota, K.; Sato, K.; Shiomi, D.; Takui, T., *ACS Central Science*, **2019**, 5, 167–175; DOI: 10.1021/acscentsci.8b00788
19. [OCU-9] *Open shell electronic structure calculations on quantum computers: A quantum circuit for the preparation of configuration state functions based on Serber construction,* Sugisaki, K.; Yamamoto, S.; Nakazawa, S.; Toyota, K.; Sato, K.; Shiomi, D.; Takui, T., *Chemical Physics Letters: X*, **2019,** 1, 100002; DOI: 10.1016/j.cpletx.2018.100002
20. [OCU-8] *Microscopic behavior of active materials inside a TCNQ-based lithium ion rechargeable battery by in-situ 2D ESR measurements* Kanzaki, Y,; Mitani, S.; Shiomi, D.; Morita, Y.; Takui, T.; Sato, K., *ACS Nano. Interface*, **2019**, 10, 43631-43640; DOI: 10.1021/acsami.8b14967
21. [OCU-7] *Intramolecular Magnetic Interaction of Spin-Delocalized Neutral Radicals through m-Phenylene Spacers*, Murata, T. ; Asakura, N. ; Ukai, S. ; Ueda, A. ; Kanzaki, Y. ; Sato, K. ; Takui, T. ; Morita, Y., *ChemPlusChem,* **2019**, 84, 680-685; https://doi.org/10.1002/cplu.201800662
22. [OCU-6] *ESR analyses of picket fence Mn^{II} and 6th ligand coordinated Fe^{III} porphyrins (S = 5/2) and a Co^{II}(hfac) complex (S = 3/2) with sizable ZFS parameters revisited: A full spin Hamiltonian approach and quantum chemical calculations.* Yamane, T.; Sugisaki, K.; Matsuoka, H.; Sato, K.; Toyota, K.; Shiomi, D.; Takui, T., *Dalton Transactions*, **2018**, 47, 16429–16444; DOI: 10.1039/C8DT02988A
23. [OCU-5] *Reversible solution π-dimerization and long multicenter bonding in a stable phenoxyl radical.* Bonanno, N. M.; Poddutoori, P. K.; Sato, K.; Sugisaki, K.; Takui, T.; Lough, A. J.; Lemaire, M. T., *Chemistry A European Journal*, **2018**, 24, 14906–14910; DOI: 10.1002/chem.20182204
24. [OCU-4] *Fe-transferrins or their homologues in ex-vivo mushrooms as identified by ESR spectroscopy and quantum chemical calculations: A full spin-Hamiltonian approach for*

the ferric sextet state with intermediate zero-field splitting parameters. Nakazawa, S.; Kanno, T.; Sugisaki, K.; Kameya, H.; Matsui, M.; Ukai, M.; Sato, K.; Takui, T., *Food Chemistry*, **2018**, 266, 24–30; DOI: 10.1016/j.foodchem.2018.05.092

25. [OCU-3] *Using optimal control methods with constraints to generate singlet states in NMR,* Rodin, B.A. ; Kiryutin, A. ; Yurkovskaya, A.V. ; Ivanov, K.L. Yamamoto, S. ; Sato, K. ; Takui, T., *Journal of Magnetic Resonance*, **2018**, 291, 14-22. DOI: 10.1016/j.jmr.2018.03.005

26. [OCU-2] *Charge-transfer character drives Möbius antiaromaticity in the excited triplet state of twisted [28]hexaphyrin.* Ema, F.; Tanabe, M.; Saito, S.; Yoneda, T.; Sugisaki, K.; Tachikawa, T.; Akimoto, S.; Yamauchi, S.; Sato, K.; Osuka, A.; Takui, T.; Kobori, Y. *The Journal of Physical Chemistry Letters*, **2018**, 9, 2685–2690; DOI: 10.1021/acs.jpclett.8b00740

