IBS CONFERENCES 2019

# IBS Conference on
# Quantum Nanoscience

**September 25th - 27th, 2019**

Lee SamBong Hall,
Ewha Womans University, Seoul

## ABSTRACT BOOK

# PROGRAM

## Day — 1 —

**Wednesday,** September 25, 2019

| | |
|---|---|
| 09:00-09:15 | **Participants Registration** |
| 09:15-09:30 | **Opening Remarks from Andreas Heinrich** |
| | **Session 1**<br>What is Quantum Nanoscience? |
| 09:30-10:00 | General Introduction<br>Andreas Heinrich |
| 10:00-10:30 | William D. Oliver |
| 10:30-11:00 | Yonuk Chong |
| 11:00-11:30 | Andrew Dzurak |
| 11:30-13:00 | **Lunch** |
| | **Session 2**<br>Quantum Sensing with Nanoscale Systems |
| 13:00-13:45 | General Introduction<br>Ania Jayich |
| 13:45-14:15 | Jörg Wrachtrup |
| 14:15-14:30 | Sangyun Lee |
| 14:30-15:00 | **Coffee Break** |
| 15:00-15:15 | Jungbae Yoon |
| 15:15-15:30 | Kyunghoon Jung |
| 15:30-16:00 | Donghun Lee |
| 16:30-17:30 | **QNS Building Tour** |
| 18:00-20:00 | **Official Dinner** |

## Day — 2 —

**Thursday,** September 26, 2019

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| 09:00 - 09:15 | **Coffee break** |
| | **Session 3**<br>Theory Challenges in Quantum Nanoscience |
| 09:15-10:00 | General Introduction<br>Daniel Loss |
| 10:00-10:30 | Jelena Klinovaja |
| 10:30-11:00 | Martin B. Plenio |
| 11:00-11:15 | Stanislav Avdoshenko |
| 11:15-11:30 | Hosung Seo |
| 11:30-13:00 | **Lunch** |
| 13:00-14:00 | **Poster Session (Daesan Gallery)** |
| 14:00-14:30 | **Coffee Break** |
| 14:30-15:30 | **Poster Session (Daesan Gallery)** |
| | **QNS Dedication Ceremony** |
| 16:00-16:15 | Ewha President |
| 16:15-16:30 | IBS Acting President |
| 16:30-17:30 | Don Eigler |
| 17:30-18:00 | **Art Contest Awards** |
| 18:30-22:00 | **Excursion** |

## Day — 3 —

**Friday,** September 27, 2019

| | |
|---|---|
| 09:00 - 09:15 | **Coffee break** |
| | **Session 4**<br>Quantum Surface Science at the Nanoscale |
| 09:15-10:00 | General Introduction<br>Taeyoung Choi |
| 10:00-10:30 | Harald Brune |
| 10:30-10:45 | Deungjang Choi |
| 10:45-11:00 | Saiful Islam |
| 11:00-11:40 | Fabio Donati |
| 11:40-13:00 | **Lunch** |
| | **Session 5**<br>A Chemical Route to Quantum Nanoscience |
| 13:00-13:45 | General Introduction<br>Roberta Sessoli |
| 13:45-14:05 | Yujeong Bae |
| 14:05-14:25 | Taner Esat |
| 14:25-15:00 | **Coffee Break** |
| 15:00-15:20 | Mykola Telychko |
| 15:20-15:40 | Ruoning Li |
| 15:40-16:00 | Danna Freedman |
| 16:00-16:30 | Wolfgang Wernsdorfer |
| 16:30-17:00 | Arzhang Ardavan |
| 17:00-17:15 | **Poster Awards** |
| 17:15-17:30 | **Closing remarks from Andreas Heinrich** |
| 17:30-17:45 | **Group Photo** |



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2019 IBS Conference on Quantum Nanoscience

# COMMITTEE MEMBERS

## Organizing Committee

### International

**Andreas Heinrich**
IBS Center for Quantum Nanoscience, Seoul, Korea (chair)

**Roberta Sessoli**
University of Florence, Italy

**Daniel Loss**
University of Basel, Switzerland

**Lieven Vandersypen**
Delft University, The Netherlands

**Ania Jayich**
University of California at Santa Barbara, USA

**Andrea Morello**
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**Young Kuk**
Daegu Gyeongbuk Institute of Science & Technology

**Yonuk Chong**
Korea Research Institute of Science and Standards, Daejeon, Korea

**Donghun Lee**
Korea University, Seoul, Korea



## Welcome Message

Bringing the quantum nanoscience community together

Welcome to the first international conference on quantum nanoscience.

The organizers believe that it's time that we bridge our various specialties as an overarching community of quantum nanoscience researchers. With the growth of the number of researchers, funding, and importance of the wide-ranging impact of quantum coherent functionality the timing to do this is now.

Our goal for this conference is to share as a field in order for us to recognize the collaboration opportunities that can span the comprehensive nature of quantum nanoscience. Whether this is your first time to Korea or your tenth, we hope you'll enjoy the beauty of Seoul in the Fall by going with your colleagues for walks full of discussions or alight in the many excellent cafes our city has to offer.

Thank you for joining this exciting first conference on quantum nanoscience and being an important member of this growing community.

Chair

Director,
IBS Center for Quantum Nanoscience,
Seoul, Korea

IBS Conference on

# Quantum Nanoscience

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1
DAY

**Wednesday,** September 25, 2019

- SESSION **1**
- SESSION **2**

IBS Conference on

# Quantum Nanoscience

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## ABSTRACT BOOK



# SESSION 01

## What is Quantum Nanoscience?

Quantum nanoscience is the intersection of quantum science and nanoscience. In this session, we will describe a working definition as well as interesting concepts and examples of quantum systems at the nanoscale that enable quantum-coherent functionality.

**Andreas Heinrich** invited

*Director of IBS Center for Quantum Nanoscience, Seoul, South Korea*

"What is Quantum Nanoscience?"

**William D. Oliver** invited

*MIT Department of Physics and Director at MIT Lincoln Laboratory, Boston, USA*

"Quantum Nanoscience and Engineering of Superconducting Qubits"

**Yonuk Chong** invited

*University of Science and Technology (UST), South Korea*

"Brief summary of the quantum computing strategic planning 2017-2018, and quantum computing research program in Korea 2019"

**Andrew Dzurak** invited

*School of Electrical Engineering and Telecommunications, UNSW, Australia*

"Silicon-based quantum computing: The path from the laboratory to industrial manufacture"

# What is Quantum Nanoscience?

**Andreas Heinrich**

*Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea.*
*Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea.*
**heinrich.andreas@qns.science*

Quantum mechanics was born out of the necessity to describe the physics of particles, atoms and molecules. At the scale of nanometers, the quantum uncertainty principle completely rules the static and dynamic properties of matter and fields. Does this mean that all of quantum physics is “nano”, and all of nanoscience is “quantum”? We suggest, provocatively, that the answer should be “no”. We propose instead an aspirational definition of Quantum Nanoscience: the search for quantum coherence-enhanced functionality at the nanoscale, see figure 1. This definition helps identify a field of research where quantum physics and nanoscience are not just a mutual necessity, but a mutual benefit.

Quantum computing is a clear example where coherence-enhanced functionality is key to providing a radical departure from the mere operation of nanometer-scale devices. Semiconductors can host quantum information encoded in buried dopant atoms or quantum dots. Purely superconducting qubits, while physically much larger than the nanoscale, require accurate control over atomic-scale defects and nanometer-thin Josephson junctions. Bottom-up strategies for building quantum bits include chemically-synthesized magnetic molecules and atomic-scale devices built by scanning probes.

Coherent quantum states are extremely sensitive to their environment. This can be exploited to design quantum-enhanced sensors, capable of detecting e.g. magnetic and electric fields, or temperature, with unprecedented sensitivity. Their nanometer size allows the sensing to occur at the scale of molecules or cells, of great interest for chemical or medical applications.

We believe that the time is right to start an international conference on Quantum Nanoscience, since the interest in the community has strongly increased over the last decade and scientists now believe that there is great value in harnessing the quantum-coherent behavior of nanoscale systems.

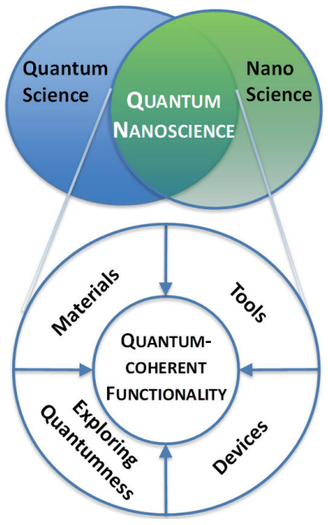


**Figure 1.** Quantum nanoscience strives for quantum-coherent functionality of nanostructures.



Notes

# Quantum Nanoscience and Engineering of Superconducting Qubits

**William D. Oliver**
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*Research Laboratory of Electronics, and MIT Lincoln Laboratory*
*Massachusetts Institute of Technology*
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Superconducting qubits are coherent artificial atoms assembled from electrical circuit elements and microwave optical components[1]. Their lithographic scalability, compatibility with microwave control, and operability at nanosecond time scales all converge to make the superconducting qubit a highly attractive candidate for the constituent logical elements of a quantum information processor[2,3]. In this talk, we review the promise, progress, and challenges of engineering systems of superconducting qubits, with an emphasis on the important role quantum nanoscience will play in this endeavor[4,5].

**References**

[1] P. Krantz, M. Kjaergaard, F. Yan, T.P. Orlando, S. Gustavsson, W.D. Oliver, "A Quantum Engineer's Guide to Superconducting Qubits," Appl. Phys. Reviews 6, 021318 (2019) | arXiv:1904.06560
[2] M. Kjaergaard, M.E. Schwartz, J. Braumueller, P. Krantz, J.I-J. Wang, S. Gustavsson, W.D. Oliver, "Superconducting qubits: Current state of play," arXiv:1905.13641
[3] D. Rosenberg, D.K. Kim, R. Das, D. Yost, S. Gustavsson, D. Hover, P. Krantz, A. Melville, L. Racz, G.O. Samach, S.J. Weber, F. Yan, J. Yoder, A.J. Kerman, W.D. Oliver, "3D integrated superconducting qubits," npj Quantum Information 3, 42 (2017) | arXiv:1706.04116
[4] W.D. Oliver and P.B. Welander, "Materials in Superconducting Qubits," MRS Bulletin 38, 816-825 (2013)
[5] J.I-J. Wang, D. Rodan-Legrain, L. Bretheau, D.L. Campbell, B. Kannan, D. Kim, M. Kjaergaard, P. Krantz, G.O. Samach, F. Yan, J.L. Yoder, K. Watanabe, T. Taniguchi, T. P. Orlando, S. Gustavsson, P. Jarillo-Herrero, W.D. Oliver, "Coherent control of a hybrid superconducting circuit made with graphene-based van der Waals heterostructures," Nature Nanotechnology 14, 120-125 (2019) | arXiv:1809.05215



Notes

# Brief summary of the quantum computing strategic planning 2017-2018, and quantum computing research program in Korea 2019

**Yonuk Chong**
*Korea Research Institute of Standards and Science (KRISS), Daejeon 34113, Korea*
*University of Science and Technology (UST), Daejeon 34113, Korea*
**E-mail:yonuk@kriss.re.kr*

In this short talk, I will provide a brief summary of our (KRISS) past activities on the strategic planning of the quantum computing research in Korea. In 2017-2018, a team of scientists in KRISS tried to listen to the community's diverse opinions about what is really relevant to quantum computing research, what we should do first, and how we may do it best, and then tried to summarize them to generate an open document which is readable by general audience. The final document was neither satisfying nor complete, but anyway a short document was published in mid-2018. In addition, as a separate topic, I will briefly introduce the first quantum computing research program in Korea launched in 2019. Finally, for the scientific part, I will briefly introduce our own research group's activity on superconducting quantum computing research which is on-going in KRISS.

