



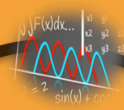
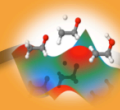
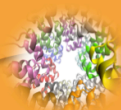
UNIVERSITÉ  
TOULOUSE III  
PAUL SABATIER



Université  
de Toulouse

# PROGRAMME

## EMTCCM 9<sup>th</sup> 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
Martial Boggio	Quantum Chemical Methods in Molecular Photochemistry
C. Meier / Fabien Gatti	Coherent Interaction of Molecules with Light

### 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.