

**SECOND YEAR OF THE MASTER**Subjects

<b>Code</b>	<b>Name</b>	<b>Acronym</b>	<b>Coordinator</b>
32523	<i>Advance Electronic Structure and Condensed Matter</i>	AES	Stefano Evangelisti (UPS)
32524	<i>Advanced Computational Techniques</i>	ACT	Manuel Alcamí (UAM)
32525	<i>Chemical and Molecular Dynamics - SM</i>	CMD	Jeremy Harvey (KUL)
32526	<i>Applications*</i>	AP	Itin. 1: Noelia Faginas (UNIPG) Itin. 2: Shirin Faraji (UGRO) Itin. 3: Arjan Berger (UPS) Itin. 4: Manuel Alcamí (UAM)

## COLOUR CODE:

Lectures	No colour
Lectures outside the Faculty (another Center, another University)	
Computer Room	
Evaluation	

\*For subject Application will be offered four different itineraries. The student will have to choose one.

## International Intensive Course (IIC) – Autonomous University of Madrid (from 10th September to 25th September)

### Advanced Electronic Structure and Condensed Matter (AES)

WEEK 07-11 SEPTEMBER

Online Sessions		
TIME	THURSDAY	FRIDAY
9:00-10:30	AES - Valence Bond	AES - Valence Bond
11:00-12:30	AES - Valence Bond	AES - Valence Bond

WEEK 14-18 SEPTEMBER

Hybrid - Online + in-class lessons					
TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
9:00-10:30	AES - Wavefunction	AES - Wavefunction	AES - Electron Correlation	AES - Electron Correlation	AES - Couple Cluster
11:00-12:30	AES - Wavefunction	AES - Wavefunction	AES - Electron Correlation	AES - Couple Cluster	AES - Couple Cluster
15:00-16:30	Practical Session Valence Bond		Practical Session Wavefunction Analysys		
16:30-19:00					

### Chemical and Molecular Dynamic (CMD)

WEEK 21-25 SEPTEMBER

Hybrid - Online + in-class lessons					
TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
9:00-10:30	CMD - Fundamentals	CMD - Fundamentals	CMD - Fundamentals	CMD - Fundamentals	CMD - Fundamentals
11:00-12:30	CMD - Fundamentals	CMD - Fundamentals	CMD - Fundamentals	CMD - Fundamentals	CMD - Fundamentals
15:00 - 16:30	Tutorials on MM AIMD QM/MM				
16:30 - 19:00					

### Applications (AP)

#### Itinerary one: Multiscale, Machine Learning and QSAR methods applied to biomolecules

Week 25 to 31 October

Hybrid - Online + in-class lessons					
TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
9:00 - 11:00	Theo I	Theo III	Theo V	Theo VII	Theo IX
11:30 - 13:30	Theo II	Theo IV	Theo VI	Theo VIII	Theo X
15:30 - 17:30	Pract I	Pract III	Pract V	Pract VII	Pract IX
18:00 - 19:30	Pract II	Pract IV	Pract VI	Pract VIII	Pract X

**Applications (AP)**  
**Itinerary two: Computational Chemistry Programming Project**  
**(Developed online)**

This itinerary will start from October 25th and it will end in December. Lessons will be available online to be followed and the students will have tutorials sessions scheduled with the professor to solve doubts.

**Advanced Computational Techniques (ACT)**  
**University of Groningen - The Netherlands**

WEEK 16-20 NOVEMBER

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
9:00 - 11:00	Theo I	Theo III	Theo V	Theo VII	Theo IX
11:30 - 13:30	Theo II	Theo IV	Theo VI	Theo VIII	Theo X
15:30 - 17:30	Pract I	Pract III	Pract V	Pract VII	Pract IX
18:00 - 19:30	Pract II	Pract IV	Pract VI	Pract VIII	Pract X

WEEK 14-18 DECEMBER

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
					Deadline Homework IIC

WEEK 11-15 JANUARY

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
8:30 - 10:00					Deadline homework ACT
17:30 - 19:30					

**Applications (AP)**

**Itinerary Three: From theory to implementation: tutorials in theoretical chemistry**  
**University Paul Sabatier Toulouse III - Winter school**

WEEK 25-29 JANUARY

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
8:00 - 10:00	Theo I	Theo II	Theo III	Theo IV	Theo V
10:30 - 12:30	Pract session	Pract session	Pract session	Pract session	Pract session
17:30 - 20:00	Pract session	Pract session	Pract session	Pract session	Pract session

WEEK 08-12 FEBRUARY

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
8:00 - 10:00	Theo VI	Theo VII	Theo VIII	Theo IX	Theo X
10:30 - 12:30	Pract session	Pract session	Pract session	Pract session	Pract session
17:30 - 20:00	Pract session	Pract session	Pract session	Pract session	Pract session

## WEEK 15-19 FEBRUARY

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
10:00 - 12:00					

**Applications (AP)**
**Itinerary Four: Theoretical methods for material simulation**

WEEK 05-09 March

<i>Hybrid - Online + in-class lessons</i>					
TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
9:00 - 11:00	Theo I	Theo III	Theo V	Theo VII	Theo IX
11:30 - 13:30	Theo II	Theo IV	Theo VI	Theo VIII	Theo X
15:30 - 17:30	Pract I	Pract III	Pract V	Pract VII	Pract IX
18:00 - 19:30	Pract II	Pract IV	Pract VI	Pract VIII	Pract X

## WEEK 5-9 JULY

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
	TFM DISSERTATIONS				

 Deadline for final marks submission: June 4<sup>th</sup>, 2021

TFM evaluation until July 9th, 2021.

 TFM official closing July 14<sup>th</sup>, 2021.

**Special Assessment**

 Deadline for final marks submission: July 6<sup>th</sup>, 2021.

 TFM evaluation until September 21<sup>st</sup>, 2021.

 TFM official closing September 23<sup>rd</sup>, 2021.