

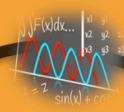
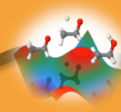
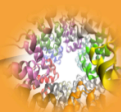


UNIVERSITÉ
TOULOUSE III
PAUL SABATIER



PROGRAMME

EMTCCM 9th ANNUAL INTENSIVE COURSE



FIRST WEEK

<i>1st-5th September</i>	Monday 1	Tuesday 2	Wednesday 3	Thursday 4	Friday 5
8h-9h	Registration	Sergio Díaz-Tendero	Didier Bégué	Laurent Maron	Laurent Maron
9h-10h	Level test	Sergio Díaz-Tendero	Didier Bégué	Laurent Maron	Laurent Maron
10h-10h30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10h30-11h30	C. Meier	Laurent Maron	Didier Bégué	M.C. Heitz	Martial Boggio
11h30-12h30	C. Meier	Laurent Maron	Didier Bégué	M.C. Heitz	Martial Boggio
Lunch					
14h-15h	C. Meier	C. Meier	C. Meier	Franck Jolibois	Franck Jolibois
15h-16h	C. Meier	C. Meier	C. Meier	Franck Jolibois	Franck Jolibois
16h-16h30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16h30-17h30	M.C. Heitz	Sergio Díaz-Tendero	Didier Bégué	Franck Jolibois	Franck Jolibois
17h30-18h30	M.C. Heitz	Sergio Díaz-Tendero	Didier Bégué	Trond Saue	

SECOND WEEK

<i>8th-12th September</i>	Monday 8	Tuesday 9	Wednesday 10	Thursday 11	Friday 12
8h-9h	Antonio Monari	Antonio Monari	Magali Benoit	Alfredo Sanchez	Germain Vallverdu
9h-10h	Antonio Monari	Antonio Monari	Magali Benoit	Alfredo Sanchez	Germain Vallverdu
10h-10h30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10h30-11h30	Martial Boggio	Nathalie Guihéry	Isabelle Baraille	Trond Saue	Mathias Rapacioli
11h30-12h30	Martial Boggio	Nathalie Guihéry	Isabelle Baraille	Trond Saue	Mathias Rapacioli
Lunch					
14h-15h	Sérgio Sousa	Nuno Cerqueira	Isabelle Baraille	Mathias Rapacioli	Germain Vallverdu
15h-16h	Sérgio Sousa	Nuno Cerqueira	Isabelle Baraille	Mathias Rapacioli	Germain Vallverdu
16h-16h30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16h30-17h30	Sérgio Sousa	Nathalie Guihéry	Nathalie Guihéry	Alfredo Sanchez	Magali Benoit
17h30-18h30	Nuno Cerqueira	Nathalie Guihéry	Nathalie Guihéry	Alfredo Sanchez	Magali Benoit

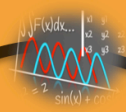
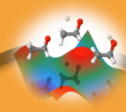
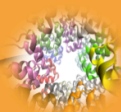


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THIRD WEEK

15th-19th September	Monday 15	Tuesday 16	Wednesday 17	Thursday 18	Friday 19
8h-9h		Arnout Ceulemans	David Sanchez	Fabien Gatti	
9h-10h		Arnout Ceulemans	David Sanchez	Fabien Gatti	
10h-10h30	Coffee break	Coffee break	Coffee break	Coffee break	
10h30-11h30	Arnout Ceulemans	David Sanchez	Jesus Ugalde	Jesus Ugalde	
11h30-12h30	Arnout Ceulemans	David Sanchez	Jesus Ugalde	Jesus Ugalde	
Lunch					
14h-15h			N. Suaud/L. Calmels	Fabien Gatti	Visit to Toulouse
15h-16h	Remco Havenith	Remco Havenith	N. Suaud/L. Calmels	Fabien Gatti	Visit to Toulouse
16h-16h30	Coffee break	Coffee break	Coffee break	Coffee break	Visit to Toulouse
16h30-17h30	Remco Havenith	Remco Havenith	Jesus Ugalde	Jesus Ugalde	Visit to Toulouse
17h30-18h30	Remco Havenith	Remco Havenith	Jesus Ugalde	Jesus Ugalde	Visit to Toulouse