* All these presentation contents are purely the opinion of the KRISS scientists. None of this presentation represents, or related to, any government policies or activities.

# Silicon-based quantum computing: The path from the laboratory to industrial manufacture

**Andrew Dzurak**
*UNSW – Sydney, Australia*
**E-mail: a.dzurak@unsw.edu.au*

In this talk I will give an overview of the development of silicon-based quantum computing (QC), from the basic science through to its prospects for industrial-scale commercialization based on CMOS manufacturing. I begin with Kane's original proposal[1] for a silicon quantum computer, conceived at UNSW in 1998, based on single donor atoms in silicon, and will review the first demonstrations of such qubits, using both electron spins[2,3] and nuclear spins[4]. I then discuss the development of SiMOS quantum dot qubits, including the demonstration of single-electron occupancy[5], high-fidelity single-qubit gates[6], and the first demonstration of a two-qubit logic gate in silicon[7], together with the most recent assessments of silicon qubit fidelities[9,10]. I will also explore the technical issues related to scaling a silicon-CMOS based quantum processor[8] up to the millions of qubits that will be required for fault-tolerant QC. Finally, I will discuss the broader effort in quantum information in Australia and a new company – Silicon Quantum Computing P/L – which was established last year to commercialize Australian research in this field.

**Acknowledgments**
We acknowledge support from the US Army Research Office (W911NF-17-1-0198), the Australian Research Council (CE11E0001017), and the NSW Node of the Australian National Fabrication Facility. The views and conclusions contained in this document are those of the author and should not be interpreted as representing the official policies, either expressed or implied, of the Army Research Office or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein.

**References**

[1] B. E. Kane, Nature 393, 133 (1998).
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[3] J.J. Pla et al., Nature 489, 541 (2012).
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[6] M. Veldhorst et al., Nature Nanotechnology 9, 981 (2014).
[7] M. Veldhorst et al., Nature 526, 410 (2015).
[8] M. Veldhorst et al., Nature Communications 8, 1766 (2017).
[9] H. Yang et al., Nature Electronics 2, 151 (2019).
[10] W. Huang et al., arXiv.1805.05027, to appear in Nature, 13 May (2019).

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## ABSTRACT BOOK



# SESSION 02

## Quantum Sensing with Nanoscale Systems

Quantum systems can make incredibly sensitive sensors of their environment. At the nanoscale this can be combined with high spatial resolution.

**Ania Jayich** invited

*Department of Physics, UCSB, USA*

"Nitrogen-vacancy center spins in diamond for quantum technologies: progress and challenges"

**Jörg Wrachtrup** invited

*Physics Department of University of Stuttgart, Germany*

"Analyzing chemical and structural composition by nanoscale NMR"

**Sangyun Lee**

*Physikalisches Institute and Research Center SCOPE and Integrated Quantum Science and Technology (IQST), University of Stuttgart, Germany*

"Electrical charge state manipulation of single silicon vacancies in a silicon carbide quantum optoelectronic device"

**Jungbae Yoon**

*Korea University, Korea*

"Quantum Sensing Based on Diamond NV centers and its application for bio samples"

**Kyunghoon Jung**

*Department of Physics and Astronomy, and Institute of Applied Physics, Seoul National University, Korea*

"Deep Learning Approach for Efficient Spectral Decomposition of Spin Resonance to Detect Nuclear Spins in Diamond"

**Donghun Lee** invited

*Physics Department of Korea University, South Korea*

"Sensing strain and magnetic field with quantum point defects"

# Nitrogen-vacancy center spins in diamond for quantum technologies: progress and challenges

**Dolev Bluvstein, Zhiran Zhang, Claire McLellan, Tim Eichhorn, Alec Jenkins, Simon Meynell, Susanne Baumann, and Ania Bleszynski Jayich***

*Department of Physics, University of California, Santa Barbara, CA 93106, USA*

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The nitrogen vacancy (NV) center defect in diamond is a powerful quantum-enabled technology, in particular in the realm of sensing and imaging with ultra-high spatial resolution. In the first part of this talk, I discuss recent experiments on NV-based, nanoscale imaging of condensed matter systems. The performance of these solid-state quantum sensors is highly dependent on their quantum coherence and charge-state stability, which are sensitive to their local environment. Surfaces are an important part of the defect's environment, in particular when targeting high spatial resolution sensing, which necessitates close proximity between the sensor and target. To identify and mitigate the deleterious environmental effects, I discuss several materials-based and quantum-control approaches. Specifically, I discuss the formation of highly-coherent NV centers via a gentle, bottom-up method of nitrogen delta-doping during chemical vapor deposition growth of diamond thin films followed by low energy (~ 150 keV) electron irradiation. I present measurements of the density and coherence properties of the NV centers formed in this way as a function of growth and irradiation parameters[1]. In the second part of the talk, I discuss the spin and charge state properties of shallow NV centers, and introduce techniques to mitigate decoherence due to paramagnetic surface spins[2] as well as charge state instabilities near surfaces[3]. These approaches to improved sensors will ultimately enable truly nanoscale spatial resolution imaging of magnetic, electric, and thermal fields in a variety of condensed matter and biological systems.

**References**

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[2] "Extending the Quantum Coherence of a Near-Surface Qubit by Coherently Driving the Paramagnetic Surface Environment", Dolev Bluvstein, Zhiran Zhang, Claire A. McLellan, Nicolas R. Williams, Ania C. Bleszynski Jayich, https://arxiv.org/abs/ 1905.06405

[3] "Identifying and mitigating charge instabilities in shallow diamond nitrogen-vacancy centers", D. Bluvstein, Z. Zhang, A. C. Bleszynski Jayich, Phys. Rev. Lett. 122, 076101 (2019)



Notes

# Analyzing chemical and structural composition by nanoscale NMR

**Jörg Wrachtrup**
*3rd Institutes of Physics and Centre for Applied Quantum Technologies, University of Stuttgart, Stuttgart, Germany*
**E-mail: j.wrachtrup@pi3.uni-stuttgart.de*

Nuclear magnetic resonance (NMR) is one of the mostly used analytical techniques in material science, biology and medicine. It provides unprecedented insight into structure and chemical composition. Yet, its sensitivity is low and hence NMR has been restricted to measuring macroscopic sample volumes so far. With the invent of nanoscale quantum sensing, however, NMR of a few and even single nuclear spins has become feasible[1]. A long standing challenge has been to achieve high spectral resolution. By using quantum memories or classical correlation methods, NMR on small sample volumes with sub-Hz spectral resolution has become feasible, unleashing the full potential of NMR on the nanoscale[2]. The talk will describe recent progress utilizing quantum algorithms to improve nanoscale NMR and show its use in measuring structures and dynamical processes[3,4].

**References**

[1] T. Staudacher, F. Shi, S. Pezzagna et al. Science 339, 561 (2013)
[2] N. Aslam, M. Pfender et al. Science 357, 67 (2017)
[3] F. Shi, Q. Zhang et al. Science 347, 1135 (2015)
[4] T. Staudacher, N. Raatz, et al. Nature Com. 6, 8527 (2015)

Notes

# Electrical charge state manipulation of single silicon vacancies in a silicon carbide quantum optoelectronic device

**Matthias Widmann[1*], Matthias Niethammer[1], Dmitry Yu. Fedyanin[2], Igor A. Khramtsov[2], Torsten Rendler[1], Ian D. Booker[3], Jawad Ul Hassan[3], Naoya Morioka[1], Roland Nagy[1], Yu-Chen Chen[1], Ivan G. Ivanov[3], Nguyen Tien Son[3], Takeshi Ohshima[4], Michel Bockstedte[5,6], Adam Gali7,8, Cristian Bonato[9], Sang-Yun Lee[1,10], and Jörg Wrachtrup[1]**

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*[5] Department Chemistry and Physics of Materials, University of Salzburg, Jakob-Haringer-Str. 2a, 5020 Salzburg, Austria*

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*[7] Wigner Research Centre for Physics, Hungarian Academy of Sciences, PO. Box 49, H-1525 Budapest, Hungary*

*[8] Department of Atomic Physics, Budapest University of Technology and Economics, Budafoki út 8., H-1111 Budapest, Hungary*

*[9] Institute of Photonics and Quantum Sciences, SUPA, Heriot-Watt University, Edinburgh EH14 4AS, UK*

*[10] Center for Quantum Information, Korea Institute of Science and Technology, Seoul, 02792, Republic of Korea*

Atomic-scale defects with stable fluorescence and long-lived spins are promising for quantum sensing and quantum information. Such point defects can exist in different charge states, each of them with its distinct optical and spin properties that can be possibly exploited for different applications. The charge state, however, can fluctuate depending on the electronic environment and on the electromagnetic excitation used for control and detection. Here, we investigate electrical charge state manipulation of individual silicon vacancies in silicon carbide, one of the leading contenders for quantum technologies. We demonstrate how to manipulate the charge state of single silicon vacancies in a silicon carbide p-i-n diode by applying a bias voltage. We also show that control of electronic environment defined by the doping profile and distribution of other defects is a key for charge state control at the nano-scale, which is evidenced by the enhanced photon emission rate under certain conditions. Our findings open a way for deterministic control over the charge state of atomic-scale defects in quantum devices and novel techniques for monitoring doping profile and voltage sensing in microscopic devices.

# Quantum Sensing Based on Diamond NV centers and its application for bio samples

**Jungbae Yoon*, Kihwan Kim, Yuhan Lee, Myeongwon Lee, and Donghun Lee**
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There are increasing demands on highly sensitive magnetic field sensors both in fundamental research and industrial fields. Diamond Nitrogen-Vacancy (NV) center is an atomic-scale quantum sensor that can meet the demands as it provides high magnetic field sensitivity over wide bandwidth of detection frequency (e.g. sensitivity < nT/Hz^1/2 and bandwidth DC ~ 1 GHz). It also provides nanometer scale spatial resolution suitable for high resolution imaging applications and miniaturized sensing devices. Moreover, as NV center even works at room temperature and is non-toxic, it is one of the powerful candidate of the nano-scale sensor for the biological or medical application. We are building up a setup for widefield view image to acquire the magnetic field distribution of magnetic samples such as magnetic nanowire. The setup and technique are going to be adapted from solid state sample to the magnetic bio samples afterwards.

