

## TCCM-ITN: Theoretical Chemistry and Computational Modelling

### Description

Theoretical Chemistry and Computational Modelling (TCCM) is emerging as a powerful tool to help in the rational design of new products and materials for pharmaceutical, chemical, energy, computer and new-materials industries. To achieve this goal, it is necessary to go beyond the traditional electronic structure studies, and merge complementary techniques that are normally not available at a single research group. The research programme of the TCCM-EJD aims at the application of computational modelling to problems demanded by the industry and with high societal relevance, namely Materials with special properties, Biomolecules at the frontier and Energy storage. The objective of the Joint Doctorate is to prepare authentic research leaders, able to develop and use multidisciplinary computational techniques (methods and software), with solid communication skills, with many contacts established through the intensive relationship with the researchers of more than 12 European universities and 14 additional partners. The TCCM-EJD launched in 2011 is based on a fully participative scientific discussion and assessment of each research project with a clear interdisciplinary character and the direct participation of the non-academic sector. The training programme puts the emphasis in common training, including 3 annual International Workshops, 3 schools on High Performance Computing and 3 tutorials. Career development opportunities are enhanced with regular inter-sectoral activities, and transferable skill education.

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