ECMOLS 2025

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4th European Conference on Molecular Spintronics

2nd - 4th June 2025 Trinity College Dublin, Ireland

ECMOLS – 4TH EDITION

The European Conference on Molecular Spintronics (ECMolS) is a biennial event that brings together researchers from the fields of organic spintronics, molecular magnetism, and molecular quantum technologies. Established in 2016, ECMolS aims to foster interdisciplinary collaboration and advance the understanding of spin-dependent phenomena in molecular systems. Through a dynamic program of talks, poster sessions, and networking opportunities, the conference encourages both established and early-career scientists to exchange ideas and build lasting scientific partnerships across Europe and beyond.

AIMS AND SCOPES

With a strong interdisciplinary focus, from chemistry, physics, materials science, and engineering, ECMolS aims to foster collaboration across disciplines, promote innovation in spin-based devices, and support the development of emerging technologies such as molecular qubits, spintronic sensors, and hybrid quantum systems.

Through a dynamic program of talks, poster sessions, and networking opportunities, the conference encourages both established and early-career scientists to exchange ideas and build lasting scientific partnerships across Europe and beyond.

PREVIOUS EDITIONS

Previous editions of the conference have taken place across various European countries, highlighting its international scope and collaborative spirit:

1st edition Bologna (Italy), 15-18 November 2016.

2nd edition Peñíscola (Castellón, Spain) 21-24 October 2018.

3rd edition Dortmund (Germany), 5-8 April 2022.

4th edition Dublin (Ireland), 2-4 June 2025.

SPONSORS



4TH EDITION ORGANIZERS AND SCIENTIFIC COMMITTEE

PROF. ALESSANDRO LUNGHI

Alessandro holds a Ph.D. in computational inorganic chemistry, received in 2016 from the University of Florence. His Ph.D. dissertation focused on the computational and theoretical investigation of molecular magnets and their interaction with typical solid-state environments. In 2016 he joined the School of Physics at Trinity College Dublin as a research fellow and started working on designing machine-learning methods for accelerating molecular dynamics simulations of solid-state materials.





PROF STEFANO SANVITO

Prof. Sanvito studied Physics in Milan, Italy, ("Laurea") and Lancaster, UK (PhD). After two years at the University of California Santa Barbara, in 2002 he joined the School of Physics at TCD. In 2006 he became associated Professor and in 2012 Professor of Condensed Matter Theory. Since 2013 he is the Director of the Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN) and for the period 2013-2015 he has been the Director of the AMBER Centre.

PROF ANDREA DROGHETTI

Andrea studied Physics at the University of Bologna, Italy, (B.Sc. and M.Sc.) and later at TCD (PhD). In 2016, he was awarded a Marie Skłodowska-Curie Individual Fellowship to work at the University of the Basque Country in Spain. In 2019, he was granted a University Research Fellowship by the Royal Society, allowing him to return to TCD as group leader. In 2024, he joined the SPIN Institute of the National Research Council of Italy as a research scientist and was later appointed Assistant Professor in Condensed Matter Theory at Ca' Foscari University of Venice. His research spans from the electronic structure of materials to the development of computational methods for quantum transport in magnetic and correlated electronic systems.



INTERNATIONAL SCIENTIFIC ADVISORY BOARD

Scientific advisory board for selecting topics, speakers and program schedule design. This edition counts with the advice of highly recognized and reputable scientists across Europe.

PROF EUGENIO CORONADO PROF ROBERTA SESSOLI PROF VALENTIN ALEK DEDIU PROF MIRKO CINCHETTI PROF FERNANDO LUIS PROF ARZHANG ARDAVAN PROF HERRE VAN DER ZANT



CONFERENCE SPEAKERS

This year's edition counts with a panel of highly distinguished researchers as Speakers, ranging from highly experienced scientists to well-established early-career researchers. All of whom have made significant contributions to the fields of molecular spintronics and molecular quantum technologies, from experimental synthesis and measurements to molecular modelling.