**References**

[1] M. Lee, et al., Nanotechnology 29, 405502 (2018)

Notes

# Deep Learning Approach for Efficient Spectral Decomposition of Spin Resonance to Detect Nuclear Spins in Diamond

**Kyunghoon Jung*, Jiwon Yun, Kiho Kim, and Dohun Kim**
*Department of Physics and Astronomy, and Institute of Applied Physics, Seoul National University, Seoul 08826, Korea*
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We present a novel machine learning approach to detect individual nuclear spins in diamond. Localizing individual nuclear spins is the essential step to build coherently controllable spin resisters, which provides us with a robust base for quantum network, quantum simulation platform, or quantum memory. So far, to find these nuclear spins, researchers have no alternative but to analyze spectrums manually so that there is no guarantee to fully find those existent spins and to obtain accurate coupling parameters, especially due to the experimental noise and its own complexity of signals.

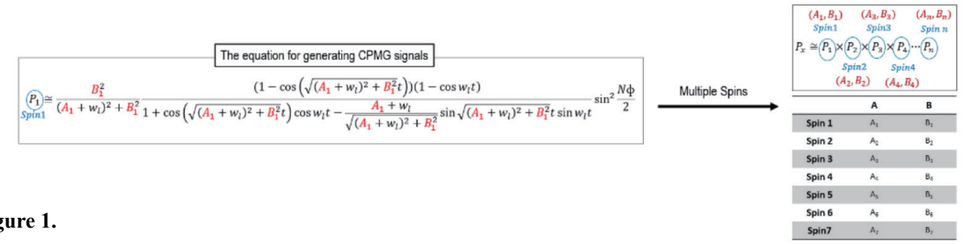


**Figure 1.**

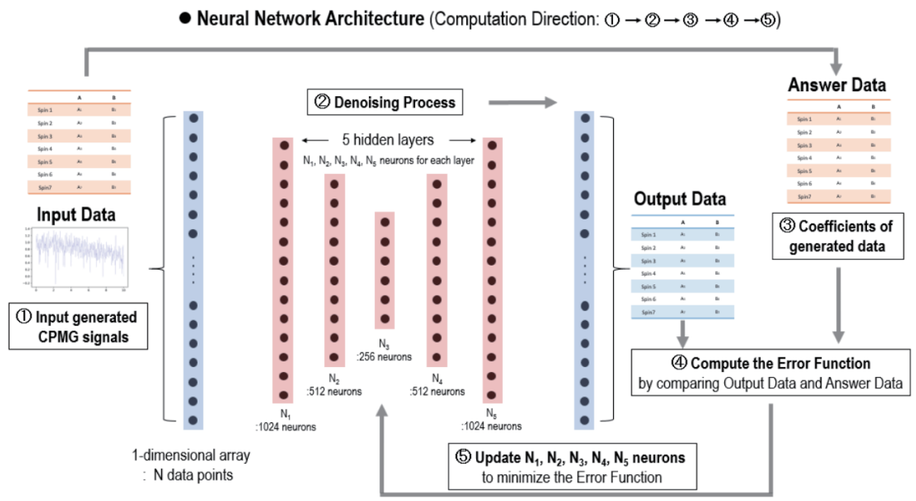


**Figure 2.** Here we introduce machine learning algorithm to automatically denoise and decompose the spectral data to identify the location and to specify the characteristic of nuclear spins in diamond.

**Acknowledgement**
The authors thank T.H. Taminiau for sharing their experimental CPMG data, which provides us with the way to implement the cross-check regarding the performance of trained deep learning model.

**References**

[1] T. H. Taminiau, Detection and Control of Individual Nuclear Spins Using a Weakly Coupled Electron Spin, Phys. Rev. Lett. 109, 137602 (2012)
[2] R. Santagati, Magnetic-Field Learning Using a Single Electronic Spin in Diamond with One-Photon Readout at Room Temperature, Phys. Rev. X 9, 021019 (2019)

Notes

# Sensing strain and magnetic field with quantum point defects

**Donghun Lee**
*Department of Physics, Korea University, Seoul, South Korea*
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Various quantum systems have been studied in the field of quantum information, quantum network and quantum metrology. Among the systems, atom-like point defect in diamond crystal has got great attention due to its unique properties for quantum applications. Particularly nitrogen-vacancy (NV) centers in diamond are solid-state spin-qubits possessing remarkable quantum properties applicable to various fields including quantum information science and quantum sensing. For instance, its atomic-scale size, long spin coherence times, and high field sensitivity are suitable for nanoscale magnetometry, electrometry, thermometry and so on.

In this talk, I will introduce current efforts and progress in our lab based on quantum point defects. Two examples will be discussed; hybrid mechanical system for quantum information application and scanning probe magnetometry for quantum sensing application. First, high-quality diamond mechanical oscillator is coupled to embedded NV centers to realize hybrid quantum systems. Coherent mechanical control of NV's spin and optical properties will be demonstrated through strain associated with the resonator's mechanical motion. Second, a novel scanning probe microscope based on NV centers will be discussed. Combination of high spatial resolution and high magnetic field sensitivity enables imaging of magnetic samples such as ferromagnetic nanowires and Permalloy structures.



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IBS Conference on

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**Thursday,** September 26, 2019

SESSION **3**

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# Quantum Nanoscience

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## ABSTRACT BOOK



# SESSION 03

## Theory Challenges in Quantum Nanoscience

Quantum Nanoscience has diverse needs for theoretical investigations ranging from modelling with high precision to the investigation and understanding of quantum coherence.

**Daniel Loss** invited

*Department of Physics, University of Basel, Switzerland*

"Ge and Si Nanowires: New Platforms for Spin and Majorana Qubits"

**Jelena Klinovaja** invited

*Prof. Jelena Klinovaja Department of Physics, University of Basel, Switzerland*

"Second Order Topological Superconductivity in π-Junction Rashba Layers"

**Martin Plenio** invited

*Institute of Theoretical Physics in University of Ulm, Germany*

"Quantum Control of Quantum Systems on the Nanoscale"

**Stanislav Avdoshenko**

*Leibniz Institute for Solid State and Materials Research Dresden, Germany*

"Theoretical study of Ho atom at MgO surface: valence electrons effect"

**Hosung Seo**

*Department of Physics and Department of Energy Systems Research, Ajou University, Korea*

"First-principles theory of single-photon emitters in two dimensional crystals for quantum information science"

# Ge and Si Nanowires: New Platforms for Spin and Majorana Qubits

**Daniel Loss**
*Dept. of Phys., Univ. of Basel, Switzerland*

I will review recent theoretical results on holes in Ge and Si nanowires and their potential for quantum computing platforms. The recent discovery[1] of an electrically induced spin-orbit interaction (SOI) of Rashba-type in the low-energy hole states of Ge/Si (core/shell) nanowires provides an attractive scenario to realize spin and topological qubits. Most remarkably, similar results apply to pure Si nanowires[2], which are fully compatible with CMOS technology. Hole spins are particularly attractive since their p-wave orbitals have minimal overlap with the nuclei resulting in long coherence times. Crucially the strong direct Rashba SOI (DRSOI) is controlled by a moderate electric field applied perpendicular to the wire[1,2,3]. This enables the electrostatic control of the coupling between the hole-spin degree of freedom and the electromagnetic field along the wire. Exploiting this feature we have proposed a scalable surface code architecture obtained by combining nanowire hole-spin qubits with a novel coplanar waveguide resonator grid structure[4]. Finally, the DRSOI also opens up the door to create Majorana fermions in such Ge or Si nanowires when proximitized by a superconductor[5].

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Notes

# Second Order Topological Superconductivity in π-Junction Rashba Layers

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Recently, a lot of interest has been raised by the generalization of conventional TIs/TSCs to so-called higher order TIs/TSCs. While a conventional d-dimensional TI/TSC exhibits (d − 1)-dimensional gapless boundary modes, a d-dimensional n-th order TI/TSC hosts gapless modes at its (d − n)-dimensional boundaries. In my talk, I will consider a Josephson junction bilayer consisting of two tunnel-coupled two-dimensional electron gas layers with Rashba spin-orbit interaction, proximitized by a top and bottom s-wave superconductor with phase difference $\phi$ close to $\pi$ [1]. In the presence of a finite weak in-plane Zeeman field, the bilayer can be driven into a second order topological superconducting phase, hosting two Majorana corner states (MCSs). If $\phi=\pi$, in a rectangular geometry, these zero-energy bound states are located at two opposite corners determined by the direction of the Zeeman field. If the phase difference $\phi$ deviates from $\pi$ by a critical value, one of the two MCSs gets relocated to an adjacent corner. As the phase difference $\phi$ increases further, the system becomes trivially gapped. The obtained MCSs are robust against static and magnetic disorder.

In the second part of my talk, I will switch from non-interacting systems [1,2], in which one neglects effects of strong electron-electron interactions, to interacting systems and, thus, to exotic fractional phases. I will show that this is indeed possible and explicitly construct a two-dimensional (2D) fractional second-order TSC. I will consider a system of weakly coupled Rashba nanowires in the strong spin-orbit interaction (SOI) regime. The nanowires are arranged into two tunnel-coupled layers proximitized by a top and bottom superconductor such that the superconducting phase difference between them is $\pi$. In such a system, strong electron-electron interactions can stabilize a helical topological superconducting phase hosting Kramers partners of Z_2m parafermion edge modes, where m is an odd integer determined by the position of the chemical potential. Furthermore, upon turning on a weak in-plane magnetic field, the system is driven into a second-order topological superconducting phase hosting zero-energy Z_2m parafermion bound states localized at two opposite corners of a rectangular sample.

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Notes

# Quantum Control of Quantum Systems on the Nanoscale

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Modern developments in quantum technologies are exploring a wide range of solid state based systems as qubits for a wide variety of purposes of applications. Unlike atomic physics systems, which are operated under extreme conditions to ensure isolation from their environment, solid state based systems are by their very nature in direct contact with the environment that is constituted by uncontrolled phonon, spin and charge degrees of freedom that form part of the host material. As a result solid state qubits suffer significantly from environmental noise. In order to address this challenge a combination of material science to improve the hardware properties and of quantum control methods to further decouple the solid state qubits from their environment while maintaining desired interactions are needed to achieve the ultimate goal of practically usable coherent quantum dynamics.

In this lecture I will present potential architectures for quantum simulation based on nuclear and electron spins on diamond[1] and discuss how we can address the control issues that arise in such devices by means of quantum control techniques. Questions such as enhanced resolution and addressing of single spins[2], high fidelity quantum gates[3,4] and cooling, i.e. polarization, of spin ensembles[5,6,7] will be considered. Methods to enhance the robustness of control procedures to control errors[8,9] as well as energy efficient control schemes[10,11] will be discussed. While much of the discussion is motivated by the aim to control NV centers in diamond, the concepts and protocols describe here are equally applicable to a wide variety of solid state qubits.