27. [OCU-1] *Trioxotriangulene: Air- and Thermally Stable Organic Carbon-centered Neutral π-Radical without Steric Protection,* Yasushi, M. ; Murata, T.; Ueda, A.; Yamada, C.; Kanzaki, Y.; Shiomi, D.; Sato, K.; Takui, T., *Bull. Chem. Soc. Japan,* **2018**, 91, 922-931. DOI: 10.1246/bcsj.20180074

Reference Materials

Presentations (by S. Hill's, M. Affronte's, and T. Takui's Group)

Presentations by S. Hill and his Group

Invited talk: *Probing Electron-Nuclear Spin Interactions via Broadband Pulsed EPR*, virtual presentation at the Intercontinental NMR Conference on Methods and Applications (ICONS2021), Feb. 10 – 12, 2021.

Invited talk: *Molecular Spins for Next Generation Quantum Technologies*, virtual presentation at the Workshop on Quantum Materials, University of South Florida, Jan. 29, 2021.

Invited talk: *Magnetic Quantum Materials and High Field Electron Spin Resonance*, at the Workshop on Quantum Science, Eddleman Quantum Institute (EQI), UCLA Luskin Conference Center, CA, Mar. 6 – 8, 2020.

Invited talk: *Molecular Spins for Next Generation Quantum Technologies*, at the Magnetism in North America (MAGNA) Conference, St. Simons Island, GA, Feb. 21 – 24, 2020.

Invited talk: *High-Frequency EPR Investigations of Spins in Molecular Systems: Recent Advances at the National High Magnetic Field Laboratory*, at the International Workshop in Spin in Molecular Systems: Theory and Application (SiMS2019), IISc Bangalore, India, Dec. 2 – 4, 2019.

Invited talk: *Molecular Lanthanide Spins for Quantum Technologies*, at the 2nd Conference on Modern Trends in Molecular Magnetism (MTMM 2019), IISER Bhopal, India, Nov. 27 – 30, 2019.

Invited talk: *Molecular lanthanide spins for quantum technologies*, at the 62nd Convention of the Polish Chemical Society – Celebrating the 100 Year Anniversary of the Society, Warsaw, Poland, Sept. 2 – 6, 2019.

Invited talk: *High-Frequency EPR Investigations of Coordination Complexes: Recent Advances at the NHMFL*, at the 6th Awaji International Workshop on "Electron Spin Science & Technology: Biological and Materials Science Oriented Applications" (6th AWEST 2019), Awaji Island, Japan, June 16 – 19, 2019.

Invited talk: *EPR Studies of Molecular Spin Qubits*, at the 12th European School on Molecular Nanoscience, Elche (Alicante), Spain, May 19 – 24, 2019.

Invited talk: *High-frequency EPR studies of exchange-coupled single-molecule magnets: possible routes to molecule-based quantum technologies*, at the ACS National Meeting and Exposition, Orlando, FL, March 31 – April 4, 2019.

Invited talk: *Molecular Lanthanide Spins for Quantum Technologies*, Rare Earth Institute of Quantum Science (REIQS) Workshop on Transformative Applications of Rare-Earth Elements and Quantum Phenomenon, UCLA Luskin Conference Center, Mar. 15 to 17, 2019.

Invited talk: *EPR Studies of Metalorganic Lanthanide Sandwich Complexes: New Routes to Molecular Spin Qubits*, 5th International Workshop on Novel Magnetic and Multifunctional Materials (5IWNMMM), Institute of Materials Science, Vietnam Academy of Science, Hanoi, Vietnam, Jan. 9 to 12, 2019.

Keynote Lecture: *An Integrated Magnetic Resonance Investigation of Metal-Metal Bonded Systems: Potential New Routes to Single-Molecule Magnets*, 3rd Joint Asia Pacific EPR/ESR Society (APES) and International EPR Society Conference, University of Queensland, Brisbane, Australia, Sept. 23 to 27, 2018.

Invited talk: *Molecular Nanomagnetism Studies Using High-Field Electron Paramagnetic Resonance*, Workshop on advanced nanomagnetism characterization, University of Campinas, Campinas, Brazil, Aug. 30-31, 2018.

