



European Workshop on Theoretical Approaches of Molecular Magnetism

Roz Armor Village Vacances. Erquy. France

May 30 - June 3 2022

Program

Monday 30

17:30 – Introduction (Boris Le Guennic)

17:40 – Ria Broer

18:00 – Frank Neese

Colour code | 60-minute talk 40-minute talk
20-minute talk Jujols X Events

Tuesday 31 | Morning #1 | 09:00 – 10:20

09:00 – Eric Collet

10:00 – Léo La Droitte

Coffee break | 10:20 – 10:50

Tuesday 31 | Morning #2 | 10:50 – 12:10

10:50 – Hélène Bolvin

11:30 – Grégoire David

Lunch break | 12:10 – 14:20

Tuesday 31 | Afternoon #1 | 14:20 – 16:00

14:20 – Nathalie Guihéry

15:00 – Barthélémy Pradines

15:20 – Nicolas Montenegro

15:40 – Aitor Sanchez

Coffee break | 16:00 – 16:30

Tuesday 31 | Afternoon #2 | 16:30 – 18:10

16:30 – Olivier Cadot

17:30 – Nicolas Foglia

17:50 – Shashank Rao

Thursday 2 | Morning #1 | 09:00 – 10:20

09:00 – Celestino Angeli

10:00 – Jean-Paul Malrieu II

Coffee break | 10:20 – 10:50

Thursday 2 | Morning #2 | 10:50 – 12:10

10:50 – Ibério de P. R. Moreira

11:30 – Daniel Santa Lucia

Lunch break | 12:10 – 14:20

Thursday 2 | Afternoon #1 | 14:20 – 16:00

14:20 – Maxime Grasser

15:00 – Nelson David Arias Olivares

15:20 – Raul Santiago

15:40 – Jordi Cirera

Coffee break | 16:00 – 16:30

Thursday 2 | Afternoon #2 | 16:30 – 17:50

16:30 – Coen de Graaf

17:10 – Roundtable

Wednesday 1 | Morning #1 | 09:00 – 10:20

09:00 – Xavier Rocquefelte

10:00 – Jordi Ribas

Coffee break | 10:20 – 10:50

Wednesday 1 | Morning #2 | 10:50 – 12:10

10:50 – Mihail Atanasov

11:30 – Jean-Paul Malrieu I

Lunch break | 12:00 – 14:30

Excursion

Friday 3 | Morning #1 | 09:00 – 11:10

09:00 – Jean-Paul Malrieu III

09:20 – Vijay Gopal

10:00 – Léo Gaspard

10:20 – Rémi Maurice

11:00 – Concluding remarks

Lunch box

Jujols X European Workshop on Theoretical Approaches of Molecular Magnetism

Roz Armor Village Vacances, Erquy, France May 30 - June 3 2022

Monday 30

17:30 – Introduction

17:40 – Ria Broer | *On the development of computational chemistry*

18:00 – Frank Neese | *Some thoughts on the future of quantum chemical software development and recent progress in multi-reference methods*

Tuesday 31

09:00 – Eric Collet | *Disentangling ultrafast electronic and structural dynamics in photomagnetic materials*

10:00 – Léo La Droitte | *Organolanthanide complexes: ab initio electronic structure investigation and magnetic properties rationalization*

Coffee break | 10:20 – 10:50

10:50 – Hélène Bolvin | *Magnetic properties of actinide complexes*

11:30 – Grégoire David | *Towards a general and consistent evaluation of magnetic exchange couplings in KS-DFT*

Lunch break | 12:10 – 14:20

14:20 – Nathalie Guihéry | *Physics of the Dzyaloshinskii-Moriya interaction*

15:00 – Barthélémy Pradines | *Impact of the electric field on magnetic parameters: disruptive Dzyaloshinskii-Moriya interaction*

15:20 – Nicolas Montenegro | *A photo-induced spin crossover based molecular switch and spin filter operating at room temperature*

15:40 – Aitor Sanchez | *Many-Electron Tight Binding model applied to singlet fission*

Coffee break | 16:00 – 16:30

16:30 – Olivier Cador | *An experimental approach of the relaxation of the magnetic moments in lanthanide-based single-molecule magnets*

17:30 – Nicolas Foglia | *Including vibrational effects in MCD calculations*

17:50 – Shashank Rao | *Ab-Initio and ligand field analysis of structural variations of an air-stable single-ion magnet displaying magnetic blocking up to 4.0 K*

Wednesday 1

09:00 – Xavier Rocquefelte | *High-Pressure tuning of magnetism and ferroelectricity in multiferroic mixed-anion cuprates*

10:00 – Jordi Ribas | *Solid-state effects on the singlet-triplet energy gaps of switchable biradicals*

Coffee break | 10:20 – 10:50

10:50 – Mihail Atanasov | *Magnetic Exchange and Valence Delocalization in a Mixed Valence $[Fe^{II}Fe^{III}Te_2]^+$ Complex: Insights From Theory and Interpretations of Magnetic and Spectroscopic Data*

11:30 – Jean-Paul Malrieu I | *The difficult exploration of a chemical utopia*

Thursday 2

09:00 – Celestino Angeli | *Multireference Perturbation Theory: the n -electron valence state approach*

10:00 – Jean-Paul Malrieu II | *Can one learn something from a Fully Contracted approach?*

Coffee break | 10:20 – 10:50

10:50 – Ibério de P. R. Moreira | *Evidence for low-lying correlated gapped states in strained graphene and graphenic 2D-COFs*

11:30 – Daniel Santa Lucia | *Antiferromagnetic Exchange and Metal–Metal Bonding in Roussin's Black Sulfur and Selenium Salts*

Lunch break | 12:10 – 14:20

14:20 – Maxime Grasser | *In silico chiroptical properties of organo-lanthanide complexes*

15:00 – Nelson David Arias Olivares | *Magnetic behavior of encapsulated Single Molecules Magnets*

15:20 – Raul Santiago | *Molecular Orbital Descriptor Approach (MODA): A Machine Learning descriptor based on first principles to predict magnetic couplings in organic magnets*

15:40 – Jordi Cirera | *Using electronic structure methods to model Spin-Crossover processes in Inorganic Systems: From molecules to crystals*

Coffee break | 16:00 – 16:30

16:30 – Coen de Graaf | *Magnetic interactions with non-orthogonal configuration interaction*

17:10 – Roundtable

Friday 3

09:00 – Jean-Paul Malrieu | *Are the formal requirements of the many-body problem made obsolete by the fantastic progresses of our computational resources?*

09:20 – Vijay Gopal | *A pedagogical discussion of the size-consistency issue for selected configuration interaction methods*

10:00 – Léo Gaspard | *Building model Hamiltonians for solids*

10:20 – Rémi Maurice | *On the CAS explosion in polynuclear transition metal complexes*

11:00 – Concluding remarks