

MASTER IN THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING

GROUP 272

FIRST SEMESTER

Subjects

Code	Name	Acronym	Coordinator
31236	Advanced Computational Techniques	ACT	Peter Reinhardt (SU)
33423	Advanced Methods in Electronic Structure, Dynamics and Molecular Modelling	AMES	Remco Havenith (RUG)
33424	Multiscale, Machine Learning and QSAR Methods Applied To Biomolecules	MML	Noelia Faginas (UNIPG)
33425	Theoretical Methods for Simulation of Materials (IMDEA)	TMSM	Johannes Gierschner
33426	Computational Chemistry Programming Project	CCPP	Jeremy Harvey (KULeuven)
33427	From Theory to Implementation: Tutorials in Theoretical Chemistry	LTTC	Nicolas Suaud (UT3)

Color coding

INFORMATICS' CLASSROOM	
CONFERENCES	
GROUP TUTORING	
EVALUATION	
LECTURES OUTSIDE THE FACULTY	

ACADEMIC COURSE 2025-2026

MASTER IN THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING

GROUP 272

UNIVERSITY OF TOULOUSE

Advanced Methods in Electronic Structure, Dynamics and Molecular Modelling

WEEK-2, FROM 15 TO 19 OF SEPTEMBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
8:15-10:05	CI/CC (Thomas Jagau)	Wavepacket Methods (Manuel Lara)	HOMEWORKS	MC Methods (NathTOie Guihery)	HOMEWORKS
10:25-12:15	Wavepacket Methods (Manuel Lara)	CI/CC (Thomas Jagau)	MC Methods (NathTOie Guihery)	VTOence Bond Theory (Remco Havenith)	VTOence Bond Theory (Remco Havenith)
12:15-16:00	BREAK	BREAK	BREAK	BREAK	BREAK
16:00-19:00	Hands-on Wavepacket Methods (Manuel Lara)	Hands-on CI/CC (Thomas Jagau)	<i>SOCIAL ACTIVITY</i>	Hand-on VTOence Bond Theory (Remco Havenith)	Hands-on MC Methods (Nicolas Suaud)

WEEK-3, FROM 22 TO 26 OF SEPTEMBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
8:15-10:05	Wavefunction AnTOysis (Angel Martin)	Non-adiabatic chemistry (Daniel Escudero)	HOMEWORKS	Relativistic Quantum Mechanics (Trond Saue)	Hands-on Relativistic Quantum Mechanics (Trond Saue)
10:25-12:15	Wavefunction AnTOysis (Angel Martin)	Non-adiabatic chemistry (Daniel Escudero)	TD-DFT (Mauro Stener)	Relativistic Quantum Mechanics (Trond Saue)	
12:15-16:00	BREAK	BREAK	BREAK	BREAK	BREAK
16:00-19:00	Hands-on Wavefunction AnTOysis (Angel Martin)	TD-DFT (Mauro Stener)	Hands-on TD-DFT (Mauro Stener)	Hands-on Non- adiabatic chemistry (Mariana Telles)	Integration Activity

WEEK-4, FROM 29 DE SEPTEMBER TO 3 DE OCTOBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
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WEEK-5, FROM 6 TO 10 DE OCTOBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
10:00-12:00					EXAM AMES IN-PERSON in each institution

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UNIVERSIDAD AUTÓNOMA DE MADRID
Advanced Computational Techniques - Quantum Computing

WEEK-7, FROM 20 TO 24 OF OCTOBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
9:00 – 13:00				ACT Pract	ACT Theory
15:00 – 19:00				ACT Pract	ACT Pract

UNIVERSIDAD AUTÓNOMA DE MADRID
Theoretical Methods for Simulation of Materials

WEEK-8, FROM 27 DE OCTOBER TO 31 OF OCTOBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
8:30 – 9:30	Introduction J. Gierschner	Molecular El. L. Zotti	BioMaterITOs P. Trouillas	Polymers J. Gamez	D. Beljonne
9:30-10:30	Exp. View 1 R. Miranda	L. Zotti	P. Trouillas	J. Gamez	D. Beljonne
11:00-12:00	R. Miranda	Het. Catalysis C. Díaz	P. Trouillas	Org. Mater. D. Beljonne	2D Mater. 2 M. Otyepka
12:00-13:00	Exp. View 2 N. Martín	C. Díaz	P. Trouillas	D. Beljonne	M. Otyepka
14:30-15:30	N. Martín	Hands-On 1 P. Aguado	Hands-On 1 P. Aguado	Hands-On 2 M. Pisarra	Hands-On 2 M. Pisarra
15:30-16:30	Intro Surfaces C. Díaz	P. Aguado	P. Aguado	M. Pisarra	M. Pisarra
17:00-18:00	2D Mater. 1 J.A. Silva	P. Aguado	P. Aguado	M. Pisarra	M. Pisarra
18:00-19:00	J.A. Silva	P. Aguado	P. Aguado	M. Pisarra	M. Pisarra

