Creating a European Space on Theoretical Chemistry and Computational Modelling (TCCM)

Worshop in Honor of Prof.
Antonio Laganà.
November 5th, 2015

Motivation:

★Crucial role of the Theoretical Chemistry and Computational Modelling on the development of modern Chemistry, modern Physics and Materials science.
(J.A. Pople and Walter Kohn. Nobel Prize in Chemistry 1998. M. Karplus, M. Levitt, A. Warshel. Nobel Prize in Chemistry 2013).

"Quantum chemistry is today used within all branches of chemistry and molecular physics [and] affords deeper understanding of molecular processes that cannot be obtained from experiments alone."

★ Need of promoting a serious and high-quality offer at the European level in this particular area.

★ Need of attaining the required critical mass to make a Master and a Doctorate viable with strong European flavor.
★ Need of an offer strongly interdisciplinary, on going from very small systems (Astrochemistry) to very large systems (proteins, catalysts, energy storage…) in a clear multi-scale approach.

Important Aspects to make our offer different

What offers our program that makes it different from other offers?

What is its European "flavor"?

It is not enough to have an excellent scientific project!!!

Transferable skills also count:
Sustainable Entrepreneurship,
Research Management,
Communication in Science (including communication to a non-expert audience)
Scientific networking,
Techniques to publish in science,
Ethical issues…

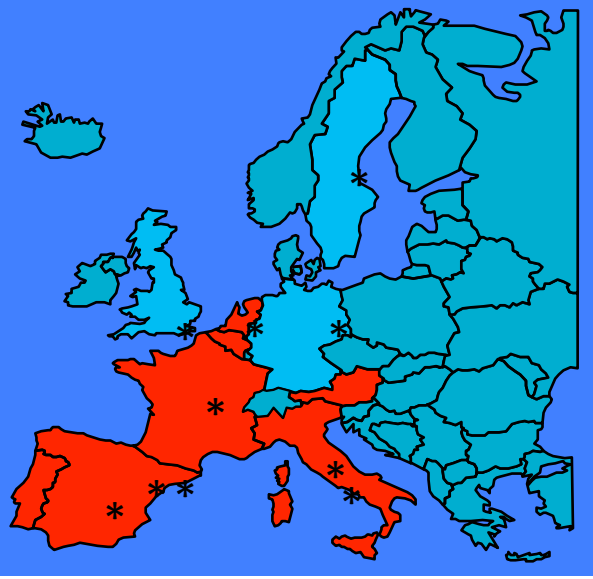
The Consortium and its structure

We did not start from scratch. Previous experience with Interuniversity Doctorate Program at the national level. Extrapolation to European level : CAM's pilot project. 2003 Meeting in El Escorial (47 Universities from 10 European countries).

In 2005 we launch a European Master on TCCM without financial support and only counting with the enthusiasm of a few. The first: Antonio

This was the first Master in Chemistry that received the Euro-Label issued by the ECTNA (European Chemistry Thematic Network Association)

First Consortium: 7 European Universities of 6 countries coordinated by the Univ. Autonoma de Madrid (UAM). For the doctorate the number was enlarged to 12 Universities and seven countries.



Main goals

★Training in an European environment, in which the students are in contact with at least three different environments.
★ Possibility of having a training in a multi-scale domain and strongly interdisciplinary, impossible to reach in a single Institution.
★ An multicultural an multilingual experience
★ Mobility strongly encouraged
★ Direct and effective contact with the productive (private) sector
★ Direct and effective contact with HPC facilities

Challenges

How is possible to offer an Integrated European Master and Doctorate with students working in different Universities and countries?

The program must ensure an homogeneous training through the organization of a large series of common mandatory activities.

But this is not enough. We must ensure homogeneity also in the evaluation of the graduates as well as in the mobility.

Structure (Master)

Two-year Master

★M1 organized locally, following common criteria which guarantee a homogeneous level.

★M2 Fully international

★ Intensive Curse on Advanced aspects and Applications. Mandatory for all students. Organized in a Rotatory base. (role of scholars)

★ Master Thesis (minimum 6 months exclusively devoted to research. Mandatory: 3 months have to be spent in a second Institution of a different country.

★ Defense in two European languages

Structure (Doctorate)

An ITN Maria S Curie program.

★ The thesis are developed in co-tutelle between two Universities of the Consortium of different countries. A double PhD title will be issued (Joint if possible).

★ In all projects the PhD candidate has to make secondments (2-10 months) in a company from the production sector.

★ Three evaluations (one per year) by an Academic Committee and experts from outside the Consortium.

★Ten common mandatory activities: Core Course, 3 Schools, 3 Tutorials, 3 Workshops.

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★ Core Course devoted to transferable skills
★ Three-body coordination (two universities and one Associate Partner.
★ Coordinated mobility along the three years of the project
★Networking among the PhD candidates through the Young Research Forum
★ A minimum of two papers accepted in peer-reviewed journals.
★ Communications to International Symposia in the last two years.
★ Defense in two European languages

Strong points:

★Possibility of choosing the best specialists in the different domains, impossible to reach in TCCM at the local level

★Interaction with other students of different countries all over the world.

★Interaction with scholars chosen among the best in non-European countries

★Possibility of working in different environments and using different techniques.

★Contact with different cultures and languages

Weak Points

★ Teaching too much concentrated during the Intensive Course

On top of that

★ Participation in teaching activities (hands-on sessions or supervising Master students)

★ Training in foreign languages

★ Enhancing science dissemination and networking : Young Researcher Forum

★ Communications to International Congresses

★ Alumni

★ Career plan and contacts with potential employers

Some final remarks

A European Joint Doctorate needs also to fulfill some other requirements:

Gender balance

Balanced distribution of the responsibilities of the Universities.

The most important risks have to be foreseen and the appropriate actions predicted.

A series of deliverables and milestones have to be well defined

A sustainability plan needs to be developed

The program should "see" beyond its end and provide the PhD candidates with some routes to explore their post-doc career.

M2 Master students in San Juan de los Reyes (Toledo) 2013

Master students in a ZCAM Course (Zaragoza) 2012

Summary:
At present TCCM (Theoretical Chemistry and Computational Modelling) is a prestigious trade mark internationally speaking, and this is the result of the enthusiasm and the many initiatives of this guy:

THANKS INDEED Antonio!!! on behalf of the whole TCCM community….. And the best for the future!!!