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**Notes**

# Theoretical study of Ho atom at MgO surface: valence electrons effect

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Detailed electronic structure of single atomic magnets is the most crucial bit in the further understanding and design of a new generation of monatomic functional elements on surfaces and in another structural setting. Recently, the inspirational single atomic experiment with Ho on MgO surfaces brought into a new light a possibility to control and manipulate the quantum states of an atom[1,2]. However, these convincing experiments are puzzling by the insufficient theoretical description. In this contribution, we looked at the exact ab initio model for the Ho atom at MgO surface under a various level of complexity in an attempt to resolve an experimental dilemma in the reported data. The research is based on the idea of the imminent need to implement the local d - and p -shell electrons of Ho atom into the active space for proper system consideration. By doing so, we have obtained the solution which complements experimental observations without any additional assumptions.

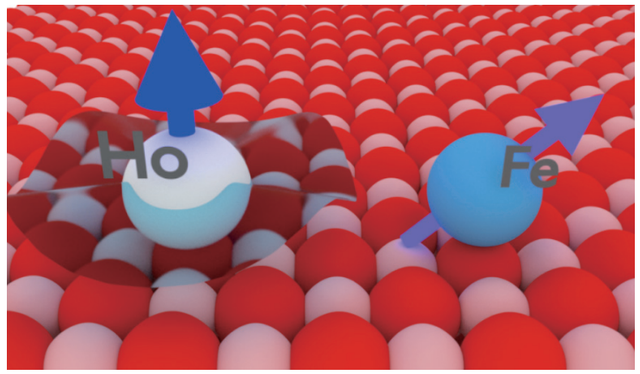


**Figure 1.** Artistic representation of a single ion EPR experiment involving a single Ho atom placed on MgO surfaces in the close proximity to Fe (sensor). Ho moment is shown as normal towards the MgO with transparent “skirt” of the dipolar field around it.

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# First-principles theory of single-photon emitters in two dimensional crystals for quantum information science

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Deep-level spin defects in wide-gap semiconductors are promising platforms for applications in quantum information processing, quantum sensing, and quantum photonics[1]. In particular, several point defects in two-dimensional materials such as h-BN have recently emerged as room-temperature single photon emitters (SPEs) with excellent optical stability and brightness[2] and potentially spin qubits[3]. In this study, we use first-principles theory to investigate the optical and spin properties of deep-level defects in two-dimensional crystals including h-BN and $MoS_2$. First, we discuss our recent combined experimental and theoretical study of Stark tuning of SPE's in h-BN[4,5]. We show that it is possible to control the SPEs' optical energy by applying an out-of-plane electric field and we suggested that the presence of the out-of-plane dipole of the SPEs may be originated from spontaneous symmetry breaking of the SPEs' defect structure[4]. We consider diverse defect candidates for SPEs in h-BN such as $V_NC_B$, $V_NN_B$ and we discuss the potential mechanism of the symmetry lowering process of the defect models and its physical implications for their application as single photon emitters[5]. In the second part of the talk, we describe spin decoherence in two-dimensional materials, using spin Hamiltonian and a cluster expansion method[6]. We show that isotopic purification could be much more effective in 2D than in 3D materials. We also discuss additional factors influencing the optimization of spin qubit hosts.

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Notes

IBS Conference on

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3 DAY

**Friday,** September 27, 2019

- SESSION **4**
- SESSION **5**

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## ABSTRACT BOOK



# SESSION 04

## Quantum Surface Science at the Nanoscale

Surfaces of materials offer the opportunity to use scanning probe techniques to measure their properties. This can be combined with atomic-scale manipulation to build structures with atomic-scale precision. Recently it has become possible to perform quantum-coherent manipulation of atoms on surfaces.

**Taeyoung Choi** invited

*IBS Center for Quantum Nanoscience and Department of Physics at Ewha, Seoul, South Korea*

"Quantum surface science at Nanoscale"

**Harald Brune** invited

*Institute of Physics, Ecole Polytechnique de Lausanne (EPFL), Lausanne*

"Hyperfine Interactions and Intra-atomic Spin Excitations in Single Atom Magnets"

**Deungjang Choi**

*Centro de Física de Materiales (MPC) CSIC-EHU, San Sebastián, Spain*

"Cooper pair tunneling through a molecular junction"

**Saiful Islam**

*Department of Chemistry, Graduate School of Science, Tohoku University, Japan*

"Scanning tunneling Microscopy study of Electronic and Spin states of Single molecule magnet"

**Fabio Donati** invited

*Center for Quantum Nanoscience and Department of Physics at Ewha, Seoul, South Korea*

"Probing the magnetism of single atoms with orbital sensitivity"

# Quantum surface science at Nanoscale

**Taeyoung Choi and Andreas Heinrich***
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Quantum nanoscience is an integrated and emerging field covering quantum physics and nanoscience. In recent years, there have been significant advances to coherently control quantum properties of matter[1] and to understand the properties of individual atoms, molecules, and their assemblies[2,3]. In particular, the center for Quantum nanoscience (QNS) mainly focuses on the researches of nanoscale quantum systems in a solid-state environment. . The first part of this talk introduces the overview of our research center and efforts - electron spin resonance (ESR) on individual atoms and molecules[4,5], Nitrogen-Vacancy (NV) center in diamond[6], and X-ray magnetic circular dichroism on atomic ensembles[7,8].

Secondly, we focus on our recent results about newly developed tool – ESR-STM. Here, we successfully reproduce single-atom ESR on individual Fe atoms adsorbed on magnesium oxide (MgO). Utilizing a 2D vector magnetic field and the local field of the magnetic STM tip, we optimize the ESR signal and characterize the role of the tip field. We demonstrate single atom ESR using only the tip-field, under zero external magnetic field, which promises to make this technique available in many existing STM systems[5].

In the summary, QNS will explore the various quantum platforms and utilize them at surfaces as quantum sensors, which possess superior spatial and energy sensitivity and possibly towards quantum bits, which might enable quantum information processing at surfaces.

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Notes

# Hyperfine Interactions and Intra-atomic Spin Excitations in Single Atom Magnets

**Harald Brune**
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The magnetic states of single surface adsorbed atoms continue to surprise us and challenge our understanding. This includes the interaction of our observation tools with the systems of interest. Very few of the investigated systems bear potential for applications in magnetic information storage or as single magnetic quantum bits. We begin to understand what makes their magnetic states stable and why other systems are paramagnetic.

Single Ho atoms on MgO(100)/Ag(100) are the smallest and most stable magnets known today[1-3]. At 8 T external field, their onset temperature for switching from the metastable to the stable state is 45 K, and up to 35 K their coercitive field is far above 8 T[3]. Their magnetic state can be read and written with tunnel electrons [2]. However, their ground state and zero-field stability remained open issues. Using anti-ferromagnetic tips with robust zero-field spin-contrast[4], we determine the ground state and find that the nuclear spin states convert avoided level crossings to real ones at zero field, while at small fields they create a series of avoided level crossings. Landau-Zener tunneling at these crossings can be used to prepare the magnetic states without implying electrons[5].

The second single-atom magnet published is Dy adsorbed on graphene/Ir(111)[6]. This system exhibits spin-contrast of up to 60 pm apparent height difference between up and down magnetization. We interpret this exceptionally large tunnel magneto resistance as 5*d* and 6*s* states being strongly polarized, due to Dy transferring almost an entire electron to graphene[7].

Together with Dy, many other rare-earth atoms adsorbed on graphene exhibit intense high energy inelastic conductance steps, see Figure to the right. Their origin is an intra-atomic spin-excitation between the 4*f* and 5*d*/6s spin-moments. For a given valence, the exchange energy between these moments is largely independent of the 4f element[8]. Consequently, we observe a linear behavior of excitation energy with filling of 4*f* levels[9].

We finally show a few systems that "don't work", *i.e.*, don't show magnetic bi-stability, and explain why.

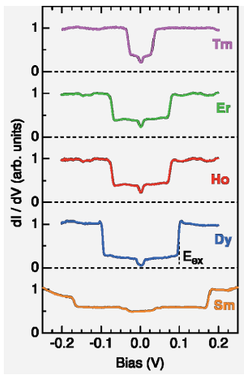


**Figure 1.**

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Notes

# Cooper pair tunneling through a molecular junction

**Cristina Mier[1], José Reina[1], Leonard Garnier[2], Benjamin Verlhac[2], Laurent Limot[2], Nicolás Lorente[1], and Deung-Jang Choi**

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The Josephson effect is the tunneling of Cooper pairs between two superconductors connected through a weak link. The tunneling takes places through Andreev bound states (ABS) localized to the weak link. The dependence of the ABS on the phase difference between the two superconductors fixes the way the Cooper pairs tunnel. ABS are a characteristic of the junction and they cannot be probed by varying the bias between the two superconductors since they take place at zero bias. This is very different from Yu-Shiba-Rusinov (YSR) in-gap state that can take place already for one superconductor and are due to the weakening of Cooper pairs produced by a magnetic impurity[1,2]. We will present experimental data and theoretical analysis characterizing the ABS of a reproducible Scanning Tunneling Microscope molecular junction giving us access to the elusive phase difference in an STM setup.

**References**

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Notes

# Scanning tunneling Microscopy study of Electronic and Spin states of Single molecule magnet

**Islam Saiful[1], S.M.F. Shahed[2], Tadahiro Komeda[2], Keiichi Katoh[1], and Masahiro Yamashita[1,3,4]**

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*[1]Department of Chemistry, Graduate School of Science, Tohoku University, Japan*

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Single molecule magnets (SMM) represent a class of compounds in which a single molecule behaves as a magnet. The reported blocking temperature, below which a single SMM molecule works as a quantum magnet, has been increasing with the development in the molecular design and synthesis techniques of multiple-decker Pc complex. Cerium intermetallics have raised a lot of interest for the past forty years thanks to their very unusual and interesting electronic and magnetic properties. This can be explained by the peculiar electronic configuration of Ce ($4f^1$) that allows different oxidation states leading to singular behavior such as quantum phase transitions, heavy-fermion behavior and the Kondo effect. Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have played an important role in the characterization of the molecule film and its interface with the metal surface. In this work, we deposited double decker cerium phthalocyanine molecule ($CePc_2$) on Au (111) substrate. We clearly found eight lobes and Kondo resonance on center and lobes. It forms two-dimensional lattice.