Invited talk: *Molecular Lanthanide Spins for Quantum Technologies*, at 2018 Gordon Research Conference on Conductivity and Magnetism in Molecular Materials, August 12 to 17, 2018, Bryant College, RI.

Keynote Lecture: *Molecular Lanthanide Spins for Quantum Technologies*, at International Conference on Coordination Chemistry (ICCC), July 30 to August 4, 2018, Sendai, Japan.

Invited talk: *Molecular Lanthanide Spins for Quantum Technologies*, at International Conference on Magnetism, July 15 to 20, 2018, San Francisco, CA.

Seminar: *Molecular Spins for Next Generation Quantum Technologies*, remote seminar via Zoom, College of Chemistry, University of California Berkeley, Berkeley, CA, November 6, 2020.

Seminar: *Molecular Lanthanide Spins for Next Generation Quantum Technologies*, remote seminar via Zoom, Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel, May 7, 2020.

Colloquium: *Molecular Spins for Next Generation Quantum Technologies*, Department of Physics, University of California at Riverside, Riverside, CA, January 23, 2020.

Seminar: *Molecular Spins for Quantum Computation*, Quantum Matter Working Group – Investigating Problems in Quantum Materials, Institute for Materials Science, Los Alamos National Lab, July 18, 2019.

Seminar: *Very High-Field/Frequency EPR Studies of Orbitally Degenerate Transition Metal Ions*, Department of Chemistry, Danish Technical University, Copenhagen, Denmark, October 25, 2018.

Seminar: *Very High-Field/Frequency EPR Studies of Orbitally Degenerate Transition Metal Ions*, Department of Chemistry, University of Copenhagen, Denmark, October 24, 2018.

Seminar: *Lanthanide Molecular Spins for Quantum Technologies*, Physical, Theoretical &

Inorganic Chemistry seminar, School of Chemistry, University of Melbourne, Australia, October 3, 2018.

Seminar: *Lanthanide Molecular Spins for Quantum Technologies*, Department of Physics, University of New South Wales, Sydney, Australia, October 2, 2018.

Seminar: *Lanthanide Molecular Spins for Quantum Technologies*, Department of Chemistry, University of Tennessee, Knoxville, TN, February 22, 2018.

Seminar: *Electro-Nuclear Clock Transitions in Lanthanide Molecular Spin Qubits*, Department of Physics, Colorado State University, Fort Collins, CO, January 26, 2018.

Contributed talk: *Investigating decoherence pathways in Ho $(W_5O_{18})_2$ via magneto-infrared spectroscopy*, Avery Blockmon,* Kendall Hughey, Ken O'Neal, Yan Duan, Aman Ullah, Luis Moreno, Mykhaylo Ozerov, Stephen Hill, Alejandro Gaita-Arino, Eugenio Coronado, Janice Musfeldt, at the ACS National Meeting and Exposition, Orlando, FL, March 31 – April 4, 2019.

Contributed talk: *Combined THz and Pulsed EPR studies on a Yb(III) Single Ion Magnet*, Jonathan Marbey*, Stergios Piligkos, Joscha Nehrkorn, Mykhaylo Ozerov, Stephen Hill, American Physical Society March Meeting, Boston, MA, Mar. 4-8, 2019.

Contributed talk: *EPR Studies of Lanthanide-Lanthanide Interactions in Triple-Decker Molecular Complexes*, Dorsa Komijani,* A. Ghirri, C. Bonizzoni, S. Klyatskaya, E. Moreno-Pineda, M. Ruben, M. Affronte, S. Hill, American Physical Society March Meeting, Los Angeles, CA, Mar. 5-9, 2018.

Poster presentation: *Radical-lanthanide ferromagnetic interaction in a Dy^{III} bis-phthalocyaninato complex*, Robert Stewart,* Dorsa Komijani, Miguel Gakiya, Mike Shatruk, Alberto Ghirri, Claudio Bonizzoni, Svetlana Klyatskaya, Eufemio Moreno-Pineda, Mario Reuben, Marco Affronte, Stephen Hill, Southeastern Section APS Meeting (Remote), Nov. 5, 2020.

