





## **First Semester**

| Subjects |   |             |                        |
|----------|---|-------------|------------------------|
| Code     | Name  | Acronym     | Coordinator            |
| 32523    | Mathematical foundations of quantum mechanics         | <i>FMMC</i> | Antonio Picón (UAM)    |
| 32524    | Statistical mechanics and applications on simulations | MEAS        | Ramón Sayós (UB)       |
| 32525    | Symmetry in atoms, molecules, and solids              | SAMS        | Pablo García (UNICAN)  |
| 32526    | Computational techniques and numerical calculations   | TC          | Pere Alemany (UB)      |
| 32527    | Theoretical chemistry methods I                       | MQT I       | Angelo Giussani (UV)   |
| 32528    | Theoretical chemistry methods II                      | MQT II      | Vícto Rayón (UB)       |
| 32529    | Deepening in methods of theoretical chemistry         | PMQT        | Marcos Mandado (UVIGO) |
| 32530    | Linux and Linux system managing                       | LIN         | Pablo Sanz (UAM)       |
| 32531    | Applied theoretical chemistry laboratory              | LQTA        | Lara Martínez (UAM)    |
| 33422    | Transversal scientific and linguistic competence      | CCLT        | Cristina Sanz (UAM)    |

#### **COLOUR CODE:**

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

<sup>\*</sup>These lessons will be held at the CCC's computer room located in Module 8.

<sup>\*\*</sup>Computer room Faculty of Science.





# Master in Theoretical Chemistry and Computational Modelling GROUP 271

#### WEEK 25-29 SEPTEMBER

| TIME         | MONDAY                                       | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|--------------|--|---------|-----------|----------|--------|
| 9:00 – 14:00 | 11:30- 14:30 UAM's Official Opening Ceremony | LIN*    | LIN*      | LIN*     | LIN*   |
|              |  |         |           |          |        |

#### WEEK 02-06 OCTOBER

| TIME         | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|--------------|--------|---------|-----------|----------|--------|
| 9:00 – 14:00 | LIN*   | LIN*    | LIN*      | LIN*     |        |
|              |        |         |           |          |        |

#### WEEK 09-13 OCTOBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY   | FRIDAY  |
|---------------|--------|---------|-----------|------------|---------|
|               |        |         |           | HOLIDAY    | HOLIDAY |
| 15:00 – 17:00 | FMMC   | MEAS    | FMMC      | (National) | HOLIDAT |
| 17:00 – 19:00 | SAMS   |         |           |            |         |

#### WEEK 16-20 OCTOBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-----------|----------|--------|
| 9:00 – 13:00  | TC*    | TC*     | TC*       | TC*      | TC*    |
| 13:00 - 15:00 |        |         |           |          |        |
| 15:00 – 17:00 | FMMC   | MEAS    | FMMC      | MEAS     | FMMC   |
| 17:00 – 19:00 | SAMS   |         |           |          | SAMS   |

#### WEEK 23-27 OCTOBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY    |
|---------------|--------|---------|-----------|----------|-----------|
| 10:00 - 11:00 | CCLT   |         | CCLT      |          | CCLT      |
| 11:00 - 12:00 | CCLT   | LQTA*   | CCLI      | LQTA*    | CCLI      |
| 12:00 – 13:00 |        |         |           |          |           |
| 13:00 - 15:00 |        |         |           |          |           |
| 15:00 – 17:00 | FMMC   | MEAS    | Sem. FMMC | MEAS     | Sem. FMMC |