To this end, we aimed at covering all key aspects of the field while allowing for researchers at different career stages to share their findings, as well as valuable insights into both fundamental principles and cutting-edge developments.

TUTORIALS	KEY-NOTES SPEAKERS
Roberta Sessoli (Florence, IT)	Pascal Ruffieux (Fribourg, CH)
Luis Hueso (San Sebastian, ES)	Mario Ruben (Karlsruhe, DE)
Fernando Luis (Zaragoza, ES)	Toeno van der Sar (Delft, NE)
	Michael Coey (Dublin, IE)
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INVITED SPEAKERS	Elke Scheer (Konstanz, DE)
María José (Pepa) Martínez-Pérez (Zaragoza, ES)	Samuel Mañas-Valero (Delft, NL)
Mirko Cinchetti (Dortmud, DE)	Amandine Bellec (Paris, FR)
Junjie Liu (London, UK)	Kasper Pedersen (Copenaghen, DK)
Sam Bayliss (Glasgow, UK)	Floriana Tuna (Manchester, UK)
Hanna Stern (Oxford, UK)	Mattia Benini (Bologna, IT)
Matteo Briganti (Florence, IT)	Yujeon Bae (Zurich, CH)
Jose Lado (Aalto, FI)	Alessandro Chiesa (Parma, IT)

CONFERENCE PROGRAM

The conference will take place from the 2nd to the 4th of June and will feature a dynamic programme of invited and contributed talks covering the latest advances in the field. Proceedings will begin with registration at the conference hall in the Hamilton Building, where attendees will receive their name tags and conference booklets. Throughout the event, participants will have the opportunity to engage with cutting-edge research and connect with leading experts. A social dinner on the second evening will offer a chance to relax, enjoy Irish culture, and foster new collaborations in an informal setting among peers and colleagues. Posters will be on display from the morning of June 2nd until the final day at Hamilton building Hall. Full details of the talks and poster presentations can be found in the following pages.

STRUCTURE AND TOPICS

The conference includes four different types of contributions from participants.

Tutorials (40 min + 5 min discussion): This section will cover the essential aspects of molecular spintronics and quantum phenomena, ranging from fundamental concepts to advanced results on the following topics:

- Organic spintronics
- Molecular electronics
- Molecular magnetism and molecular quantum technologies
- Optical and electromagnetic control of molecular spins
- Molecules at the interface

Keynote Talks (30 min + 5 min discussion): Concise tutorial-style presentations by leading speakers from some of the most prominent European research groups active in molecular spintronics and molecular quantum technologies.

Invited talks (20 min + 5 min discussion): These presentations will showcase some of the most relevant scientific advances in the above topics, delivered by well-established researchers who have made significant contributions to the field.

Contributed Talks (12 min + 3 min discussion): These short presentations will highlight some of the most recent advances delivered by a diverse group of researchers, including early-career scientists, emerging talents, and established experts.

Poster Contributions: All participants will have the opportunity to present their research results, including work that, although still in progress, can stimulate discussion. The poster session will be held on Monday, June 2nd, starting at 6 PM. However, we encourage all participants to keep their posters holding throughout the entire conference, so they can be viewed, discussed, and referenced at any time.

These contributions are organized into thematic blocks throughout the program.

Day 1 (Monday 2nd June) will focus on molecular qubits, including topics as synthesis and applications, optical activity and magnetic molecules at interfaces.

Day 2 (Tuesday 3rd June) will cover topics related to quantum devices and applications, magnetic molecules at the interfaces (including 2D materials), surface magnetism, molecular junctions.

Day 3 (Wednesday 4th June) will primarily address molecule-interface properties, quantum theory, spinelectric coupling.

