## Theoretical Chemistry and Computational Modelling

### CORE COURSE

**September 28th to October 9th**

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<td><strong>School on Sustainable Entrepreneurship</strong>&lt;br&gt;A. Lagana</td>
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<td>Supercomputing: projects and networks.&lt;br&gt;A Luna</td>
<td>Tutorial on Scientific Publication.&lt;br&gt;Rob van Daelen (Elsevier), Manuel Yáñez (UAM). Tutorial on Scopus.</td>
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<td><strong>Doctorates scientific workshop.</strong>&lt;br&gt;UAM</td>
<td>Workshop on Communication in Science I. Scientific information Unit UAM</td>
<td>Writing successful proposals I&lt;br&gt;B. Herrero</td>
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School on Sustainable Entrepreneurship

Sept 28

09:00 – 09:30 Welcome (Prof. Otilia Mo – Director of the Department of Chemistry of the Universidad Autonoma de Madrid, ES)

09:30 – 11:00 Technological foundations for innovative entrepreneurship in computational services in chemistry research and education (Prof. Antonio Laganà, University of Perugia (IT))

11:00 – 11:30 Break

11:30 – 13:30

- Isidro de Pablo (CIADE) The New Knowledge Transfer Strategy of UAM

- Alejandro Arranz, Director of the Madrid Scientific Park. Scientific Parks: design and support to innovative enterprises

13:30 – 14:30 Lunch

14:30 – 16:00 From the idea to the project and from the project to the start-up (Prof. Antonio Laganà, University of Perugia (IT))

16:00-16:30 Break

16:30-18:00 Employability Dr Ray Wallace.CVAS, Nottingham (UK)
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Sept 29

09:30 – 11:00 Success story: Master-UP a spinoff of the University of Perugia for support to research and training (Dr. Noelia Faginas Lago, President of Master-UP, University of Perugia (IT))

11:00 – 11:30 Break

11:30 – 13:00 Success story: Arctur a SME for innovative compute and data resource provision (Tomi Tomi Ilijas, Arctur CEO, Nova Gorica (SL))

13:00 – 14:30 Lunch

14:30 – 16:00 Success story: eXact Lab a spinoff for support services to advanced physical science (Dr Stefano Cozzini, SISSA, Trieste (IT))

16:00 – 16:30 Break

16:30 – 18:00 Success story: Quantitative Risk Research a spinoff to support services to advanced mathematical applications (Prof. Santiago Carrillo, Universidad Autonoma de Madrid, Madrid (ES))

Sept 30

9:30- 13:30 Tutorial 'Being an entrepreneur. Dare to explore!'.

Ana Gorostegui. (Fundación Tomillo)

a. Market (standards, objectives, competitors, potential customers)

b. Product (life cycle, needs, methods of specification, development and optimisation)
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c. Economic analysis and financial resources and risks
d. Commercial strategies, quality policy, evaluation, auditing

13:00-14:30 Lunch

16:00 – 18:00 Visit to the Madrid Scientific Park

### Supercomputing: Projects and Networks

**Lecturers:** Alberto Luna and Pablo Sanz (CCC – UAM)

**Oct 01**

**Block 1**

- Organization of a Supercomputing Center.
- Supercomputing centers in the world.
- Supercomputing centers in Spain.
- Spanish Supercomputing Network (RES).
- Partnership for advanced computing in Europe (PRACE).

**Block 2**

- Comparative: CPU, GPU, MIC (Intel Xeon Phi). What do I need for my work?
- Shared and distributed memory. Relationship with programming models. Types of jobs. Scaling the number of cores. Infiniband. Speed and Latency. When is it necessary to use such an expensive network?
• Parallelization levels. Where should I calculate if my job needs N cores?.

Block 3

CCC-UAM guided visit.

Block 4

• Myths and legends of big data.
• Electrical and cooling requirements for servers. Can I host them in my office?.
• If I apply for a project, what kind of server should I order?.

Block 5

• What can I do to apply for a project in RES?.
• Mobility programs, scholarships, training and support offered by PRACE.

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<th>Research Management and Writing Successful Proposals</th>
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Lecturer: Berta Herrero (Atria Science).

Oct 01

Research Management.

• Definition of research.
• The third mission of the University.
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- The death valley.
- Research Plans, Programmes and Projects.
- Research strategies for a group, resources and budget.

**Oct 01 and Oct 08**

**Writing successful proposals workshop**

- Overview of EU funding.
- Objectives of a proposal.
- Structure of a proposal.
- Key points in H2020.
- Evaluation criteria.
- How to find the right partners.
- How was the EJD-TCCM designed and funded?

- Workshops:
  1) Budget and resources. Calculate how much a PhD costs.
  2) Winning proposals. Evaluation criteria. Key points to write good proposals.

The workshop is a mock-up of the submission and evaluation of proposals in H2020 projects. Students first write a proposal according to some objectives and evaluation criteria. Then proposals are distributed and the students evaluate all proposals, to see the referee point of view. Finally a group discussion is made to understand panel decisions. The workshop is divided in 2 days to allow time for proposal preparation and reviewing. Day 1: Students write a one-page proposal in groups. Days 3-5: Students evaluate the proposals of other groups. Day 9: Panel evaluation and discussion of the final ranking. Lessons learnt.
Tutorial on Scientific Publication and Scopus

**Tutorial on Scientific Publication**
Lecturers: Rob van Daelen (Elsevier), Manuel Yáñez (UAM).

**Tutorial on Scopus**
To be confirmed

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**Workshop on Communication in Science**

**Oct 07**

**9:00 - 9:30** Introduction and Workshop presentation (Carmela Calés, professor and UCCUAM Director).

**9:30-10:30** General View: digital platforms for classic tools (Carmela Calés, professor and UCCUAM Director).

Social Networks (FB, Twitter, LinkedIn, Research Gate), blogs, videos, podcasts and images.

**10:45-12:30** Writing science for non-scientists (John Rojas, MA, UCCUAM Journalist and Expert in Public Communication of Science).

Twits, news and articles.

**12:30-13:45** Communicating science to listeners: the art of podcasts & radio emissions (Carmen Rodríguez, PhD and Lecturer and Director of Radio Program).

**15:00-17:00** Looking at Science: making microvideos (Paloma B. Bielicka, BSc Physics, Film Director and Expert in Public Communication of Science).

**17:00-19:00** Outreach Activities (Marta Ramos, PhD Molecular Biology, Specialist in Scientific Journalism and Communication and UCCUAM Coordinator).
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Publics and ad hoc outreach activities, hands-on and exhibitions.

**Oct 08**

**9:30-13:30** Workshop Tutorial (John Rojas, Carmen Rodríguez, Paloma B., Bielicka, Marta Ramos (1h/each)).

**15:00-19:00** Presentations (Jury: John Rojas (2h), Carmen Rodríguez (2h), Paloma B. Bielicka (2h), Marta Ramos (2h), Carmela Calés (4h)).

*Based on the workshops on:*