PROGRAMME

EMTCCM 9th ANNUAL INTENSIVE COURSE
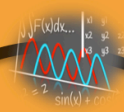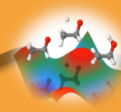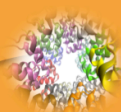
FIRST WEEK

1st-5th September	**Monday 1**	**Tuesday 2**	**Wednesday 3**	**Thursday 4**	**Friday 5**
8h-9h	Registration	Laurent Maron	Didier Bégué	Laurent Maron	Laurent Maron
9h-10h	Level test	Laurent Maron	Didier Bégué	Laurent Maron	Laurent Maron
10h-10h30	*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*
10h30-11h30	C. Meier	Sergio Díaz-Tendero	Didier Bégué	M-C. Heitz	Martial Boggio
11h30-12h30	C. Meier	Sergio Díaz-Tendero	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		

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 Guihery
11h30-12h30	Martial Boggio	Mathias Rapacioli	Isabelle Baraille	Mathias Rapacioli	Nathalie Guihery
Lunch					
14h-15h	Sérgio Sousa	Nuno Cerqueira	Isabelle Baraille	Nathalie Guihery	Germain Vallverdu
15h-16h	Sérgio Sousa	Nuno Cerqueira	Isabelle Baraille	Nathalie Guihery	Germain Vallverdu
16h-16h30	*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*
16h30-17h30	Sérgio Sousa		Nathalie Guihery	Alfredo Sanchez	Magali Benoit
17h30-18h30	Nuno Cerqueira		Nathalie Guihery	Alfredo Sanchez	Magali Benoit
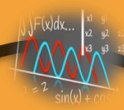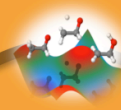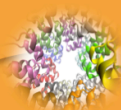
THIRD WEEK

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	
15h-16h	Remco Havenith	Remco Havenith	N. Suaud/L. Calmels	Fabien Gatti	
16h-16h30	*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*	
16h30-17h30	Remco Havenith	Remco Havenith	Jesus Ugalde	Jesus Ugalde	
17h30-18h30	Remco Havenith	Remco Havenith	Jesus Ugalde	Jesus Ugalde	

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	
9h-10h	K. Raghavachari	K. Raghavachari	K. Raghavachari	Angel Pendas	
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	**Visit to Toulouse**
15h-16h	N. Suaud/ L. Calmels	N. Suaud/ L. Calmels		Angel Pendas	**Visit to Toulouse**
16h-16h30	*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*	*Visit to Toulouse*
16h30-17h30	Gervasi Osvaldo	Gervasi Osvaldo	Angel Pendas		**Visit to Toulouse**
17h30-18h30	Gervasi Osvaldo	Gervasi Osvaldo	Angel Pendas		**Visit to Toulouse**
20h00					**Closing dinner**
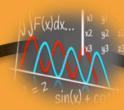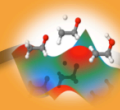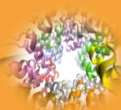
FIRST WEEK

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
Martial Boggio	Quantum Chemical Methods in Molecular Photochemistry
C. Meier / Fabien Gatti	Coherent Interaction of Molecules with Ligh

SECOND WEEK

8th-12th September

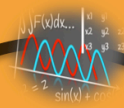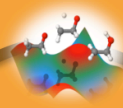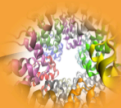|	Title
Antonio Monari	QM/MM Methods in Modelling Biochemical Process
Martial Boggio	Quantum Chemical Methods in Molecular Photochemistry
Sérgio Sousa / Mathias Rapacioli / Nuno Cerqueira	Introduction to Molecular dynamics simulations. A portable intermolecular potential for molecular dynamics studies Modelling Biochemical Systems.
Magali Benoit	Nanostructured graphene: A 2D playground
Isabelle Baraille / Germain Vallverdu	Solids and their surfaces
Nathalie Guihery/ Alfredo Sanchez	Multireference Calculations for the Treatment of Both Non-Dynamic and Dynamic Correlations.

THIRD WEEK

15th-19th September

	Title
Arnout Ceulemans	Classical and Non-classical aromaticity
Remco Havenith	Valence Bond Theory
David Sanchez	Linux for Scientific 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.
O. Gervasi A. Scemama/ N. Renon	Modern trends and challenges in high performance/high throughput Computing Parallel Computing and Programming.
Angel Pendas	Wavefunction Analysis