	Monday - 2/6		Tuesday - 3/6		Wednesday - 4/6	
08:00	Registration					
08:30	Opening					
09:00	R. Sessoli	09:00	F. Luis	09:00	L. Hueso	
09:45	M. Ruben	09:45	T. van der Sar	09:45	M. Coey	
10:20	F. Tuna	10:20	H. Stern	10:20	J. Liu	
10:45	Coffee break	10:45	Coffee break	10:45	Coffee break	
11:15	K. Pedersen	11:15	S. Mañas-Valero	11:15	M. Benini	
11:40	M. Ozerov	11:40	P. Martizez-Perez	11:40	M. Sharma	
	S. Chorazy	12:05	M. Senge		D. Janas	
	A. Powell		M. Mannini		A. Riminucci	
12:25	Lunch	12:35	Lunch		A. Ferretti	
14:15	S. Bayliss	14:15	P. Ruffieux	12:40	Lunch	
14:40	A. Chiesa	14:50	Y. Bae	14:30	J. Lado	
15:05	S. Ciuti	15:15	P. Wilke	14:55	L. Mariano	
	S. Gorgon		M. Slota		G. Lupi	
	M. Galante	15:45	Coffee break		E. Macaluso	
15:50	Coffee break	16:15	E. Scheer	15:40	Coffee break	
16:20	A. Bellec	16:40	J. Thomas	16:10	M. Cinchetti	
16:45	M. Briganti		P. Gehring	16:35	W. T. Morrillo	
17:10	E. Rentschler	17:10			M. Pizzochero	
	C. Sanudo		Group Picture	K. Radhika		
	C. Calzado		17:20 Closing		Closing	
18:00	Poster Session	17:30	Bus to Social Dinner		Closing	

Tutorials	40' talk + 5' discussion	
Key-note	20' talk +5' discussion	
Invited	20' talk + 5' discussion	
Contributed	12' talk +3' discussion	

TALKS DETAILS

Speaker	Title
Y. Bae	Atomic-Scale Quantum Science with Spins on Surfaces
S. Bayliss	Chemically tuneable room-temperature optically detected coherent spin control for quantum sensing
A. Bellec	Spin-crossover molecules / ferromagnetic interfaces
M. Benini	The Emergence of Correlated Ferromagnetic Glass in FM/Molecule hybrid systems
M. Briganti	Metallocene Pawns on the Surface Chessboard: an Ab Initio Perspective
C. Calzado	Spin-state switching of strapped Ni-porphyrin complexes deposited on metal surfaces
A. Chiesa	Chirality-Induced Spin Selectivity in Donor-Acceptor Molecules: a resource for quantum technologies
S. Chorazy	Controlling charge and properties of luminescent lanthanide molecular nanomagnets through the attachment of cyanido metalloligands
M. Cinchetti	Light-driven modulation of proximity-enhanced spin precession frequency in the Co/C60 interface
S. Ciuti	Light-induced behaviour of Cr-based antiferromagnetically-coupled heterometallic systems
J. M. D Coey	Amorphous Rare-earth Transition Metal Alloys Revisited
A. Ferretti	Antiferromagnetic spinterfaces based on transition metal oxides
M. Galante	Quantum spin decoherence in radical pairs mediated by chiral bridges
P. Gehring	Enhancing the performance of Molecular Heat Engines by Correlations
S. Gorgon	Energetic requirements for luminescence in radical molecules
L. Hueso	Tuning 2D magnetic materials with molecular layers
D. Janas	Exploring electron correlation at 3d ferromagnetic-organic interfaces
R. Kataria	Enabling Electrical Readout of Molecular Quantum Bits
J. Lado	Hamiltonian learning triplons and high-order topological order in nanoscale quantum magnets
J. Liu	Chemical Tuning of the Quantum Spin-Electric Coupling in Molecular Nanomagnets
F. Luis	Quantum circuits with molecular spins: opportunities and challenges
G. Lupi	Hamiltonian learning quantum magnets with non-local impurity tomography
E. Macaluso	Simulating Open Quantum Systems with Molecular Spin Qudits
S. Mañas-Valero	A twist on 2D spintronics: from van der Waals magnets to single spin magnetometry
M. Mannini	Thiahelicene-based junctions to explore CISS effect in self-assembled monolayers
L. Mariano	The role of electronic excited states in spin-lattice relaxation of molecular qubits
M. J. Martinez- Perez	Van der Waals magnonic cavities
W. Morrillo	Ab initio design of molecular qubits with electric field control
M. Ozerov	Spectroscopic unveiling of spin-phonon coupling in Yb(trensal)
K. Pedersen	Chemical Engineering of Quantum Phenomena and Emergent Properties in 2D Molecule- Based Nets
M. Pizzochero	Electrically-tunable ultra-flat bands and π -electron magnetism in graphene nanoribbons
A. Powell	Toroidal magnetic moments and dark states
E. Rentschler	Magnetic Anisotropy in mixed 3d-4f Metallacrowns: from bulk to surface
A. Riminucci	Spintronic advantage of molecular spin-valves for neuromorphic computing
M. Ruben	Quantum Computing with Molecules
P. Ruffieux	Nanographene Spin Chains

