

First Semester

Subjects

| Code | Name | Acronym | Coordinator |
|-------------|--|----------------|--------------------------|
| 31236 | Advanced Computational Techniques | ACT | Ramón Sayós (UB) |
| 33423 | Advanced Methods in Electronic Structure, Dynamics and Molecular Modelling | AMES | Manuel Alcamí (UAM) |
| 33424 | Multiscale, Machine Learning and QSAR Methods Applied To Biomolecules | MML | Iñaki Tuñón (UV) |
| 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 | TTC | Nicolas Suaud (UPS) |

COLOUR CODE:

| | |
|---|-----------|
| Lectures | No colour |
| Lectures outside the Faculty (another Centre, another University) | |
| Computer Room | |
| Evaluation | |
| Doubs/Exercises resolution | |
| Conferences | |

UNIVERSITY OF VALENCIA

WEEK 18-22 SEPTEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|---------------|---------------|---------------|---------------|---------------|
| 9:00 – 13:00 | AMES - Theory | AMES - Theory | AMES - Theory | AMES - Theory | AMES - Theory |
| 15:00 – 19:00 | AMES - PRACT | AMES - PRACT | AMES - PRACT | AMES - PRACT | AMES - PRACT |

WEEK 25-29 SEPTEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|---------------|---------------|---------------|---------------|---------------|
| 9:00 – 11:00 | AMES - Theory | AMES - Theory | AMES - Theory | AMES - Theory | AMES - Theory |
| 15:00 – 19:00 | AMES - PRACT | AMES - PRACT | AMES - PRACT | AMES - PRACT | AMES - PRACT |

WEEK 02-06 OCTOBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------------|--------------|--------------|--------------|--------------|
| 9:00 – 13:00 | MML - Theory | MML - Theory | MML - Theory | MML - Theory | MML - Theory |
| 15:00 – 19:00 | MML - Pract | MML - Pract | MML - Pract | MML - Pract | MML - Pract |
| | CCPP* | | | | |

* The course will be focused on Coding of a program to compute the semi empirical density-functional theory tight binding energy of simple molecules.

WEEK 09-13 OCTOBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-----------------------|------------------------------|--------|
| 10:00 – 12:00 | | | EXAM - AMES online | HOLIDAY (National) | |
| 15:00 – 17:00 | | | | | |
| 17:00 – 19:00 | | | | | |

WEEK 16-20 OCTOBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-----------|----------|---------------------|
| 10:00 – 12:00 | | | | | EXAM - ML online |
| 15:00 – 19:00 | | | | | |

Master in Theoretical Chemistry and Computational Modelling GROUP 272

Advanced Computational Techniques

WEEK 23-27 OCTOBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | 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 |

WEEK 30 OCTOBER -03 NOVEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-------------------------------|----------|--------|
| 10:00 – 11:00 | | | HOLIDAY (National) | | |
| 11:00 – 12:00 | | | | | |
| 12:00 – 13:00 | | | | | |
| 13:00 – 15:00 | | | | | |
| 15:00 – 17:00 | | | | | |
| 17:00 – 19:00 | | | | | |

WEEK 06-10 NOVEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|------------------------------|----------------------------------|---|
| 10:00 – 12:00 | | | EXAM - ACT online | HOLIDAY (Madrid City) | HOLIDAY (Faculty of Science-UAM) |
| 15:00 – 17:00 | | | | | |
| 17:00 – 19:00 | | | | | |

WEEK 13-17 NOVEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--|---------|-----------|----------|--------|
| 10:00 – 14:00 | Deadline to submit 2 homework | | | | |

WEEK 20-24 NOVEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-----------|----------|--------|
| 10:00 – 11:00 | | | | | |
| 11:00 – 12:00 | | | | | |

WEEK NOVEMBER 27 TO DECEMBER 01

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|---------------|---------------|---------------|---------------|---------------|
| 9:00 – 13:00 | TMSM - Theory | TMSM - Theory | TMSM - Theory | TMSM - Theory | TMSM - Theory |
| 15:00 – 19:00 | TMSM - Pract | TMSM - Pract | TMSM - Pract | TMSM - Pract | TMSM - Pract |

WEEK 4-08 DECEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
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Master in Theoretical Chemistry and Computational Modelling GROUP 272

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|---------------|--|--|-------------------------------|--|-------------------------------|
| | | | HOLIDAY (National) | | HOLIDAY (National) |
| 13:00 - 15:00 | | | | | |
| 15:00 - 17:00 | | | | | |

WEEK 11-15 DECEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|-------------------------------|---------|--------------------|----------|--------|
| 10:00 - 12:00 | Deadline to submit 2 homework | | Exam MML online | | |
| 15:00 - 17:00 | | | | | |

WEEK 18-22 DECEMBER

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-----------|----------|-------------------------------|
| 10:00 - 11:00 | | | | | Deadline to submit 3 homework |
| 11:00 - 12:00 | | | | | |

UNIVERSITY PAUL SABATIER TOULOUSE III - FRANCE

WEEK 22-26 JANUARY

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------------|--------------|--------------|--------------|--------------|
| 9:00 - 13:00 | TTC - Theory | TTC - Theory | TTC - Theory | TTC - Theory | TTC - Theory |
| 15:00 - 19:00 | TTC - Pract | TTC - Pract | TTC - Pract | TTC - Pract | TTC - Pract |

WEEK 29 JANUARY TO 2 FEBRUARY

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------------|--------------|--------------|--------------|--------------|
| 9:00 - 13:00 | TTC - Theory | TTC - Theory | TTC - Theory | TTC - Theory | TTC - Theory |
| 15:00 - 19:00 | TTC - Pract | TTC - Pract | TTC - Pract | TTC - Pract | TTC - Pract |

SECOND SEMESTER

Subjects

| Code | Name | Acronym | Coordinator |
|-------|---------------|---------|-----------------------|
| 31239 | Master Thesis | TFM | Alicia Palacios (UAM) |

COLOUR CODE:

| | |
|---|-----------|
| Lectures | No colour |
| Lectures outside the Faculty (another Centre, another University) | |
| Computer Room | |
| Evaluation | |
| Doubs/Exercises resolution | |

WEEK 12-16 FEBRUARY

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|---------------------|----------|--------|
| 10:00 - 12:00 | | | EXAM TTCM online | | |

WEEK FEBRUARY 26 TO MARCH 01

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-----------|----------|---------------------------------|
| 10:00 - 11:00 | | | | | Deadline to submit TTC homework |

WEEK 3-7 JULY

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|--------------|--|---------|-----------|----------|--------|
| 9:00 - 13:00 | TFM defense will take place this week. The date must be fixed yet. | | | | |

TFM evaluation deadline July 5, 2024.

WEEK 3-7 JULY

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|--------------|--|---------|-----------|----------|--------|
| 9:00 - 13:00 | TFM defense will take place this week. The date must be fixed yet. | | | | |

Closing date for TFM records: July 11, 2024.

SUPPLEMENTARY ASSESSMENT

WEEK 03-06 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
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WEEK 10-14 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
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Master in Theoretical Chemistry and Computational Modelling GROUP 272

WEEK 17-21 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|-------------------------------------|
| | | | | | Deadline to submit retake exercises |
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WEEK 24-28 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
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Closing date for records, July 3, 2024.
TFM evaluation deadline: September 17, 2024.
Closing date for TFM records: September 19, 2024.