

EJD: TCCM
Theoretical Chemistry
and Computational Modelling

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Intervenant : M. CALATAYUD

Motivation

- Crucial role of Computational Chemistry and Modelling on the development of modern chemistry, physics, biochemistry, pharmacy and material science.

Nobel prize Chemistry: J.A. Pople and Walter Kohn (1998)

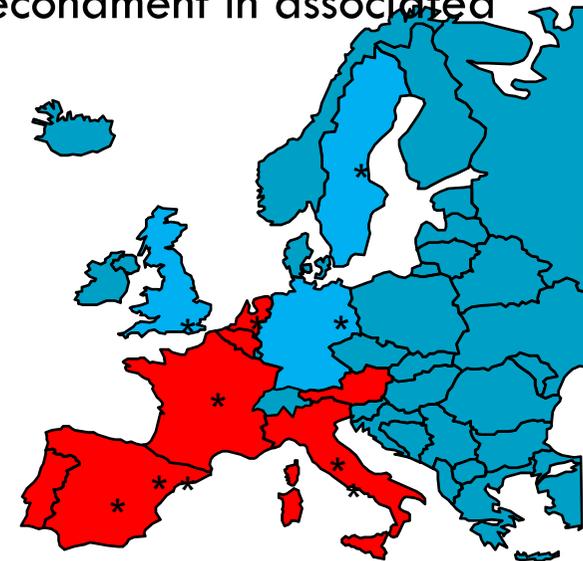
M. Karplus, M. Levitt, A. Warshel (2013)

“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 to create a European offer in this important area**
- **Need of having a minimum critical mass**
- **Need of making a rational offering in a strong interdisciplinary field (goes from very small systems (astrochemistry) to very large (proteins, catalysts...))**

The consortium & the structure

- Previous experience in a joint European Master TCCM
 - Erasmus Mundus & ECTN Euromaster
- European Doctorate already running without dedicated funds
- **Consortium** : 12 universities (beneficiaries) coordinator: UAM (Madrid, Spain)
14 partners* (non-academic): supercomputing centres, materials, bioinformatics, doctoral schools, universities
- **Structure**: Cotutelle agreement (2 beneficiaries) + secondment in associated partner



The goals

- Participation in a Europe-wide training environment
- A unique research environment. A multi-scale approach
- A multicultural and multilingual experience
- A significant mobility

- **Challenge: go beyond cotutelle to make an integrated Doctorate program**
 - Secondments in associate partners
 - Fully coordinated follow-up of the training and the research activity of the doctoral candidates
 - Common activities:
 - mandatory core course in transferable skills (no training – that should be done at Master level)
 - Annual meetings
 - Tutorials, etc.

The evaluation

- Preparation of the proposal
 - Previous experience with Master
 - Previous unsuccessful proposals EM & ITN
 - Coordination between pedagogical and administrative staff
- **Evaluation:**
 - 95.4 /100 , based on criteria: excellence, impact, implementation
 - Strong points: multisectorial exposure, role of associate partners in training, quality and experience of supervisors, sustainable joint doctorate structure
 - Weak points: soft skills training, entrepreneurship and company management, risk mitigation plan poorly described

The implementation

- Currently signing contracts, budget ~3.5 MEUR
- *Recruitment of 15 PhD candidates*
- *Scientific and personal career follow-up*
- *Organization of activities*
- *Evaluation & reporting*

Problems

- Cotutelle agreement: no “universal” convention model, needs approval of 2 universities in different countries. Usually long and complex
- Diploma: diploma supplement signed by all the universities in the consortium
- Project management

The EJD-TCCM

- ✓ **Multidisciplinary training in theoretical chemistry and computational modelling**
- ✓ **Mobility**
- ✓ **Common activities**
- ✓ **Exposure to non-academic sector**
- ✓ **Build a European training network**