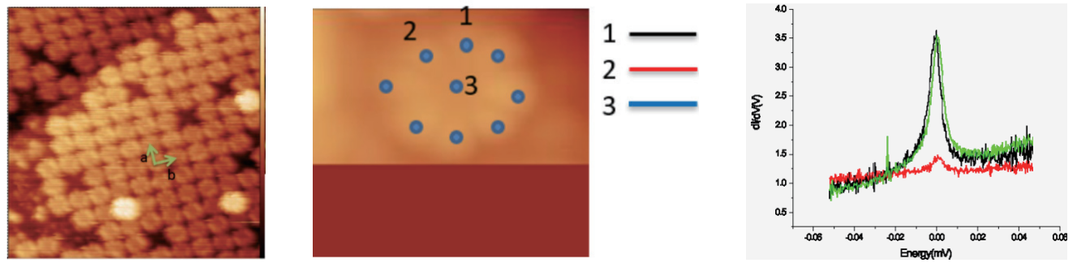


**Figure 1.** (i) STM image of the double-decker $CePc_2$ molecule (ii) dI/dV spectra position in a $CePc_2$ molecule (iii) Corresponding dI/dV spectra

**References**

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Notes

# Probing the magnetism of single atoms with orbital sensitivity

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Magnetic storage devices such as hard drives and magnetic tapes are massively used in conventional high-capacity storage units. The increasing data-storage needs motivate the research towards novel fundamental alternatives to achieve ever-larger bit density. Individual atoms adsorbed on a surface, with each atom being able to store a single bit of data, could potentially allow maximal storage density in a solid-state system. However, in order to store and process information, it is required to stabilize the electron spin of the magnetic atoms against thermal and quantum fluctuations.

In the first part of this talk, I will present the rapid evolution of this field and the sequence of advancements that led to the discovery of the first single atom magnet, namely a holmium atom on a magnesium oxide ultra-thin film. Using x-ray magnetic circular dichroism (XMCD), we found these atoms to be magnetically stable up to 40 K even in absence of an external magnetic field[1]. In addition, they can be read and written individually using a scanning tunneling microscope[2,3].

In the second part, I will present the most recent advances towards the understanding of their magnetic properties and the design of novel single atom magnets. We used XMCD to investigate the different transitions accessible in the soft x-rays range to probe the spin magnetic moments with orbital sensitivity and understand the magnetic level scheme of rare earth atoms on MgO/Ag(100). Finally, I will discuss the strategies to realize novel single atom magnets with enhanced structural and magnetic stability, as well as the first results obtained in this direction.

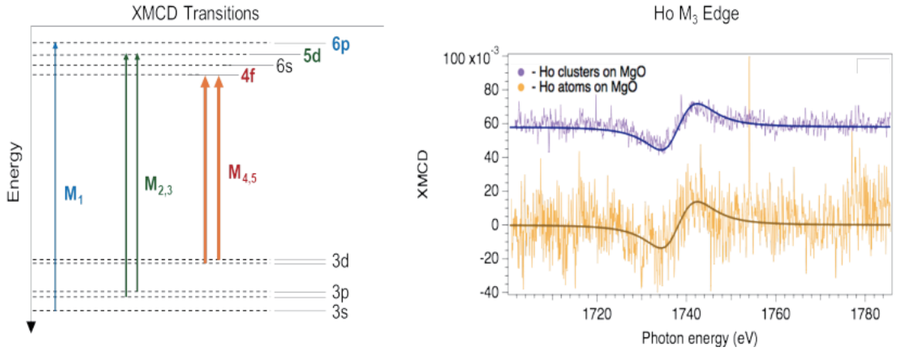


**Figure 1.** x-ray magnetic circular dichroism of single atoms with orbital sensitivity. Left: schematics of the soft-x-rays absorption transitions. Right: XMCD signal of the M3 edge acquired on 0.10 ML (clusters) on 0.03 ML (atoms) of Ho on MgO/Ag(100). Black lines show simulated transitions obtained from multiplet calculations.

**References**

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Notes

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## ABSTRACT BOOK



# SESSION 05

## A Chemical Route to Quantum Nanoscience

We will explore possible pathways from quantum coherent effects in interesting molecules to the future dream of self-assembled quantum computers.

**Roberta Sessoli** invited

*Department of Chemistry, University of Florence, Italy*

"Magnetic molecules for the second quantum revolution: potential and challenge"

**Yujeong Bae**

*Center for Quantum Nanoscience and Department of Physics at Ewha, Seoul, South Kore*

"Controlling spin transport through exchange coupled molecules using an STM"

**Taner Esat**

*Center for Quantum Nanoscience and Department of Physics at Ewha, Seoul, South Kore*

"A standing molecule as a single-electron field emitter"

**Mykola Telychko**

*Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117543, Singapore.*

"Atomically precise bottom-up synthesis of π-extended [5]triangulene"

**Ruoning Li**

*Key Laboratory for the Physics and Chemistry of Nanodevices, Peking University, China*

"Observation of biradical spin coupling through hydrogen bonds"

**Danna Freedman**

*Department of Chemistry, Northwestern University, USA*

"Chemical approaches to quantum information science"

**Wolfgang Wernsdorfer** invited

*Department of Physics, KIT Karlsruhe, Germany*

"Operating quantum states in individual magnetic molecules"

**Arzhang Ardavan** invited

*Department of Physics, Oxford University, United Kingdom*

"Using DNA to assemble molecular electronic devices"

# Magnetic molecules for the second quantum revolution: potential and challenge

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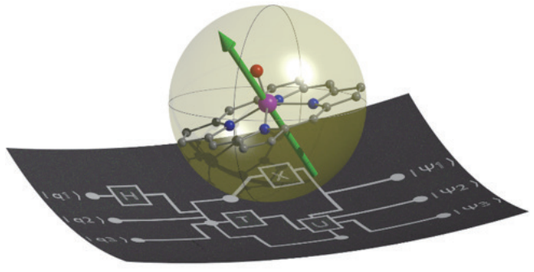
Implementation of modern Quantum Technologies might benefit from the remarkable quantum properties shown by molecular spin systems. The spin is intrinsically a two-level quantum system which can easily be manipulated by electromagnetic radiations, as magnetic resonance techniques have been showing us for almost 80 years. Molecular chemistry has already demonstrated to be a rich playground for the preparation of tailormade molecules that can serve for the realization of potential components of a quantum computer. Molecules with a large spin and strong magnetic anisotropy showing magnetic bistability at the single molecule level (single-molecule magnets, SMMs) have been proposed since 1990s as the ideal miniaturization of memory units with the possibility to harness quantum effects to control the spin dynamics. More recently molecules with significant spin coherence are investigated as possible realization of multiqubit architectures for quantum gates implementation.

Even if the use and manipulation of molecular spin systems for QT applications appears a step behind to alternative physical realizations, such as superconducting circuits, quantum dots, etc. remarkable advancements have been already achieved, while plenty of room for significant improvements is still available[1].Of relevance is the high tunability of single center spin Hamiltonian parameters, in particular the spin manifold, the anisotropy of the *g* tensor and of the hyperfine coupling, as well as quadrupolar interaction for lanthanide ions. The organization of molecular spin centers in bi- and three-dimensional architectures, e.g. in metal-organic frameworks[2], and the possibility to evaporate magnetic molecules on clean surfaces and to control the interaction with the substrate[3] are also very appealing.

The current state of our research on magnetic molecules showing spin coherence, in particular on coordination compounds containing light elements, will be presented here.



**References**
[1] M. Atzori and R. Sessoli, J. Am. Chem. Soc., in press. Doi:10.1021/jacs.9b00984.
[2] T. Yamabayashi, T. et al. J. Am. Chem. Soc. **140**, 12090 (2018).
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# Controlling spin transport through exchange coupled molecules using an STM

**Yujeong Bae[1], Kai Yang[2], Andreas J. Heinrich[1,3,*], and Christopher P. Lutz[2,*]**
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The single atom or molecule represents the ultimate limit in high-density magnetic memory storage. Shrinking spin-based devices to such a limit requires the ability to control and probe the spin states at the atomic scale. The scanning tunneling microscope (STM) provides the capability to study the quantum states of single atoms and molecules on a surface. Here, we present that the correlation between two exchange coupled spin systems determines the spin selectivity of electric currents through these coupled spins. Using inelastic electron tunneling spectroscopy in the STM, we study the spin-dependent transport through exchange-coupled two nickelocen (Nc) molecules: one at the apex of STM tip and one on a surface of two monolayers of MgO. While the Nc molecule attached to the tip apex preserves its spin properties, we are able to continuously control the coupling strength and the resulting quantized states by controlling the tip-sample distance. Increasing the coupling strength results in a strong asymmetry in the differential conductance, which indicates spin-polarized tunneling transport. We find the coupling and spin excitation can be controlled by changing the adsorption geometry of the Nc molecule at the tip apex, where the spin state of Nc stays same at different geometries. We also show the spin states of the Nc molecule can be tuned by assembling it with an adjacent Fe atom, which enhances the spin contrast of the STM tip by 20 times compared to a typical spin-polarized STM tip.

# A standing molecule as a single-electron field emitter

**Taner Esat[1,2,3*], Niklas Friedrich[1,2], F. Stefan Tautz[1,2] and Ruslan Temirov[1,2]**

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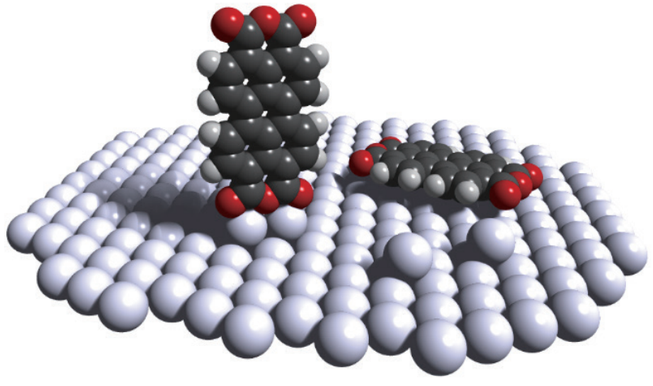
The unique strength of scanning probe microscopy (SPM) is the combination of superior imaging and spectroscopy capabilities with the possibility to manipulate and excite objects at the nanoscale. This has brought atom-scale devices on surfaces into reach. However, a serious limitation to date is that SPM experiments and the produced devices are confined to two-dimensional flatlands, because surfaces are sticky and erecting nanoscale structures that project out of a surface is extremely difficult.

Here, we demonstrate that SPM-based manipulation can rise above this limitation. Specifically, we lift a flat molecule which under all known circumstances adsorbs in the surface plane from a metal and place it on its edge (see Figure)[1].

The atypical orientation of the molecule allows us to exploit molecular anisotropy, thereby creating an unusual functional relationship between metal and molecule that lends itself to the construction of a coherent single-molecule field emitter. From the interference pattern in the field emission current the phase of the emitter's quantum mechanical wave function can be reconstructed[1]. Our results demonstrate that manipulation experiments with scanning probe microscopes can be extended to handle anisotropic molecules with orientational control, opening the door to three-dimensional molecular architectonics on surfaces. Evidently, the access to the third dimension offers unmatched freedom in the design of functional molecular nanostructures.



