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 fiel 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 ».** Flaurent 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 ». Nicholus 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 BETKHOSHVILI, 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.