WEEK-9, FROM 3 TO 7 OF NOVEMBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
10 – 12:00					EXAM - TMSM IN-PERSON in each institution

WEEK-10, FROM 10 TO 14 OF NOVEMBER

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MASTER IN THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING

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TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
	FESTIVO				FESTIVO FACULTAD DE CIENCIAS

UNIVERSITY OF TOULOUSE
Advanced Computational Techniques
WEEK-11, FROM 17 TO 21 OF NOVEMBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
09:00 – 13:00	ACT - Theory	ACT - Theory	ACT - Theory	ACT - Theory	ACT - Theory
15:00 – 19:00	ACT - Pract	ACT - Pract	ACT - Pract	ACT - Pract	ACT - Pract

UNIVERSITY OF TOULOUSE
Multiscale, Machine Learning and QSAR
WEEK-12, FROM 24 TO 28 OF NOVEMBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
8:30 – 10:15	Introduction (L. Storch)	(F. Santini)	(M. Brut)	(R. Poteau)	(V. Poggioni)
10:30-12:15	(Simon Cross)	(M. Pezzella)	(M. Quadrini)	(F. Feixas)	(D. Laage)
12:15-13:30	LUNCH				
13:30-15:30	Introduction (L. Storch)	Hands-on (F. Santini)	Hands-on (M. Brut)	Hands-on (R. Poteau)	Hands-on (V. Poggioni)
16:00-18:00	Hands-on (Simon Cross)	Hands-on (M. Pezzella)	Hands-on (M. Quadrini)	Hands-on (F. Feixas)	Hands-on (D. Laage)

WEEK-13, FROM 1 TO 5 OF DECEMBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
					EXAM - ACT IN-PERSON in each institution

ACADEMIC COURSE 2025-2026

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WEEK-14, FROM 8 TO 12 OF DECEMBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
	FESTIVO				EXAM - MML IN-PERSON in each institution

WEEK-15, FROM 15 TO 19 OF DECEMBER

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
					Deadline to submit homework (AMES)

HOLIDAYS: 20/12/2025 TO 7/01/2025

WEEK-16, FROM 5 TO 9 DE JANUARY

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
	HOLIDAYS				Deadline to submit homework (MML, ACT and TMSM)

UNIVERSITY OF TOULOUSE

From Theory to Implementation: Tutorials in Theoretical Chemistry

WEEK-17, FROM 12 TO 16 OF JANUARY

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
9:00 – 13:00			LTTC - Theory	LTTC - Theory	LTTC – Theory
15:00 – 19:00			LTTC - Pract	LTTC - Pract	LTTC - Pract

WEEK-18, FROM 19 TO 23 DE JANUARY

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
9:00 – 13:00	LTTC - Theory	LTTC - Theory	LTTC - Theory	LTTC - Theory	
15:00 – 19:00	LTTC - Pract	LTTC - Pract	LTTC - Pract	LTTC - Pract	

ACADEMIC COURSE 2025-2026

MASTER IN THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING

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SECOND SEMESTER

Subjects

Code	Name	Acronym	Coordinator
31239	Master Thesis	TFM	Juan José Nogueira (UAM)

WEEK-3, FROM 9 TO 13 OF FEBRUARY

TIME	MONDAY 9	TUESDAY 10	WENDSDAY 11	THURSDAY 12	FRIDAY 13
10:00 – 12:00					EXAM - LTTC IN-PERSON in each institution

HOLIDAYS: FROM 28/03 TO 06/04

FROM 30 DE MARZO TO 3 OF APRIL

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
	HOLIDAYS				

WEEK-10, FROM 6 TO 10 OF APRIL

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
	HOLIDAYS				

WEEK-17, FROM 26 TO 30 OF MAYO

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
	Master thesis defense will take place this week. The date must be fixed yet				

Closing of records until 4th of June 2026 at 14:00

Evaluation of TFM, until 3rd of July 2026
Closing record of TFM, until 9th of July 2026

ACADEMIC COURSE 2025-2026

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SECOND CALL EVALUATION

WEEK FROM 15 TO 19 OF JUNE

TIME	MONDAY	TUESDAY	WENDSDAY	THURSDAY	FRIDAY
MAÑANA					Deadline to send retake exercises.
TARDE					

Closing record 1st of July 2026

Evaluation of TFM, until 22nd of September 2026
Closing record of TFM, until 24th of September 2026