

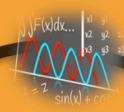
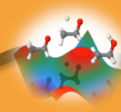
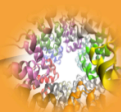


UNIVERSITÉ
TOULOUSE III
PAUL SABATIER



PROGRAMME

EMTCCM 9th ANNUAL INTENSIVE COURSE



FIRST WEEK

1st-5th September	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

8th-12th September	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	Mathias Rapacioli	Isabelle Baraille	Mathias Rapacioli	Nathalie Guihéry
11h30-12h30	Martial Boggio	Mathias Rapacioli	Isabelle Baraille	Mathias Rapacioli	Nathalie Guihéry
Lunch					
14h-15h	Sérgio Sousa	Nuno Cerqueira	Isabelle Baraille	Nathalie Guihéry	Germain Vallverdu
15h-16h	Sérgio Sousa	Nuno Cerqueira	Isabelle Baraille	Nathalie Guihéry	Germain Vallverdu
16h-16h30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16h30-17h30	Sérgio Sousa	Trond Saue	Nathalie Guihéry	Alfredo Sanchez	Magali Benoit
17h30-18h30	Nuno Cerqueira	Trond Saue	Nathalie Guihéry	Alfredo Sanchez	Magali Benoit

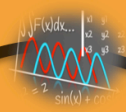
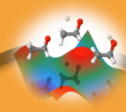
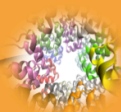


UNIVERSITÉ
TOULOUSE III
PAUL SABATIER



PROGRAMME

EMTCCM 9th ANNUAL INTENSIVE COURSE



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



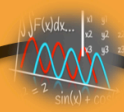
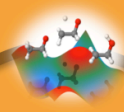
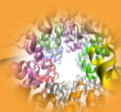
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PROGRAMME

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 / Mathias Rapacioli	Introduction to Molecular dynamics simulations. A portable intermolecular potential for molecular dynamics studies Modelling Biochemical Systems
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.

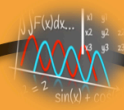
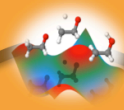
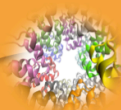


UNIVERSITÉ
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PROGRAMME

EMTCCM 9th ANNUAL INTENSIVE COURSE



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