**References**

[1] Esat, T., Friedrich, N., Tautz, F.S. and Temirov, R. A standing molecule as a single-electron field emitter. Nature 558, 573 (2018).

# Atomically precise bottom-up synthesis of π-extended [5]triangulene

**J. Su[1,2†], M. Telychko[1,2†], P. Hu[1†], G. Macam[3†], P. Mutombo[6], H. Zhang[1], Y. Bao[1,2], F. Cheng[1,2], Z. Q. Huang[3], Z. Qiu[1,4], S. J. R. Tan[1,4], H. Lin[5], P. Jelínek[6,7], F. C. Chuang[3], J. Wu[1] , and J. Lu[1,2]**

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*[3]Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan.*
*[4]NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, 28 Medical Drive, Singapore 117456, Singapore.*
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*[6] Institute of Physics, The Czech Academy of Sciences, Prague 16200, Czech Republic.*
*[7] Regional Centre of Advanced Technologies and Materials, Palacký University, Olomouc 78371, Czech Republic.*
*† These authors contributed equally*
**E-mail: chmluj@nus.edu.sg (J. Lu)*

The zigzag-edged triangular graphene molecules (ZTGMs) have been predicted to host ferromagnetically coupled edge states with the net spin scaling with the molecular size, which affords large spin tunability crucial for next-generation molecular spintronics. However, the scalable synthesis of large ZTGMs and the direct observation of their edge states have been long-standing challenges due to the molecules' high chemical instability. Here we report the bottom-up synthesis of π-extended [5]triangulene with atomic precision via surface assisted cyclodehydrogenation of a rationally-designed molecular precursor on metallic surfaces. We apply atomic force microscopy and scanning tunneling spectroscopy measurements to reveal edge-localized electronic states. Bolstered by density functional theory calculations, our results show that [5]triangulenes synthesized on Au(111) retain the open-shell π-conjugated character with magnetic round states.

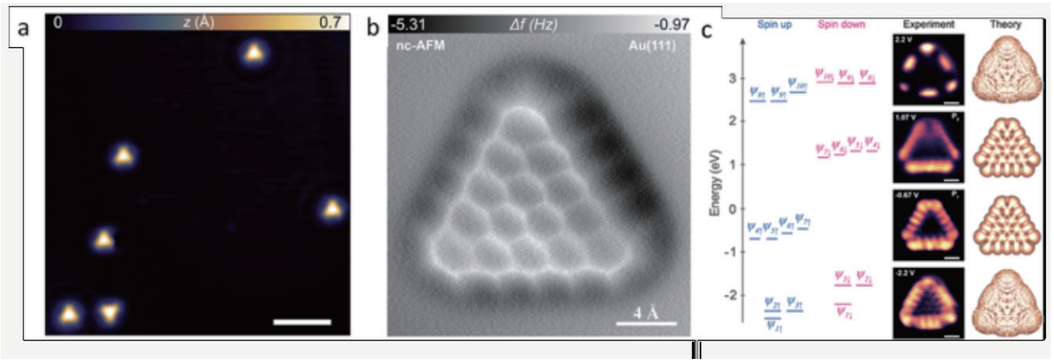


**Figure 1.** Figure: a) Large scale STM image of [5]triangulene molecules on Au(111). b) High-resolution nc-AFM image of individual [5]triangulene taken with CO functionalized tip. c) Energetic diagram of [5]triangulene and set of dI/dV maps acquired at different biases.

Notes

# Observation of biradical spin coupling through hydrogen bonds

**Yang He[1], Na Li[1], Ivano Eligio Castelli[2], Ruoning Li[1], Jing-Tao Lü[3,*], Kai Wu[4,*], Per Hedegård[5,*], and Yongfeng Wang[1,*]**

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Investigation of intermolecular electron spin interaction is of critical importance to understand quantum effects in chemical and biological reactions. Quantum coherence of radical pairs plays a pivotal role in chemical amplification of magnetic field effect relevant to avian magnetoreception. Although radical pairs have been intensively studied, spin interaction in single radical pairs has not been reported. Here, radical pairs of all-trans retinoic acid molecules on Au(111) are created using an ultra-low temperature scanning tunneling microscope. Antiferromagnetic coupling between two radicals is identified by magnetic-field dependent spectroscopy. The measured exchange energies are on the order of meV. The biradical spin coupling is mediated through O-H···O hydrogen bonds, as elucidated from analysis combining density functional theory and a modern version of valence bond theory.

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[2] M. Ternes, Spin excitations and correlations in scanning tunneling spectroscopy New J. Phys. 17, 063016 (2015).
[3] S. Karan, N. Li, Y. Zhang, Y. He, I.-P. Hong, H. Song, J.-T. Lü, Y. Wang, L. Peng, K. Wu, G. S. Michelitsch, R. J. Maurer, K. Diller, K. Reuter, A. Weismann, R. Berndt, Spin manipulation by creation of single-molecule radical cations. Phys. Rev. Lett. 116, 027201 (2016).

# Chemical approaches to quantum information science

**Danna Freedman*, Joseph Zadrozny, Michael Graham, and Majed Fataftah**
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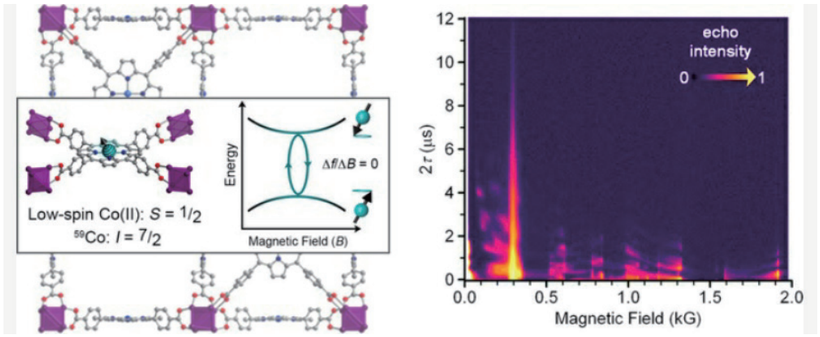
**E-mail:danna.freedman@northwestern.edu*

Chemistry offers a unique bottom up approach to the design of qubits, the smallest unit of a QIS system. We harness this angstrom scale precision to develop fundamental insight into the spin dynamics of electronic spin-based qubits. Results on increasing coherence time, constructing qubit arrays, and understanding the impact of nuclear spin on electronic spin coherence time will be presented.







**References**

[1] Fataftah, M.S.; Freedman, D. E. Progress towards creating optically addressable qubits Chem. Commun. **2018**, 54, 13773–13781

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[3] Graham, M. J.; Zadrozny, J. M.; Fataftah, M. S.; Freedman, D. E. Forging Solid-State Qubit Design Principles in a Molecular Furnace Chem. Mater. **2017**, 29, 1885–1897.

[4] Graham, M. J.; Yu, C.; Krzyaniak, M.; Wasielewski, M.; Freedman, D. E. Synthetic Approach to Determine the Effect of Nuclear Spin Distance on Electronic Spin Decoherence J. Am. Chem. Soc. **2017**, 139, 3196–3201.

# Operating quantum states in individual magnetic molecules

**Wolfgang Wernsdorfer**
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The endeavour of quantum electronics is driven by one of the most ambitious technological goals of today's scientists: the realization of an operational quantum computer. We start to address this goal by the new research field of molecular quantum spintronics, which combines the concepts of spintronics, molecular electronics and quantum computing. The building blocks are magnetic molecules, i.e. well-defined spin qubits. Various research groups are currently developing low-temperature scanning tunnelling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors, Fig. 1) to read and manipulate the spin state and perform basic quantum operations. We will present our recent measurements of geometric phases, the iSWAP quantum gate, the coherence time of a multi-state superposition, and the application to Grover's algorithm[1-5].

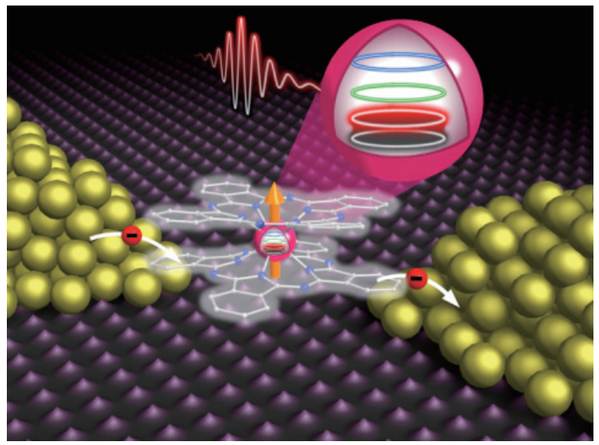

**Figure 1.** A molecular spin transistor based on a single TbPc2 molecular magnet

**References**
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# Using DNA to assemble molecular electronic devices

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Molecules represent the ultimate limit for miniaturization of functional materials. Devices in which individual molecules are probed and manipulated will push classical electronic circuit architectures to the limits of their performance. Furthermore, this is the scale at which quantum phenomena dominate properties: single-molecule structures can provide fundamental tests of quantum theory as well as components for future quantum technologies.

Such considerations have motivated several decades of basic research into electronic devices with molecular active elements, but, despite the promise, this effort has failed to deliver transferable technologies suitable for industrial deployment. This is because there are fundamental shortcomings in the existing “top-down” approaches to assembling single-molecule electrical devices. At the molecular scale, an approach exploiting self-assembly holds more promise. This can be achieved using DNA nanotechnology to design components with specific interactions, offering a route to high yield, scalable, functional molecular electronic circuits.

