

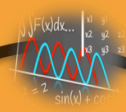
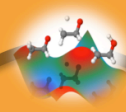
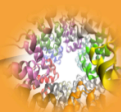


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PAUL SABATIER



# PROGRAMME

## EMTCCM 9<sup>th</sup> ANNUAL INTENSIVE COURSE



### FIRST WEEK

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

### SECOND WEEK

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

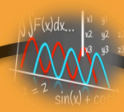
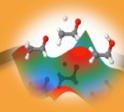
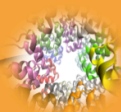


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# PROGRAMME

## EMTCCM 9<sup>th</sup> ANNUAL INTENSIVE COURSE



### THIRD WEEK

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

### FOURTH WEEK

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



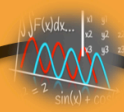
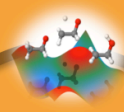
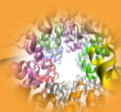
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# PROGRAMME

## EMTCCM 9<sup>th</sup> ANNUAL INTENSIVE COURSE



### FIRST WEEK

*1st-5th September*

#### Title

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

### SECOND WEEK

*8th-12th September*

#### Title

Antonio Monari	<a href="#">QM/MM Methods in Modelling Biochemical Process</a>
Martial Boggio	<a href="#">Quantum Chemical Methods in Molecular Photochemistry</a>
Sérgio Sousa / Mathias Rapacioli	<a href="#">Introduction to Molecular dynamics simulations. A portable intermolecular potential for molecular dynamics studies</a> <a href="#">Modelling Biochemical Systems</a>
Nuno Cerqueira	<a href="#">Molecular Docking and Virtual Screening</a>
Magali Benoit	<a href="#">Ab Initio Molecular Dynamics for Extended Systems: Applications to geological systems</a>
Isabelle Baraille / Germain Vallverdu	<a href="#">Solids and their surfaces</a>
Nathalie Guihéry/ Alfredo Sanchez	<a href="#">Multireference Calculations for the Treatment of Both Non-Dynamic and Dynamic Correlations.</a> / <a href="#">Cholesky decomposition.</a>

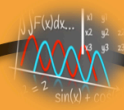
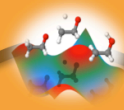
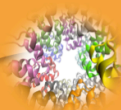


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# PROGRAMME

## EMTCCM 9<sup>th</sup> ANNUAL INTENSIVE COURSE



### THIRD WEEK

*15th-19th September*

#### Title

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

### FOURTH WEEK

*22th-26th September*

#### Title

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