

JUJOLS XII

« *European Workshop on Theoretical approaches of Molecular Magnetism.* »

Fischer auditorium, Faculty of Chemistry, 4 Rue Blaise Pascal, 67000 Strasbourg - France.

May 26th-30th, 2025

Organizers: Vincent ROBERT (vrobert@unistra.fr), Oussama BINDECH (obindech@unistra.fr), Emilie RANCHON (eranchon@unistra.fr), Guillaume ROUAUT (rouaut@unistra.fr) - Laboratory of Quantum Chemistry of Strasbourg.

Monday, May 26th

1:45 PM - 2:00 PM Opening words from the organizing team.

2:00 PM - 2:30 PM « Many-electron tight binding parametrized by NOCI-F ». Coen DE GRAAF, Quantum Chemistry Group, URV, Tarragona - Spain.

2:30 PM - 3:00 PM « NOCI calculations on stacks of indolonaphtyridine moieties ». Xavier LÓPEZ, Rovira i Virgili University - Spain.

3:00 AM - 3:30 AM « Treatments of periodic correlated materials ». Jean-Paul MALRIEU, Laboratory of Quantum Chemistry and Physics, Toulouse - France

3:30 PM - 4:00 PM Discussion

4:00 PM - 4:30 PM Coffee break

4:30 PM - 5:00 PM « Impact of the electric field on the interactions of the anisotropic spin Hamiltonian ». Nathalie GUIHERY, Laboratory of Quantum Chemistry and Physics, Toulouse - France.

5:00 PM - 5:30 PM « Approximate fourth-order n-electron valence state perturbation theory: implementation and application ». Emily KEMPFER, Max-Planck Institut für Kohlenforschung, Department of Theory and Spectroscopy - Germany.

5:30 PM - 6:00 PM « Hyperfine transitions in lanthanide complexes ». Hélène Bolvin, Laboratory of Quantum Chemistry and Physics, Toulouse - France.

6:00 PM - 6:30 PM Discussion

Tuesday, May 27th

- 9:00 AM - 9:30 AM « Electronic Structure, Spectroscopy and Decompositions of Carbon Dioxide and its Mono- and Dianions ». Mihail ATANASOV, Max-Planck Institut für Kohlenforschung, Department of Theory and Spectroscopy - Germany.
- 9:30 AM - 10:00 AM « NOCI-F Calculations on stacks up to 10 Indolonaphthyridine molecules ». Ionut-Octavian STAN, Rovira i Virgili University, Tarragona - Spain.
- 10:00 AM - 10:15 AM Discussion

10:15 AM - 10:45 AM Coffee break

- 10:45 AM - 11:15 AM « Study of the microscopic interactions underlying the properties of spin liquids in Kagome networks of spin 1/2 ». Flaurant HEULLY-ALARY, Laboratory of Quantum Chemistry and Physics, Toulouse - France.
- 11:15 AM - 11:45 AM « Paramagnetic NMR Chemical Shifts of An(IV)DOTA complexes ». Victor ADEBAYO, Laboratory of Quantum Chemistry and Physics, University of Toulouse - France.
- 11:45 AM - 12:00 AM Discussion

12:00 AM - 1:45 PM Lunch

- 2:00 PM - 2:30 PM « Spin-Crossover (SCO) iron (II) complex deposite on Cu(111): a combined study using wavefunction and DFT-based approaches ». Julieta ALDAY, Department of Physical Chemistry, University of Seville - Spain.
- 2:30 PM - 3:00 PM « Modelling one- and two-phonon magnetic relaxation pathways lanthanide SMMs ». Shashank VITTAL RAO, Max-Planck Institut für Kohlenforschung, Department of Theory and Spectroscopy - Germany.
- 3:00 PM - 3:30 PM Discussion

