Agenda of the annual meeting of the MolQif PEPR Quantique Project

Monday February 9, Amphi Becquerel

14.15-14.30, Introduction
Talal Mallah

14.30-18.00, Coffee break 30 minutes at 16.00
Alessandro Lunghi, Trinity College, Dublin, Ireland
Relaxation mechanisms I, theory

19h- Dinner at Le 19 Bar Restaurant

Tuesday February 10, Amphi Becquerel

9h00-12h00, Coffee Break 30 minutes at 10.30
Alessandro Lunghi, Trinity College, Dublin, Ireland
Relaxation mechanisms II, theory

12.00-14.00 Lunch

14.00-17.30, Coffee break 30 minutes at 15.30
Serge Gambarelli, CEA-Grenoble
Pulsed EPR, experiment

17.45-18h45: Plenary meeting

19.00: Dinner at Le 19 Bar Restaurant

Wednesday February 11, Room 66

9.00-12.30, Coffee break 30 minutes at 10.30
Arzhang Ardavan, University of Oxford, UK
Computing with molecules

See page 2 for the detail of the lectures

See page 3 for Useful Information

Alessandro Lunghi

Background (1h):
1. intro to density matrix formalism; mixed vs pure states; time evolution; magnetization and FID
2. Phenomenological intro to relaxation and decoherence; T-dependence; commonly held beliefs on the mechanisms
3. Intro to the concept of ab initio open quantum systems theory
4. Open quantum systems theory: reduced density matrix; time convolutionless master equations; Markov approximation; Lindblad theorem
5. Ab initio simulations: wavefunction theory; variational principle; casscf; DFT

Relaxation time (3h):
6. History of T_1 theory: Waller, Van Vleck, Orbach, etc
7. A modern formalism for T_1 and its ab initio implementation
8. spin Hamiltonian formalism; Phonons; spin-phonon coupling
9. Direct relaxation in spin-1/2 (with examples)
10. Raman relaxation in spin-1/2 (with examples)
11. Orbach and Raman relaxation in spin>1/2 (with examples)
12. Relaxation in solid-state defects (with examples)
13. Summary of relaxation theory and chemical strategies for modulating it

Decoherence (1h):
14. Relaxation vs Dephasing; flip-flops
15. Correlation Cluster Expansion simulations
16. Dipolar interactions: electron vs nuclear spin baths; effect of dilutions and deuteration
17. Phonon-induced dephasing
18. Summary on contributions to dephasing and chemical strategies for modulating it
19. Final overview and future perspectives

Serge Gambarelli lecture's program

Introduction to pulsed EPR
1. Pulses, FID, echoes
2. The main simple pulse sequences, phase cycling

Measurement of relaxation times
1. Basic principles
2. ESEEM, spectral diffusion, and instantaneous diffusion
3. Advanced sequences for measuring T_1: saturation recovery, hole burning, etc.
4. Advanced sequences for measuring T_2 and introduction to dynamical decoupling

How to measure electronic dipolar couplings and hyperfine couplings in a complex system
1. DEER, or how to precisely measure electron–electron dipolar coupling

Arzhang Ardavan lecture's program
1. Pulsed magnetic resonance to make sure the terminology overlaps with Serge's
2. What quantum information is, and what the basic operations are in spin language
3. Examples of simple multi-spin Hamiltonians how these operations can be implemented using magnetic resonance
4. Survey the kinds of errors that can occur in single-qubit rotations (gates) and how to measure them precisely using multi-pulse sequences
5. BB1 composite pulses for correction of the dominant error (rotation angle errors), an example of "fault tolerance"
6. Principles of active "error correction" in contrast to "fault tolerance"
7. The Parma scheme for implementing active error correction on qudits
8. Recent experiment implementing the above using a S=1/2 electron spin qubit hyperfine coupled to a S=3/2 nuclear qubit.

Useful Information

•MolQif website: https://www.pepr-quantique.fr/projet/molqif/, where you can download this Agenda

•To join the WhatsApp group: https://chat.whatsapp.com/FykU8WzKbsBJJsIoAUWQ2v?mode=gi_t

•Restaurant address:
Le 19 Bar Restaurant, 19 Cours Gilbert Simondon, 91120 Palaiseau
https://www.destination-paris-saclay.com/fr/fiche/restauration/le-19-bar-restaurant-palaiseau_TFO6358507/

•Buses from Massy RER Station to Marguerite Péry Stop (15 minutes)
Line 4606: https://www.bonjour-ratp.fr/lignes-bus/rd-saclay-ligne-4606-c01567/ (Freq=10 min)
Line 5154: https://www.bonjour-ratp.fr/lignes-bus/francilite-express-ouest-ligne-5154-c01571/ (Freq=1 h)

•It is possible to have lunch at Polytechnique if you arrive a bit early on Monday and at the end of the meeting on Wednesday, just tell us (WhatsApp).