# Master in Theoretical Chemistry and Computational Modelling GROUP 271

|               |        |            | I               | I             |               |
|---------------|--------|------------|-----------------|---------------|---------------|
| 17:00 – 19:00 | SAMS   |            |                 |               | SAMS          |
|               |        |            |                 |               | •             |
|               |        |            | ER -03 NOVEMBER | I             |               |
| TIME          | MONDAY | TUESDAY    | WEDNESDAY       | THURSDAY      | FRIDAY        |
| 10:00 – 11:00 | CCLT   |            |                 |               | CCLT          |
| 11:00 – 12:00 |        | LQTA*      |                 | LQTA*         |               |
| 12:00 – 13:00 |        |            | HOLIDAY         |               |               |
| 13:00 – 15:00 |        |            | (National)      |               |               |
| 15:00 – 17:00 | FMMC   | MEAS       | (National)      | MEAS          | FMMC          |
| 17:00 – 19:00 |        | SAMS       |                 | SAMS          |               |
| <u>'</u>      |        | WEEK 06-10 | O NOVEMBER      |               | -             |
| TIME          | MONDAY | TUESDAY    | WEDNESDAY       | THURSDAY      | FRIDAY        |
| 10:00 - 11:00 | 00LT   |            |                 |               |               |
| 11:00 – 12:00 | CCLT   | LQTA*      |                 | HOLIDAY       |               |
| 12:00 - 13:00 |        |            |                 |               | HOLIDAY       |
| 13:00 - 15:00 |        |            |                 | (Madrid City) | (Faculty of   |
| 15:00 – 17:00 | FMMC   | MEAS       |                 | (Maaria City) | Science)      |
| 17:00 – 19:00 |        | SAMS       |                 |               |               |
| ·             |        | WFFK 13-1  | 7 NOVEMBER      |               | •             |
| TIME          | MONDAY | TUESDAY    | WEDNESDAY       | THURSDAY      | FRIDAY        |
| 10:00 - 11:00 |        |            |                 |               |               |
| 11:00 – 12:00 | CCLT   | LQTA*      | CCLT            | LQTA*         | CCLT          |
| 12:00 – 13:00 |        |            |                 |               |               |
| 13:00 – 15:00 |        |            |                 |               |               |
| 15:00 – 17:00 | FMMC   |            | FMMC            |               | FMMC          |
| 17:00 – 19:00 |        | SAMS       |                 |               | LINUX Deadlin |

#### WEEK 20-24 NOVEMBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |  |  |
|---------------|--------|---------|-----------|----------|--------|--|--|
| 10:00 - 11:00 | CCLT   | LQTA**  | CCLT      |          | CCLT   |  |  |
| 11:00 - 12:00 | CCLT   |         | CCLT      | LQTA**   | CCLT   |  |  |
| 12:00 – 13:00 |        |         |           |          |        |  |  |
| 13:00 - 15:00 |        |         |           |          |        |  |  |
| 15:00 – 17:00 | FMMC   | тс      | FMMC      | TC       | MQT I  |  |  |
| 17:00 – 19:00 |        |         |           |          |        |  |  |

Homework





# Master in Theoretical Chemistry and Computational Modelling GROUP 271

#### WEEK NOVEMBER 27 TO DECEMBER 01

| TIME          | MONDAY          | TUESDAY | WEDNESDAY  | THURSDAY | FRIDAY |
|---------------|-----------------|---------|------------|----------|--------|
| -             | IVIONDAT        | TOLSDAT | WEDINESDAT | THURSDAT | TRIDAT |
| 10:00 – 11:00 | CCLT            |         | CCLT       |          |        |
| 11:00 - 12:00 | CCLI            | LQTA*   | LQTA*      |          |        |
| 12:00 - 13:00 |                 |         |            |          |        |
| 13:00 – 15:00 |                 |         |            |          |        |
| 15:00 – 17:00 | MQTI            | TC      | MQTI       | тс       | MQT I  |
|               | TC 1 Decelling  |         |            |          |        |
| 17:00 - 19:00 | TC 1 - Deadline |         |            |          |        |
| 17.00 15.00   | Homework        |         |            |          |        |

#### WEEK 4-08 DECEMBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY   | THURSDAY | FRIDAY     |
|---------------|--------|---------|-------------|----------|------------|
|               |        |         | HOUDAY      | HOUDAY   | HOLIDAY    |
| 13:00 – 15:00 |        |         | (National)  | HOLIDAY  | (National) |
| 15:00 - 17:00 | MQT I  | PMQT    | (Ivational) |          |            |

#### WEEK 11-15 DECEMBER

| TIME          | MONDAY      | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY                    |
|---------------|-------------|---------|-----------|----------|---------------------------|
| 10:00 - 11:00 | MEAS part I |         |           |          |                           |
| 11:00 - 12:00 | deadline    | LQTA*   |           | LQTA*    | LQTA Deadline<br>Homework |
| 12:00 - 13:00 | Homework    |         |           |          | Homework                  |
| 13:00 - 15:00 |             |         |           |          |                           |
| 15:00 – 17:00 | MQTI        |         | MQTI      |          | MQT I                     |