# INFORMATION

## Campus Map of Ewha Womans University

Ewha Womans University, 52 Ewhayeodae-gil, Daehyeon-dong, Seodaemun-gu
04344 Seoul, Republic of Korea

**Coordinates for your navigator** 37.561176, 126.946389


## Venue

**Conference** | Lee SamBong Hall, Ewha Campus Complex (ECC) B4
**Dedication Ceremony** | Graduate School Building (Emerson Chapel)
**Building Tour & Lab Tour** | Research Cooperation Building(QNS)

## Directions to Ewha Womans University

Hongik Univ ▸ Ewha Womans Univ


### By bus

· Take the green bus 7737 at Exit 9 (bus stop 14-015)
· Exit at Ewha Womans University station
· 500m walking distance to Ewha Campus Complex (ECC)
· Bus fare: 1,200 KRW (1 USD)

### By subway

· Take the subway line 2 (Green Line) at Hongik Univ. station
· Exit at Ewha Womans Univ. station (Exit 2 and 3)
· 500m walking distance to Ewha Campus Complex (ECC)
· Subway fare: 1,200 KRW (1 USD)

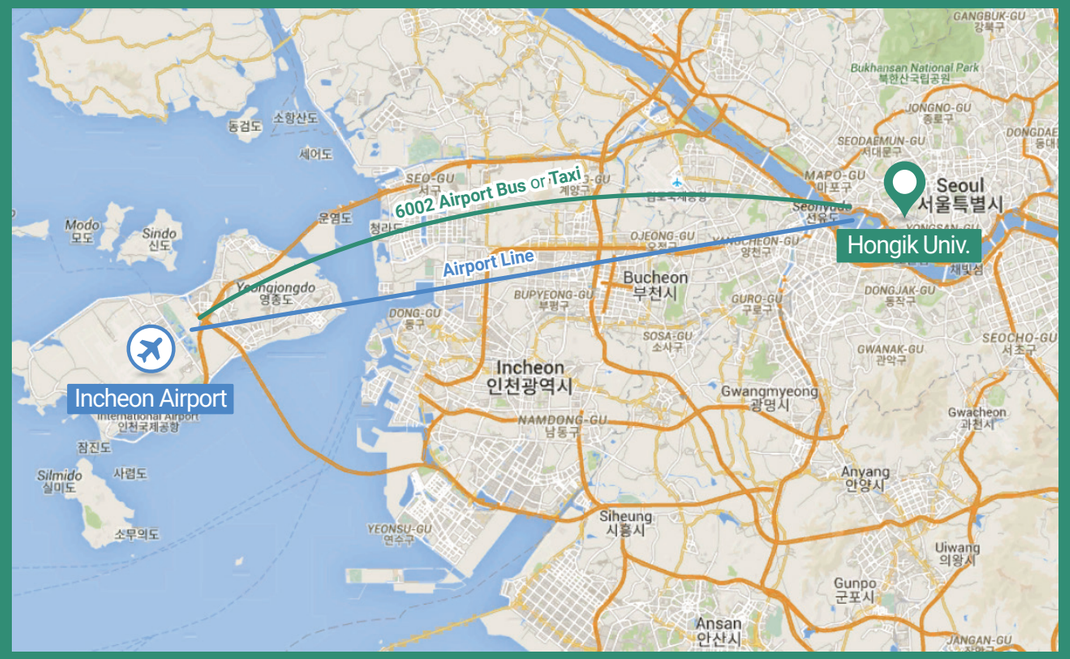
### By taxi

· Destination: Ewha Campus Complex (이화여자대학교캠퍼스복합단지)
· Approx. 15~20 minutes distance
· Taxi fare: 5,000~6,500 KRW (5.50 USD)

# INFORMATION

## Directions to Incheon International Airport

Hongik Univ ▸ Incheon International Airport




### By bus

· Take the airport bus 6002 at Exit 9 (bus stop 14-015)
· Exit at Incheon International Airport Terminal 1 or 2(Approx. 75 minutes)
· Bus fare: 10,000 KRW (10 USD)

### By subway

· Take the Airport Rail Road at Hongik Univ. station
· Exit at Incheon International Airport Terminal 1 or 2 (Approx. 65 minutes)
· Subway fare: 4,050 KRW (4 USD)

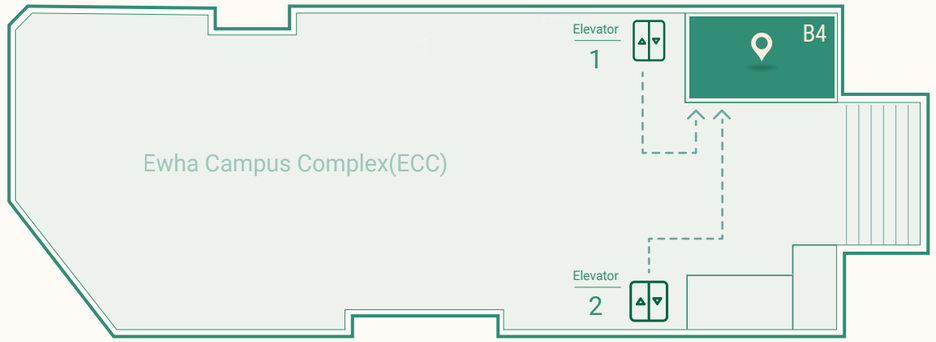
### By taxi

· Destination: Incheon International Airport Terminal 1 or 2 (Approx. 55 minutes)
· Taxi fare: 60,000~65,000 KRW (60 USD)



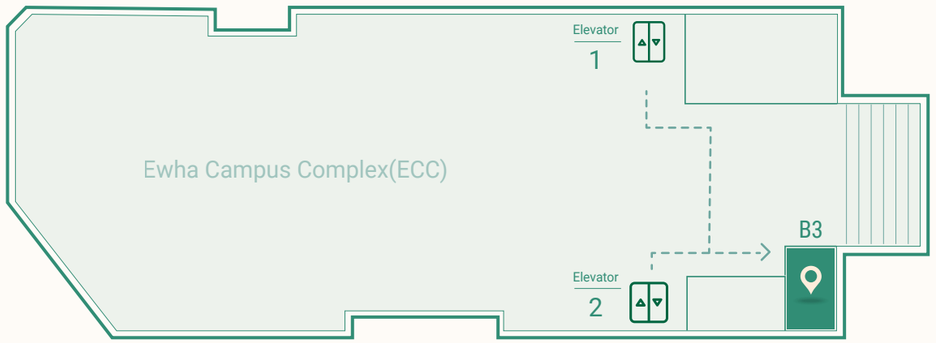
# ECC MAP

## ECC Hall B4




Conference Lee SamBong Hall

## ECC Hall B3




Poster Session Daesan Art Gallery

# DAY 1

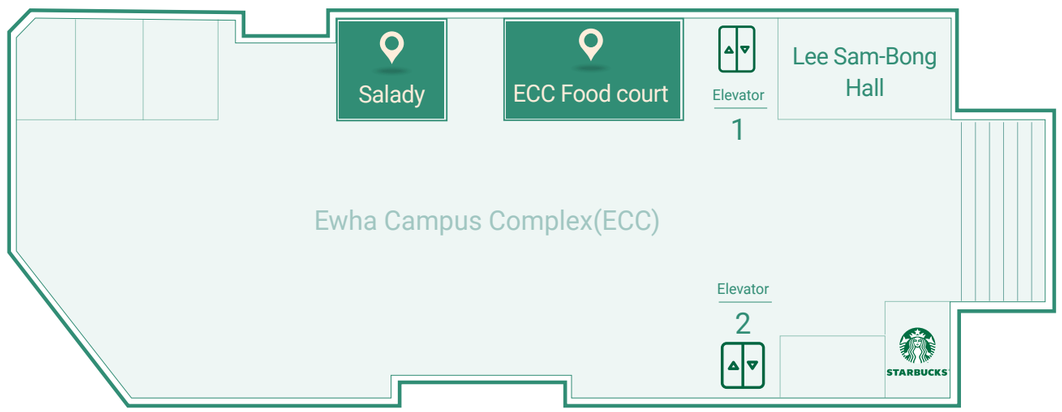
## Wednesday, September 25th

### Lunch

**Time** 11:30 – 13:00 (90')

**Participants**

Participants may use lunch voucher at ECC food court or Salady (B4, ECC)




### Dinner

**Time** 18:00 – 20:00 (120')

**Participants**

Venue: Research Cooperation Building(1st floor) The Hub at QNS





# DAY 2

## Thursday, September 26th

### Lunch

**Time** 11:30 – 13:00 (90')

**Participants**

Participants may use lunch voucher at ECC food court or Salady (B4, ECC)

### Dinner

**Time** 18:00 – 20:00 (120')

#### for Invited Sepakers

Venue: House dinner at Aryeng-dang **with the Ewha President**

#### for Excursion Participants

Venue: to be announced

*** Take the bus in front of the Emerson Chapel after the dedication ceremony**

Bus 1 **- Night Tour**

Seoul Tower + Nam Mountain

Bus 2 **- Market Tour**

Kwangjang Market + Chunggye Stream

# DAY 3

Friday, September 27th

## Lunch

**Time** 11:40 – 13:00 (70')

**Participants**

Participants may use lunch voucher at ECC food court or Salady (B4, ECC)






2020

# Center for Quantum Nanoscience

## IBS Conference on Quantum Surface Science

**Topic** Spins on Surfaces and quantum surface science

- Electron spin resonance and scanning tunneling microscopy
- Electron spin resonance at sub-monolayer resolution
- Combining optical spectroscopy with STM
- Low-temperature, high-resolution spectroscopy

**Date** October, 2020

**Venue** Seoul, Korea

**Website** https://ibsconference.org/2020/icqns/
( * To be opened in October )

**Contact Info**

Jihee Min(Currently) / Seokyoung Choi(in 2020) | **conference@qns.science**

# About Quantum Nanoscience

## About Us

The Center for Quantum Nanoscience (QNS) at Ewha Womans University aims to investigate quantum effects in solid state systems to further our understanding of this crucially important, but as of yet, poorly understood basic research field. Our goal is to become recognized as the best place to perform quantum research on the atomic scale in a solid-state environment and be a destination for leading domestic and international researchers.

## Research Groups

### Quantum Properties of Individual Spin Systems on Surfaces
Quantum-coherent control of single atom and molecule spins on surfaces.

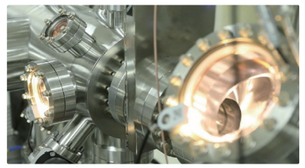
### Ensemble Measurements of Spins on Surfaces
Quantum properties of molecules and atoms on surfaces with x-ray absorption spectroscopy and electron spin resonance.

### Optics combined Scanning Probe Microscopy
Quantum-coherent manipulation of atoms and defects on surfaces combining optical spectroscopy and scanning probe microscopy (STM+AFM).

### Development of NV Center-Based Scanning Magnetometry at Low Temperatures
Nanoscale quantum sensing using nitrogen-vacancy centers in a diamond.

### Theory of Quantum Systems at Surfaces
Predictive computational methods based on density functional theory.

## Equipment



Scanning Tunnelling Microscope (STM)

Electron Spin Resonance STM

### Scanning Tunnelling Microscope (STM) at 10 millikelvin (mK)
Home-built combination of STM with a dilution refrigeration system to operate at the coldest temperatures currently available for quantum control at extremely cold temperatures. System includes two-axis magnetic field.

### Electron Spin Resonance STM
QNS is developing several STM systems with high-frequency capabilities to perform ESR on single atoms and molecules on surfaces. Operation temperature of about 0.5K and vector magnetic fields will be available. High frequency sources up to 50GHz with pulsed capabilities.

### Surface Science Electron Spin Resonance (ESR)
Spatially-averaging ESR at temperatures from 2 to 400 Kelvin and is optimized to work on clean surfaces. Sensitivity of ESR to sub-monolayer spin density.

### Low Temperature STM + Atomic Force Microscopy (AFM)
QNS operates several low-temperature STM and AFM systems.
AFM systems with cold preamp are designed for spin-dependent measurements operating between 1K and 10K.

### Optics STMs
QNS has focused on designing low-temperature STM systems with good optical access to detect photons from the STM and to shine laser light onto STM tip-sample junctions.

### Growth Systems for Atomically-Controlled Thin Films
QNS operates several growth systems for atomically controlled sample growth, including molecular beam epitaxy for growth of thin-film materials.