E. C. Sañudo	Integrating molecules in devices: surface deposition of 2D arrays of qubits
E. Scheer	Conventional versus Singlet-Triplet Kondo Effect in Blatter Radical Molecular Junctions: Zero- bias Anomalies and Magnetoresistance
M. Senge	Rigid Hydrocarbon Scaffolds as Isostere Tectons for On-surface Chemistry
R. Sessoli	Toward Quantum Technologies with Magnetic Molecules: What is Missing?
M. Slota	Magnetic States in Quantum Carbon and Rare-Earth Porphyrin Units
H. Stern	A quantum coherent spin defect in hexagonal boron nitride at ambient conditions
J. Thomas	Single-molecule electrical measurements of intramolecular exchange interactions
F. Tuna	Quantum Decoherence in Molecular Qubits Probed by EPR
T. van der Sar	Magnetic imaging of spin waves and supercurrents using spins in diamond
P. Willke	Quantum Spin-Engineering in On-Surface Molecular Ferrimagnets

POSTER SESSION DETAILS

Presenter	Title of your Abstract	no.
R. Ahmed	Substitution Position and Pattern-Controlled Constructive and Destructive Quantum Interference in Isoelectronic BN-Embedded Coronene	1
J. Alday	Spin-Crossover (SCO) iron (II) complex deposite on Cu(111): a combined study using wavefunction and DFT-based approaches	2
E. Aoustin	Towards switchable magnetic tunnel junction based on polyoxometalates monolayer	3
J. Arnold	Scanning Tunneling Microscopy and Spectroscopy of YbPc2 Molecules	4
L. Bauder	Self-Assembled Monolayers of Molecular Spin Qubits	5
C. Bigelli	Study of magnetic anisotropy of lanthanide complexes through ab initio methodologies	6
J. Braun	Shining Light on Relaxation Dynamics in 3d-4f Single Molecule Magnets	7
V. Briganti	Predicting spin-phonon relaxation with machine learning	8
S. Chakraborty	Modulating Spin States and Magnetic Properties in Molecular Adsorbates on CrI3 for Spintronic Applications	9
N. Chanda	On the formulation of fourth- and sixth-order time-local generators in spin-phonon relaxation theory	10
J. Chomiuk	Spin modification by chemical oxidation of paramagnetic porphyrin oligomers	11
C. del Río Bueno	Remote polariton-polariton interactions mediated by superconducting circuits for quantum applications	12
D. Dzierżek	Octacyanoniobate(IV) as an electronic spin qubit and a potential 10-level electronuclear spin qudit	13
M. Fornasarig	Electronic Structure of Organic Hydrocarbon Radicals: A Multi-Methodological Study	14
L. Frangoulis	Accelerating High Throughput Studies of Single Ion Magnets	15
G. Fratesi	Adsorption of phthalocyanines and porphyrins for tuning and functionalization of transition metal oxide surfaces	16
T. Georgiou	Quantum Spin Effects in Chiral Molecules: Enantiospecific NMR as a Tool for Chiral Discrimination	17
S. Gimenez- Santamarina	A fully ab initio exploration of Spin–Lattice Relaxation in Gadolinium-based complexes	18
A. Halkseven	Understanding the Influence of Electronic Configuration on Magnetic Coupling in Multispin Systems	19
C. Hogan	Ab Initio Description of Vibronic Emission Bands in a Yb(III) Complex	20