#### WEEK 18-22 DECEMBER

| TIME          | MONDAY                | TUESDAY                   | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|-----------------------|---------------------------|-----------|----------|--------|
| 10:00 - 11:00 |                       | 001775 111                |           |          |        |
| 11:00 - 12:00 | LQTA<br>Oral present. | CCLT Deadline<br>Homework |           |          |        |
| 12:00 - 13:00 |                       | Homework                  |           |          |        |





# UNIVERSITY OF OVIEDO INTENSIVE COURSE (3 WEEKS)

#### WEEK 8-12 JANUARY

| TIME          | MONDAY       | TUESDAY      | WEDNESDAY    | THURSDAY     | FRIDAY       |  |
|---------------|--------------|--------------|--------------|--------------|--------------|--|
| 8:30 - 10:00  | FMMC         | FMMC         | FMMC         | FMMC         | FMMC         |  |
| 10:15 - 11:45 | MQT I        |  |
| 12:00 - 13:30 | FMMC         | FMMC         | FMMC         | FMMC         | FMMC         |  |
| 13:30 – 15:00 | LUNCH TIME   |              |              |              |              |  |
| 15:00 – 17:00 | MEAS         | MEAS         | MEAS         | MEAS         | MEAS         |  |
| 17:30 – 19:30 | MEAS (Pract) |  |

#### WEEK 15-19 JANUARY

| TIME          | MONDAY     | TUESDAY | WEDNESDAY   | THURSDAY    | FRIDAY      |  |
|---------------|------------|---------|-------------|-------------|-------------|--|
| 9:00 - 11:00  | SAMS       | SAMS    | SAMS(Pract) | SAMS(Pract) | SAMS(Pract) |  |
| 11:30 - 13:30 | SAMS       | SAMS    | SAMS        | SAMS        | SAMS        |  |
| 13:30 – 15:00 | LUNCH TIME |         |             |             |             |  |
| 15:00 – 17:00 | TC         | TC      | TC          | TC          | TC          |  |
| 17:30 - 19:30 | MQT I      | MQTI    | MQTI        | MQT I       | MQT I       |  |

#### WEEK 22-26 JANUARY

| TIME          | MONDAY         | TUESDAY        | WEDNESDAY      | THURSDAY       | FRIDAY         |  |  |
|---------------|----------------|----------------|----------------|----------------|----------------|--|--|
| 9:00 - 11:00  | PMQT           | PMQT           | PMQT           | PMQT           | PMQT           |  |  |
| 11:30 - 13:30 | PMQT (Pract)   | PMQT (Pract)   | PMQT           | PMQT (Pract)   | PMQT (Pract)   |  |  |
| 13:30 - 15:00 |                | LUNCH TIME     |                |                |                |  |  |
| 15:00 – 16:30 | MQT II         |  |  |
| 16:45 – 18:15 | MQT II         |  |  |
| 18:30 – 20:00 | MQT II (Pract) |  |  |

#### WEEK 29 JANUARY TO 2 FEBRUARY

| TIME | MONDAY  | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|---------|---------|-----------|----------|--------|
|      | HOLIDAY |         |           |          |        |



# Master in Theoretical Chemistry and Computational Modelling GROUP 271

### **SECOND SEMESTER**

| _           |     |     |
|-------------|-----|-----|
| <b>VIII</b> | nıa | rtc |
| Su          | שוע | cıs |

| Code  | Name  | Acronym | Coordinator            |
|-------|---|---------|------------------------|
| 32528 | Theoretical chemistry methods II              | MQT II  | Víctor Rayón (UVA)     |
| 32529 | Deepening in methods of theoretical chemistry | PMQT    | Marcos Mandado (UVIGO) |
| 30576 | Dynamics of the chemical reactions            | DRQ     | Pablo Gamallo (UB)     |
| 31246 | Excited states                                | EE      | Javier Cerezo (UAM)    |
| 31248 | Solids  | S       | Antonio Márquez (US)   |
| 32532 | Lasers  | LA      | Alicia Palacios (UAM)  |
| 32533 | Computational biochemistry                    | ВС      | Vicent Moliner (UJI)   |

#### COLOUR CODE:

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

#### WEEK 05-09 FEBRUARY

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-----------|----------|--------|
| 10:00 – 11:00 | MOTIL  | DNAOT   | MOTIL     | DNAOT    |        |
| 11:00 – 12:00 | MQT II | PMQT    | MQT II    | PMQT     |        |