### Quantum Control of Atomic-Scale Defects in Solids (NV AFM)
In collaboration with researchers from Korea University QNS has built an AFM system with individual nitrogen vacancy (NV) centers in the AFM tip.

### Computing Cluster
Medium-scale computing cluster to perform density-functional and quantum chemistry modelling of atoms and molecules.

## Social Media

Follow us in Social Media - @QNSscience
Visit our website - qns.science

# Student Opportunities at QNS

## Ewha Womans University Opportunities at QNS

### 1 Ewha Undergraduate Internship

Available to all full-time Ewha Students studying in a related field.
This is a good opportunity to get hands-on experience in the lab and learn from our Postdocs, PIs, and Graduate students.
Apply via Ewha's "Physics Department"

### 2 Become a QNS Graduate Student

Available to all Ewha Students.
Ewha Womans University and QNS offer a graduate student placement. If you are an Ewha graduate student who is interested in doing your research in the field of "Quantum Nanoscience" you are welcome to apply!
Apply via Ewha's "Office of Admissions"

### 3 International Summer School Internship Program

Available to International Students through the Ewha Summer School program who are studying outside of Korea.
This summer school program allows you to take classes related to Quantum Nanoscience that are taught by experts at QNS. Some students who enroll in the summer school have an opportunity to apply for the QNS Internship program, where you can receive experience working in our labs.
Apply via Ewha "Office of International Affairs"

### 4 High School Student Program "High Ewha, Hi Ewha"

Available to Korean High School Students.
A one-day domestic summer program for Korean high school students.
Apply via Ewha "Office of Admissions"

## Non-Ewha Student Opportunities at QNS

### International Student Research Stay

This opportunity is provided by QNS for International students to come to QNS for a research stay. Requires advisor's approval.
Apply via email | **hr@qns.science**

### Domestic PhD Korean University Research Stay

This opportunity is provided to graduate students in Korea to QNS as a researcher. Requires advisor's approval.
Apply via email | **hr@qns.science**



# Open job position

## Post-Doc Position in **ESR-STM Lab**

The ESR-STM lab at QNS is looking for several postdoctoral candidates. One opening is focused on revealing the spin structures of molecules and nanostructures with sub-nm resolution using the recently developed ESR-STM technique based on a Unisoku 3-He STM. QNS is one of the few labs around the world that have demonstrated ESR STM at the single atom level. In this project we want to utilize ESR-active atoms on surfaces as quantum sensors to detect the magnetic properties of nearby 'unknown' species.
A second and possibly third postdoctoral position is available utilizing home-built ESR STM systems. One system is built inside a dilution fridge which operates below 10mK and a second one in a closed-cycle Joule-Thomson system. These two systems will offer temperatures from 10mK to 40K as well as magnetic fields in several vector geometries. Both systems are being finalized in 2019 and will be in the testing and debugging phase at the beginning of 2020. We plan to be fully operational by summer of 2020. Candidates for these positions should have some experience and a strong interest in developing home-built instrumentation. The research goals include ESR STM as well as quantum-coherent manipulation of spins on surfaces for possible quantum computing applications.

**Requirement**

- Ph.D. in Physics, Chemistry, or Material Science or related areas
- Excellent experimental skills
- Strong communication and interpersonal skills for interacting with a diverse group of researchers and technical staff
- Experience with SPM (STM, AFM)

**Preferred experience**

- Experience with programming languages such as MATLAB or Python
- Experience with high frequency measurements
- Surface science sample preparation and characterization
- Interest in living in the Sinchon area in Seoul, an amazing metropolis at the heart of Asia

## Post-Doc Position in **NV Center Lab**

The Quantum Sensing lab at QNS is looking for a postdoctoral candidate. Scanning magnetometry at the nanometer scale has garnered world-wide attention since enhanced spatial resolution in magnetic resonance technique will enable the investigation of chemical structures of bio-molecules and materials at the atomic level.
In this Nitrogen Vacancy (NV) center project, we are developing novel scanning probe microscopes based on diamond NV centers. These centers are nanoscale spin qubits possessing long spin coherence time and high magnetic field sensitivity even at ambient conditions. We are utilizing the NV center as a probe tip of SPM, enabling three dimensional mapping of magnetic samples and molecules with nanoscale resolution. In 2020, we are integrating this scanning NV magnetometry with a low temperature cryostat. Although the NV centers exhibit excellent quantum properties at ambient condition, the quantum properties of the NV centers could be greatly enhanced at low temperatures. For instance, low temperature experiments will reduce thermal and mechanical drift, minimize phonon background, and lengthen spin coherence time, enabling sub-nanometer spatial resolution with greater magnetic field sensitivity.

**Requirement**

- Ph.D. in Physics, Chemistry, or Material Science or related areas
- Excellent experimental skills
- Strong communication and interpersonal skills for interacting with a diverse group of researchers and technical staff

**Preferred experience**

- Optical measurement techniques
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- Programming in Labview, MATLAB or Python
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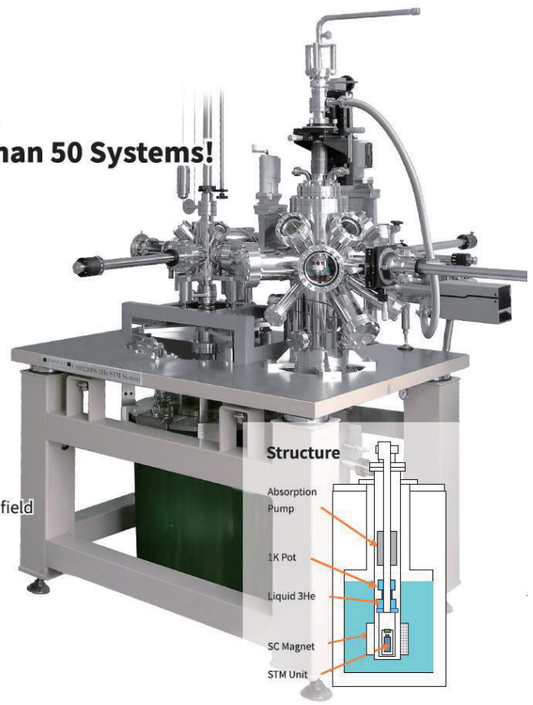


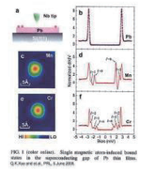

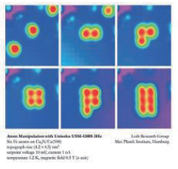

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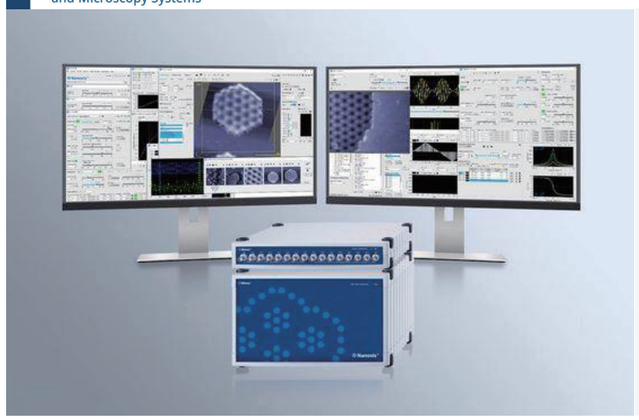

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IBS Conference on

# Quantum Nanoscience

**September 25th - 27th, 2019**

Lee SamBong Hall,
Ewha Womans University, Seoul

# PROGRAM

## Day — 1 —

**Wednesday,** September 25, 2019

| | |
|---|---|
| 09:00-09:15 | **Participants Registration** |
| 09:15-09:30 | **Opening Remarks from Andreas Heinrich** |
| | **Session 1**<br>What is Quantum Nanoscience? |
| 09:30-10:00 | General Introduction<br>Andreas Heinrich |
| 10:00-10:30 | William D. Oliver |
| 10:30-11:00 | Yonuk Chong |
| 11:00-11:30 | Andrew Dzurak |
| 11:30-13:00 | **Lunch** |
| | **Session 2**<br>Quantum Sensing with Nanoscale Systems |
| 13:00-13:45 | General Introduction<br>Ania Jayich |
| 13:45-14:15 | Jörg Wrachtrup |
| 14:15-14:30 | Sangyun Lee |
| 14:30-15:00 | **Coffee Break** |
| 15:00-15:15 | Jungbae Yoon |
| 15:15-15:30 | Kyunghoon Jung |
| 15:30-16:00 | Donghun Lee |
| 16:30-17:30 | **QNS Building Tour** |
| 18:00-20:00 | **Official Dinner** |

## Day — 2 —

**Thursday,** September 26, 2019

| | |
|---|---|
| 09:00 - 09:15 | **Coffee break** |
| | **Session 3**<br>Theory Challenges in Quantum Nanoscience |
| 09:15-10:00 | General Introduction<br>Daniel Loss |
| 10:00-10:30 | Jelena Klinovaja |
| 10:30-11:00 | Martin B. Plenio |
| 11:00-11:15 | Stanislav Avdoshenko |
| 11:15-11:30 | Hosung Seo |
| 11:30-13:00 | **Lunch** |
| 13:00-14:00 | **Poster Session (Daesan Gallery)** |
| 14:00-14:30 | **Coffee Break** |
| 14:30-15:30 | **Poster Session (Daesan Gallery)** |
| | **QNS Dedication Ceremony** |
| 16:00-16:15 | Ewha President |
| 16:15-16:30 | IBS Acting President |
| 16:30-17:30 | Don Eigler |
| 17:30-18:00 | **Art Contest Awards** |
| 18:30-22:00 | **Excursion** |

## Day — 3 —

**Friday,** September 27, 2019

| | |
|---|---|
| 09:00 - 09:15 | **Coffee break** |
| | **Session 4**<br>Quantum Surface Science at the Nanoscale |
| 09:15-10:00 | General Introduction<br>Taeyoung Choi |
| 10:00-10:30 | Harald Brune |
| 10:30-10:45 | Deungjang Choi |
| 10:45-11:00 | Saiful Islam |
| 11:00-11:40 | Fabio Donati |
| 11:40-13:00 | **Lunch** |
| | **Session 5**<br>A Chemical Route to Quantum Nanoscience |
| 13:00-13:45 | General Introduction<br>Roberta Sessoli |
| 13:45-14:05 | Yujeong Bae |
| 14:05-14:25 | Taner Esat |
| 14:25-15:00 | **Coffee Break** |
| 15:00-15:20 | Mykola Telychko |
| 15:20-15:40 | Ruoning Li |
| 15:40-16:00 | Danna Freedman |
| 16:00-16:30 | Wolfgang Wernsdorfer |
| 16:30-17:00 | Arzhang Ardavan |
| 17:00-17:15 | **Poster Awards** |
| 17:15-17:30 | **Closing remarks from Andreas Heinrich** |
| 17:30-17:45 | **Group Photo** |