Poster presentation: *Spectroscopic Evidence of Spin-Phonon Coupling in an Yb(trensal) Single-Molecule Magnet*, Jonathan Marbey,* Jon Kragskow, Joscha Nehrkorn, Mykhaylo Ozerov, Nick Chilton, Stergios Piligikos, Stephen Hill, at the Magnetism in North America (MAGNA) Conference, St. Simons Island, GA, Feb. 21 – 24, 2020.

Poster presentation: *Suppression of 2nd Order Axial Anisotropy in a Trigonal $[Mn^{III}]_3$ Complex*, Jonathan J. Marbey,* Pei-Rung Gan, En-Che Yang, Stephen Hill, 16th International Conference on Molecule-Based Magnets (ICMM), Rio de Janeiro, Brazil, Sept. 1 to 5, 2018.

Poster presentation: *Combined THz and Pulsed EPR studies on a Yb(III) Single Ion Magnet,* Jonathan Marbey,* Stergios Piligikos, Joscha Nehrkorn, Mykhaylo Ozerov, Stephen Hill, 3rd Gordon Research Conference on Conductivity and Magnetism in Molecular Materials, Bryant College, RI, Aug. 12-17, 2018.

Poster presentation: *Double Quantum Transitions in Ni(II) Systems,* Robert Goff,* Samuel M. Greer, Jonathon Marbey, Andrew Ozarowski, Stephen Hill, 46th Southeastern Magnetic Resonance Conference, Tallahassee, FL, Oct. 27-29, 2017.

Poster presentation: *EPR Study of Lanthanide (III) Double- and Triple-Decker Phthalocyanine Complexes,* Dorsa Komijani,* A. Ghirri, C. Bonizzoni, S. Klyatskaya, E. Moreno-Pineda, and M. Ruben, M. Affronte, S. Hill, 46th Southeastern Magnetic Resonance Conference, Tallahassee, FL, Oct. 27-29, 2017.

Presentations of the project results at International events by M. Affronte and his Group:

2019: Invited talk at Joint European Magnetic Symposia, Uppsala SW, August 26-30, 2019.

2019: Keynote presentation at The 6th AWEST, June 16-20, in Awaji Island, Japan.

2019: 5th International Workshop on Novel Magnetism and Multifunctional Materials Hanoi Vietnam Jan 9th-12th

2018: Invited talk at The 16th International Conference on Molecular Magnets, Rio de Janeiro, Brazil, Sept. 3-6, 2018.

2019: Results have been also presented by Dr. Alberto Ghirri and Dr. Claudio Bonizzoni in 6 more International workshops. Dr. Bonizzoni also participated to the Workshop NMMM in Hanoi in 2019.

2021: The performances of the *Active Technologies* Arb Rider AWG with our setup in Modena have been presented by Dr. Claudio Bonizzoni (CNR Modena) in a webinar on "Quantum Computing with AWG" on 25th February 2021 10:00 AM PST time for US customers. More than 180 participants attended this presentation of the new generation of AWG by Active Technologies for the North America area (rebranded for Berkeley Nucleonics as distributor). This testifies interest of our technological achievements to the specialized communities.

<u>Presentations by T. Takui (only major ones):</u>

Invited Lecture: The 5th International Workshop on Novel Magnetic and Multifunctional Materials, Hanoi, Vietnam, Jan. 9-12, 2019.

Plenary Lecture, Rising Stars Symposium at The 16th International Conference on Molecular Magnets, Rio de Janeiro, Brazil, Sept. 3-6, 2018.

Invited Lecture, The VIII International Conference "High Spin Molecules and Molecular Magnets", Astrakhan, Russia, Sept. 17-21, 2018.

Change in Research Objectives: None

Change in Program Officer: Dr. Christopher Vergien, L Maj USAF PACAF AFOSR/AFMC/AFRL/AFOSR/IOA

Extensions Granted/Milestones Slipped: None

End of Report.