#### WEEK 12-16 FEBRUARY

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY       |
|---------------|--------|---------|-----------|----------|--------------|
| 10:00 - 11:00 | МQТ ІІ | PMQT    | MOTIL     | PMQT     | Som MOT I    |
| 11:00 – 12:00 |        | PIVIQI  | MQT II    | PIVIQI   | Sem. MQT I   |
| 12:00 – 15:00 |        |         |           |          |              |
| 15:00 – 16:00 |        |         |           |          | Seminar SAMS |

#### WEEK 19-23 FEBRUARY

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY                               |
|---------------|--------|---------|-----------|----------|--------------------------------------|
| 10:00 - 11:00 |        |         |           |          | Deadline<br>homework 1 <sup>st</sup> |
| 11:00 – 12:00 | MQT II | PMQT    |           | PMQT     | week of the IC<br>(Except MEAS)      |

#### WEEK FEBRUARY 26 TO MARCH 02

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY                                    |
|---------------|--------|---------|-----------|----------|---|
| 10:00 - 11:00 |        |         |           |          | Seminar MQT II                            |
| 11:00 – 12:00 |        | PMQT    |           |          | Deadline<br>homework IC –<br>MEAS (PRACT) |





# Master in Theoretical Chemistry and Computational Modelling GROUP 271

#### WEEK 04-08 MARCH

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY                   |
|---------------|--------|---------|-----------|----------|--------------------------|
| 15:00 – 16:00 |        |         |           |          | Deadline                 |
|               |        |         |           |          | homework 2 <sup>nd</sup> |
| 16:00 – 17:00 |        |         |           |          | week of the IC.          |

#### WEEK 11-15 MARCH

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|--------|---------|-----------|----------|--------|
| 15:00 - 16:00 |        |         |           | EXAM     |        |
| 16:00 - 17:00 |        |         |           | MQTI     |        |

#### WEEK 18-22 MARCH

| TIME          | MONDAY | TUESDAY       | WEDNESDAY | THURSDAY | FRIDAY                   |
|---------------|--------|---------------|-----------|----------|--------------------------|
| 15:00 – 16:00 |        | TENTATIVE     |           |          | Deadline                 |
| 16.00 17.00   |        | HOLIDAY       |           |          | homework 3 <sup>rd</sup> |
| 16:00 – 17:00 |        | (Madrid city) |           |          | week of IC               |

#### WEEK 25-29 MARCH

| TIME | MONDAY | TUESDAY | WEDNESDAY          | THURSDAY | FRIDAY |
|------|--------|---------|--------------------|----------|--------|
|      |        | HC      | LIDAYS (Easter Wee | ek)      |        |

#### WEEK 01-05 APRIL

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
|      |        | EXAM    |           |          |        |
|      |        | POMT    |           |          |        |

### **OPTATIVE SUBJECTS (subject to modifications at ZCAM node)**

UNIVERSITY OF ZARAGOZA (ZCAM)

#### Lasers

#### WEEK 08-12 APRIL

| TIME        | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY  |
|-------------|--------|---------|-----------|----------|---------|
| 9:00-11:00  | Theo-1 | Theo-2  | Theo-3    | Theo-5   | Pract-7 |
| 11:30-13.30 | Theo-1 | Theo-2  | Prac-3    | Prac-5   | Pract-8 |
| 15:00-17:00 | Prac-1 | Prac-2  | Theo-4    | Theo-6   |         |
| 17:30-19:00 | Prac-1 | Prac-2  | Prac-4    | Prac-6   |         |

### **Computational Biochemistry**

#### WEEK 15-19 APRIL

|             |        | _       | -         |          |         |
|-------------|--------|---------|-----------|----------|---------|
| TIME        | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY  |
| 9:00-11:00  | Theo-1 | Theo-2  | Theo-3    | Theo-5   | Pract-7 |
| 11:30-13.30 | Theo-1 | Theo-2  | Prac-3    | Prac-5   | Pract-8 |
| 15:00-17:00 | Prac-1 | Prac-2  | Theo-4    | Theo-6   |         |
| 17:30-19:00 | Prac-1 | Prac-2  | Prac-4    | Prac-6   |         |