FOURTH WEEK

22th-26th September	Monday 22	Tuesday 23	Wednesday 24	Thursday 25	Friday 26
8h-9h	K. Raghavachari	K. Raghavachari	K. Raghavachari	Angel Pendas	Final
9h-10h	K. Raghavachari	K. Raghavachari	K. Raghavachari	Angel Pendas	Test
10h-10h30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10h30-11h30	A. Scemama/ N. Renon	A. Scemama/ N. Renon	A. Scemama/ N. Renon	A. Scemama/ N. Renon	A. Scemama/ N. Renon
11h30-12h30	A. Scemama/ N. Renon	A. Scemama/ N. Renon	A. Scemama/ N. Renon	A. Scemama/ N. Renon	A. Scemama/ N. Renon
Lunch					
14h-15h	N. Suaud/ L. Calmels	N. Suaud/ L. Calmels		Angel Pendas	Internship
15h-16h	N. Suaud/ L. Calmels	N. Suaud/ L. Calmels		Angel Pendas	Presentation
16h-16h30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16h30-17h30	Osvaldo Gervasi	Osvaldo Gervasi	Angel Pendas		Internship
17h30-18h30	Osvaldo Gervasi	Osvaldo Gervasi	Angel Pendas		Presentation
20h00					Closing dinner



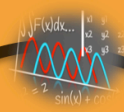
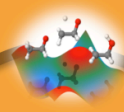
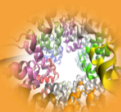
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PROGRAMME

EMTCCM 9th ANNUAL INTENSIVE COURSE



FIRST WEEK

1st-5th September

Title

M.-C. Heitz	Nonadiabatic dynamics with mixed quantum-classical methods
Laurent Maron	DFT for organometallics reactivity
Sergio Díaz-Tendero	Molecular Materials
Didier Bégué	Vibrational spectroscopy
Franck Jolibois	Theoretical NMR
Trond Saue	Introduction to Relativistic Effects in Chemistry
Martial Boggio	Quantum Chemical Methods in Molecular Photochemistry
C. Meier / Fabien Gatti	Coherent Interaction of Molecules with Light / Introduction to Molecular Quantum Dynamics

SECOND WEEK

8th-12th September

Title

Antonio Monari	QM/MM Methods in Modelling Biochemical Process
Martial Boggio	Quantum Chemical Methods in Molecular Photochemistry
Sérgio Sousa	Molecular Dynamics Simulations in Modeling Biochemical Systems
Mathias Rapacioli	Tight Binding Approaches
Nuno Cerqueira	Molecular Docking and Virtual Screening
Magali Benoit	Ab Initio Molecular Dynamics for Extended Systems: Applications to geological systems
Isabelle Baraille / Germain Vallverdu	Solids and their surfaces
Nathalie Guihéry/ Alfredo Sanchez	Multireference Calculations for the Treatment of Both Non-Dynamic and Dynamic Correlations. / Cholesky decomposition.

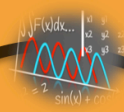
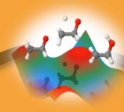
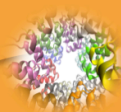


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THIRD WEEK

15th-19th September

Title

Arnout Ceulemans	Classical and Non-classical aromaticity
Remco Havenith	Valence Bond Theory
David Sanchez	Linux for Scientifical Environments
Jesus Ugalde	Advanced Density Functional Theory
N. Suaud/ L. Calmels	Magnetism in Solids: A Theoretical Study

FOURTH WEEK

22th-26th September

Title

K. Raghavachari	Advanced Correlated Methods. Composite Electronic Structure Methods. Strategies for Accurate Calculations on Large Molecules.
O. Gervasi	Modern trends and challenges in high performance/High Throughput Computing
A. Scemama/ N. Renon	Parallel Computing and Programming
Angel Pendas	Wavefunction Analysis