	J. Hurtado	Mechanoelectric sensitivity reveals destructive quantum interference in single- molecule junctions	21
	J. Janetzki	Magnetic Anisotropy of a Potential Nickel(II) Molecular Spin Qubit	22
	Z. Khatibi	Spin polarized VHE in proximitized graphene	23
	N. Montenegro- Pohlhammer	Voltage-induced modulation of the magnetic exchange in binuclear Fe(III) complex deposited on Au(111) surface	24
	M. Muppal	Effect of Film Thickness and Substrate on Spin Crossover Molecules Grown on Graphene	25
	Moritz Nau	Electrically Conductive Macrocycles with an Antiaromatic 8π Electron Core	26
	S. Oh	Surface characterization and electronic properties of YPc2 molecular spin qubit candidate interfaced with Cu (111)	27
	S. Oh	Room-Temperature Quantum Sensing of Magnetic fields Using 15N@C60 Molecular Spins	28
	F. Pereyra	Simulation of spin-phonon interaction for molecular quantum bit systems	29
	J. Pirard	Seebeck coefficient as a spectroscopy technique for molecular junctions	30
	E. Powell	Chiral Diradicals for Quantum Technologies: Spin-Optical Control in a Trityl– Binaphthalene System	31
L	L. Rieger	Molecular conductance of diaryl amine capped carbon-bridged oligo(phenylene vinylene)s	32
	C. Ryan	Decoherence of molecular spins in crystals: nuclear vs electronic dipolar spin baths	33
	R. Sánchez-de- Armas	Co2+ and Cu2+ magnetic dimeric metal-porphyrin rings mechanically-bonded around carbon nanotubes: how nanotube defects modulate magnetic properties	34
	G. Sansone	Decoherence Mitigation in Molecular Qudits via Eigenstates Engineering	35
	F. Santanni	Porphyrins as platforms to engineer exchange coupling interactions in multi-qubit architectures	36
	A. Sarkar	Probing the Electronic Excitations of Vanadyl and Copper Tetraphenylporphyrinate using Multiconfigurational Methods	37
	J. Strohsack	Dynamical proximity-induced magnetism at cobalt/molecular interfaces	38
	V. Wakchaure	Stable Carbazole-Based Chichibabin Diradicaloid with Redshifted Absorption and Enhanced Photoluminescence	39
	J. Zolg	Design Strategies for High Performance Light-emitting Triarylmethyl-derived Radicals	40
	M. Zychowicz	Ab initio simulations of the complex A.C. susceptibility for single-molecule magnets embedded in coordination networks	41

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TRINITY COLLEGE DUBLIN (TCD)

The 4th Edition of ECMolS will take place in Dublin, at the historic and internationally renowned Trinity College Dublin. Founded in 1592 by Queen Elizabeth I, Trinity College Dublin is Ireland's oldest and most prestigious university. Located in the heart of Dublin, the college blends historic grandeur with cutting-edge research. Its iconic campus features elegant Georgian architecture and the renowned Long Room Library, home to the 9th-century Book of Kells, one of the world's most treasured manuscripts.

With a legacy of excellence spanning over four centuries, Trinity has produced celebrated alumni such as Oscar Wilde, Samuel Beckett, and Mary Robinson. Today, it stands as a globally recognized institution, offering world-class education and research across disciplines. Trinity continues to shape the future while proudly preserving its rich intellectual and cultural heritage.