### **Dynamics of the Chemical Reactions**

WEEK 22-26 APRIL

| TIME        | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY                      |
|-------------|--------|---------|-----------|----------|-----------------------------|
| 9:00-11:00  | Theo-1 | Theo-2  | Theo-3    | Theo-5   | Theo-7                      |
| 11:30-13.30 | Theo-1 | Theo-2  | Prac-3    | Prac-5   | Prac-7                      |
| 15:00-17:00 | Prac-1 | Prac-2  | Theo-4    | Theo-6   | Final test<br>(13:30-14:30) |
| 17:30-19:30 | Prac-1 | Prac-2  | Prac-4    | Prac-6   |                             |

#### WEEK APRIL 29 TO MAY 03

| TIME | MONDAY                         | TUESDAY | WEDNESDAY             | THURSDAY                 | FRIDAY                               |
|------|--------------------------------|---------|-----------------------|--------------------------|--------------------------------------|
|      | Deadline<br>homework<br>Lasers |         | HOLIDAY<br>(National) | HOLIDAY<br>(Madrid City) | Deadline<br>homework<br>Biochemistry |

### **UNIVERSITY OF ZARAGOZA (ZCAM)**

#### **Solid States**

University of Zaragoza (ZCAM)

WEEK 6-10 MAY

| TIME        | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY  |
|-------------|--------|---------|-----------|----------|---------|
| 9:00-11:00  | Theo-1 | Theo-2  | Theo-3    | Theo-5   | Pract-7 |
| 11:30-13.30 | Theo-1 | Theo-2  | Prac-3    | Prac-5   | Pract-8 |
| 15:00-17:00 | Prac-1 | Prac-2  | Theo-4    | Theo-6   |         |
| 17:30-19:00 | Prac-1 | Prac-2  | Prac-4    | Prac-6   |         |

#### **Excited States**

**WEEK 13-17 MAY** 

| TIME        | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY  |
|-------------|--------|---------|-----------|----------|---------|
| 9:00-11:00  | Theo-1 | Theo-2  | Theo-3    | Theo-5   | Pract-7 |
| 11:30-13.30 | Theo-1 | Theo-2  | Prac-3    | Prac-5   | Pract-8 |
| 15:00-17:00 | Prac-1 | Prac-2  | Theo-4    | Theo-6   |         |
| 17:30-19:00 | Prac-1 | Prac-2  | Prac-4    | Prac-6   |         |

#### **WEEK 20-24 MAY**

| TIME | MONDAY   | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY       |
|------|----------|---------|-----------|----------|--------------|
|      | Deadline |         |           |          | Deadline     |
|      | homework |         |           |          | homework     |
|      | Dynamics |         |           |          | Solid States |





## Master in Theoretical Chemistry and Computational Modelling GROUP 271

| WEEK 27-31 MAY |       |        |                |        |         |  |  |
|----------------|-------|--------|----------------|--------|---------|--|--|
| HORA           | LUNES | MARTES | MIÉRCOLES      | JUEVES | VIERNES |  |  |
|                |       |        | Deadline       |        |         |  |  |
|                |       |        | homework       |        |         |  |  |
|                |       |        | Excited States |        |         |  |  |

### Closing date of records June 06, 2024.

### TFM evaluation deadline July 5, 2024.

#### WEEK 3-7 JULY

| TIME         | MONDAY | TUESDAY             | WEDNESDAY           | THURSDAY           | FRIDAY |
|--------------|--------|---------------------|---------------------|--------------------|--------|
| 9:00 - 13:00 | TFM    | defense will take p | lace 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 |
|------|--------|---------|-----------|----------|--------|
|      |        |         |           |          |        |
|      |        |         |           |          |        |

#### WEEK 10-14 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY      |
|------|--------|---------|-----------|----------|-------------|
|      |        |         |           |          | Deadline to |
|      |        |         |           |          | send retake |
|      |        |         |           |          | exercises.  |

#### **WEEK 17-21 JUNE**

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
|      |        |         |           |          |        |
|      |        |         |           |          |        |

#### WEEK 24-28 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
|      |        |         |           |          |        |
|      |        |         |           |          |        |

Closing date for records, July 3, 2024.

TFM evaluation deadline: September 17, 2024. Closing date for TFM records: September 19, 2024.