3:30 PM - 4:00 PM Coffee break

- 4:00 PM - 4:30 PM « Spin-state switching at the single-molecule level by distortion of the coordination sphere: validation based on quantum-chemistry calculations ». Nicolas MONTENEGRO-POHLHAMMER, University of Seville - Spain.
- 4:30 PM - 5:00 PM « Tuning the spin-crossover properties of Fe(II) complexes embedded in carbon nanohoops ». Arnau GARCIA-DURAN, University of Barcelona, Institute of Theoretical and Computational Chemistry - Spain.
- 5:00 PM - 5:30 PM « Simple models to rationalize magnetic anisotropy in single molecule magnets ». Daniel ARAVENA, University of Santiago of Chile - Chile.
- 5:30 PM - 6:00 PM Discussion

Wednesday, May 28th

9:00 AM - 9:30 AM « A rigorous model Hamiltonian based analysis of open-shell conjugated organic molecules. » Amisadai LORENZO REYES, CTOM, Institute of Molecular Sciences of Marseille - France.

9:30 AM - 10:00 AM « Nitrobenzenide radical formation through single electron transfer: A density functional theory study ». Nicholas BHATTACHARJEE, Donostia International Physics Center, San Sebastián - Spain.

10:00 AM - 10:15 AM Discussion.

10:15 AM - 10:45 AM Coffee break

10:45 AM - 11:15 AM « Rational Design of Fully π -Conjugated Organic Polyradicals with Any Ground-State Multiplicity ». Sergi BETKHOSVILI, IQTCUB, Barcelona - Spain.

11:15 AM - 11:45 AM « High spin organic diradicals based on intramolecular charge transfer ». Arnau CORTÉS LLAMAS, University of Barcelona - Spain.

11:45 AM - 12:00 AM Discussion.

12:00 AM - 1:45 PM Lunch

2:00 PM - 2:30 PM « Solid-State Effects on the Competition between pi-Pairs and C-C sigma-Dimers in bis-1,2,3-Dithiazolyl Radical-based Materials ». Jordi RIBAS, University of Barcelona - Spain.

2:30 PM - 3:00 PM « From antiferromagnetic ordering to spin frustration in 2D covalent organic frameworks: a case study on graphphenyl analogues ». Iberio DE PINHO RIBEIRO MOREIRA. University of Barcelona - Spain.

3:00 AM - 3:30 AM Discussion.

3:30 PM - 4:00 PM Coffee break

4:00 PM - 4:30 PM « Towards describing f-element complexes CPL spectra using wavefunction methods ». Mathieu GASCOIN, Institute of Chemical Sciences of Rennes - France.

4:30 PM - 5:00 PM « Open-shell coupled-cluster for magnetic molecules ». Vijay GOPAL CHILKURI, CTOM/ISM2, University of Aix-Marseille - France.

5:00 PM - 5:30 PM « The very final talk with the decomposition method: can we use it beyond magnetic coupling? ». Grégoire DAVID, Institute of Chemical Sciences of Rennes - France.

5:30 PM - 6:00 PM Discussion.

Thursday, May 29th _____

3:00 PM - 5:00 PM Guided visit of Strasbourg

7:30 PM Dinner, Restaurant l'Homme Sauvage, 58 Rue Saint-Urbain, 67100 Strasbourg

Friday, May 30th

- 9:30 AM - 10:00 AM « Local potential Functional Embedding Theory ». Wafaa Makhlouf, Laboratory of Quantum Chemistry of Strasbourg - France.
- 10:00 AM - 10:30 AM « Quantum algorithm for polaritonic chemistry ». Even CHIARI, Laboratory of Quantum Chemistry of Strasbourg - France.
- 10:30 AM - 11:00 AM « Development of analytic geometric gradients of molecular properties. ». Petra PIKULOVÁ, Max-Planck Institut für Kohlenforschung, Department of Theory and Spectroscopy - Germany.
- 11:00 AM - 11:30 AM Coffee break
- 11:30 AM - 12:00 AM General Discussion & closing adress.