To learn more about TCD's history: TCD history

SCHOOL OF PHYSICS

The School of Physics at Trinity College Dublin has a distinguished history dating back to 1710, with earlier contributions from alumni like William Molyneux. Early figures such as Richard Helsham helped shape physics education, while the 19th century marked a golden era with renowned scholars like Hamilton, Lloyd, and Fitzgerald, who influenced modern physics and helped establish the Physical Laboratory. In the 20th century, Nobel laureate Ernest Walton, famous for splitting the atom, became a leading figure. Today, the School holds a prominent position in Irish and European physics research.

More information can be found here: <u>SoP history</u>

AMBER AND CRANN RESEARCH CENTRE

CRANN is Trinity College Dublin's largest research institute and Ireland's leading centre for nanoscience, uniting over 300 researchers across various disciplines, including Physics, Chemistry, Medicine, Engineering and Pharmacology. It co-hosts the SFI-funded AMBER Centre, which collaborates with academic and industry partners to develop advanced materials for sectors like ICT and healthcare. CRANN operates from two state-of-the-art facilities, including the Naughton Institute and the Advanced Microscopy Laboratory, home to Ireland's most advanced microscopy equipment. More information can be found here: <u>CRANN</u> webpage

AMBER is the Research Ireland (formerly Science Foundation Ireland) Centre for Advanced Materials and BioEngineering Research. The Centre brings a multidisciplinary partnership between leading academics in Advanced Materials Science, BioEngineering and Industry. Working collaboratively, we develop new materials and devices for the ICT, medical devices, energy, and sustainable industrial technology sectors. Today, society is faced with many technological and environmental challenges, from sustainability and reducing its carbon footprint to next-generation personalised healthcare. By partnering with highly specialist Research faculties across Ireland, AMBER brings excellence in advanced research, innovation, and knowledge from multiple industry sector projects to our collaborative partners, industry, and society at a national and global level.

AMBER is hosted by Trinity College Dublin, in partnership with CRANN (Centre for Research on Adaptive Nanostructures and Nanodevices) and the Trinity Centre for Biomedical Engineering, RCSI University of Medicine and Health Sciences, University College Cork, University of Galway, Dublin City University, TU Dublin, Tyndall National Institute, University of Limerick, University College Dublin and the Technological University of the Shannon: Midland West.



How to get to Trinity College Dublin

Traveling from Dublin Airport to Trinity College is simple and convenient. Both **Aircoach** and **Dublin Express** buses operate directly from **outside Terminal 2**, offering frequent services to the city centre. A one-way ticket costs approximately €10. These buses stop within walking distance of Trinity College Dublin. Tickets can be purchased at the kiosk located next to the bus stop or booked online in advance at the following links:

<u>Aircoach</u>

Dublin Express



WHERE IS LUNCH SERVED?

Lunch will be served in Trinity College's historic **Dining Hall**, a magnificent space built in 1790 that stands as a testament to the university's rich architectural and cultural heritage.

The hall is in the northern part of campus, overlooking Parliament Square and right next to the College Chapel. Please note that the Dining Hall is approximately a **10-minute walk** from the Hamilton Building. We kindly recommend all attendees to keep an eye on the schedule to ensure a timely return for the afternoon sessions.

WHERE IS THE CONFERENCE HALL?

The conference will be held in the **MacNeill Theatre**, **Hamilton Building**, located on the southeast side of Trinity College Dublin. It is easily accessible from both the **Pearse Street Gate** and the **Lincoln Place Gate**.

The conference hall is located on the 1st floor. Upon arrival, please proceed to the registration desk, located at the Hall next to entrance, where our staff will assist you with your registration, name tags, and provide your conference booklet.

SOCIAL DINNER VENUE

The Social Dinner will take place at the Merry Ploughboy Gastro Pub, an award-winning venue celebrated for its authentic Irish music and dance performances. This traditional pub offers a unique and immersive cultural experience, allowing attendees to enjoy delicious food and drinks while soaking in the vibrant atmosphere of Irish hospitality. **Transportation has been arranged for all participants.** Please make sure to be at the Hamilton building entrance **no later than 17:30** for departure.