## **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   | <b>AMES</b> | Manuel Alcamí (UAM)      |
| 33424    | Multiscale, Machine Learning and QSAR Methods                     | MML         |                          |
|          | Applied To Biomolecules   |             | Iñaki Tuñón (UV)         |
| 33425    | Theoretical Methods for Simulation of Materials (IMDEA)           | TMSM        | Johannes Gierschner      |
| 33426    | Computational Chemistry Programming Project                       | ССРР        | 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   |           |



# Master in Theoretical Chemistry and Computational Modelling GROUP 272

#### **UNIVERSITY OF VALENCIA**

#### WEEK 18-22 SEPTEMBER

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

#### WEEK 25-29 SEPTEMBER

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

#### WEEK 02-06 OCTOBER

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

<sup>\*</sup> 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 |            |        |
| 10:00 – 12:00 |        |         | online      | HOUDAY     |        |
| 15:00 – 17:00 |        |         |             | (National) |        |
| 17:00 – 19:00 |        |         |             |            |        |

#### WEEK 16-20 OCTOBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY    |
|---------------|--------|---------|-----------|----------|-----------|
| 10.00 12.00   |        |         |           |          | EXAM - ML |
| 10:00 – 12:00 |        |         |           |          | online    |
|               |        |         |           |          |           |
| 15:00 – 19:00 |        |         |           |          |           |
| ==:::: ==:::  |        |         |           |          |           |



# Master in Theoretical Chemistry and Computational Modelling GROUP 272

# University of Barcelona Advanced Computational Techniques

#### WEEK 23-27 OCTOBER

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

#### WEEK 30 OCTOBER -03 NOVEMBER

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

#### WEEK 06-10 NOVEMBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY  | THURSDAY      | FRIDAY       |
|---------------|--------|---------|------------|---------------|--------------|
| 10:00 – 12:00 |        |         | EXAM - ACT |               |              |
| 10.00 - 12.00 |        |         | online     | HOLIDAY       | HOLIDAY      |
| 15:00 – 17:00 |        |         |            | (Madrid City) | (Faculty of  |
| 17:00 – 19:00 |        |         |            |               | Science-UAM) |

#### **WEEK 13-17 NOVEMBER**

| TIME          | MONDAY      | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|---------------|-------------|---------|-----------|----------|--------|
|               | Deadline to |         |           |          |        |
| 10:00 - 14:00 | 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 |
| 15:00 – 19:00 | TMSM - Pract  |



# Master in Theoretical Chemistry and Computational Modelling GROUP 272

#### WEEK 4-08 DECEMBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY             | THURSDAY | FRIDAY                |
|---------------|--------|---------|-----------------------|----------|-----------------------|
|               |        |         | HOUDAY                |          | HOUDAY                |
| 13:00 – 15:00 |        |         | HOLIDAY<br>(National) |          | HOLIDAY<br>(National) |
| 15:00 - 17:00 |        |         | (IvatiOffal)          |          | (IvatiOffal)          |

#### WEEK 11-15 DECEMBER

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

#### WEEK 18-22 DECEMBER

| TIME          | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY                              |
|---------------|--------|---------|-----------|----------|-------------------------------------|
| 10:00 – 11:00 |        |         |           |          | Deadline to<br>submit 3<br>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  |

#### 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  |



# Master in Theoretical Chemistry and Computational Modelling GROUP 272

### **SECOND SEMESTER**

| _       |   | •      |      |   |
|---------|---|--------|------|---|
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|         |   |        |      |   |

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 |          |        |
| 10:00 – 12:00 |        |         | online    |          |        |

#### WEEK FEBRUARY 26 TO MARCH 01

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

#### WEEK 3-7 JULY

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

# Closing date for TFM records: July 11, 2024.

#### **SUPPLEMENTARY ASSESSMENT**

#### WEEK 03-06 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
|      |        |         |           |          |        |
|      |        |         |           |          |        |

#### WEEK 10-14 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
|      |        |         |           |          |        |
|      |        |         |           |          |        |



# Master in Theoretical Chemistry and Computational Modelling GROUP 272

#### **WEEK 17-21 JUNE**

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY        |
|------|--------|---------|-----------|----------|---------------|
|      |        |         |           |          | Deadline to   |
|      |        |         |           |          | submit retake |
|      |        |         |           |          | exercises     |

#### WEEK 24-28 JUNE

| TIME | MONDAY | TUESDAY | WEDNESDAY | THURSDAY | FRIDAY |
|------|--------|---------|-----------|----------|--------|
|      |        |         |           |          |        |
|      |        |         |           |          |        |

Closing date for records, July 3, 2024. TFM evaluation deadline: September 17, 2024. Closing date for TFM records: September 19, 2024.