

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

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



THIRD WEEK					
15th-19th September	Monday 15	Tuesday 16	Wednesday 17	Thursday 18	Friday 19
8h-9h		Arnout Ceulemans	David Sanchez	<u>Fabien Gatti</u>	
9h-10h		<b>Arnout Ceulemans</b>	<b>David Sanchez</b>	<u>Fabien Gatti</u>	
10h-10h30	Coffee break	Coffee break	Coffee break	Coffee break	
10h30-11h30	Arnout Ceulemans	David Sanchez	<u>Jesus Ugalde</u>	<u>Jesus Ugalde</u>	
11h30-12h30	Arnout Ceulemans	David Sanchez	<u>Jesus Ugalde</u>	<u>Jesus Ugalde</u>	
Lunch					
14h-15h			N. Suaud/L. Calmels	Fabien Gatti	Visit to Toulouse
15h-16h	Remco Havenith	Remco Havenith	N. Suaud/L. Calmels	<u>Fabien Gatti</u>	Visit to Toulouse
16h-16h30	Coffee break	Coffee break	Coffee break	Coffee break	Visit to Toulouse
16h30-17h30	Remco Havenith	Remco Havenith	<u>Jesus Ugalde</u>	<u>Jesus Ugalde</u>	Visit to Toulouse
17h30-18h30	Remco Havenith	Remco Havenith	<u>Jesus Ugalde</u>	<u>Jesus Ugalde</u>	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				
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				
Lunch					
14h-15h	N. Suaud/ L. Calmels	N. Suaud/ L. Calmels		Angel Pendas	Intership
15h-16h	N. Suaud/ L. Calmels	N. Suaud/ L. Calmels		Angel Pendas	Presentation
16h-16h30	Coffee break				
16h30-17h30	Osvaldo Gervasi	Osvaldo Gervasi	Angel Pendas		Internship
17h30-18h30	Osvaldo Gervasi	Osvaldo Gervasi	Angel Pendas		Presentation
20h00					Closing dinner



## **FIRST WEEK**

### 1st-5th September

Title

M.-C. Heitz Nonadiabatic dynamics with mixed quantum-classical methods

Laurent Maron <u>DFT for organometallics reactivity</u>

Sergio Díaz-Tendero Molecular Materials

Didier Béqué <u>Vibrational spectroscopy</u>

Franck Jolibois Theoretical NMR

Trond Saue <u>Introduction to Relativistic Effects in Chemistry</u>

Martial Boggio <u>Quantum Chemical Methods in Molecular Photochemistry</u>

C. Meier / Coherent Interaction of Molecules with Ligh / Introduction to Molecular Quantum

<u>Dynamics</u>

## **SECOND WEEK**

Fabien Gatti

### 8th-12th September

Title

Antonio Monari OM/MM Methods in Modelling Biochemical Process

Martial Boggio Quantum Chemical Methods in Molecular Photochemistry

Sérgio Sousa <u>Molecular Dynamics Simulations in Modeling Biochemical Systems</u>

Mathias Rapacioli <u>Tight Binding Approaches</u>

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/ Multireference Calculations for the Treatment of Both Non-Dynamic and Dynamic

Alfredo Sanchez <u>Correlations</u>. / <u>Cholesky decomposition</u>.



# **THIRD WEEK**

#### 15th-19th September

Title

Arnout Ceulemans Classical and Non-classical aromaticity

Remco Havenith Valence Bond Theory

David Sanchez <u>Linux for Scientifical Environments</u>

Jesus Ugalde <u>Advanced Density Functional Theory</u>

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 <u>Wavefunction Analysis</u>