



Theoretical Chemistry and Computational Modelling

Acronimo: **TCCM**

Call: **H2020-MSCA-ITN-2014**

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Abstract: The Perugia Joint Doctoral Program (JDP) ITN-EJD-642294 in Theoretical Chemistry and Computational Modelling (TCCM) is carried out within a consortium including Madrid Autonoma (the coordinator), Barcelona, Pais Vasco, Groningen, Leiden, Leuven, Paris VI, Pisa, Porto, Stockholm, Stuttgart, Toulouse and Valencia. The JDP TCCM aims at training the students to lead the design and use of computational technologies for the application of Molecular sciences to research and industry in the field of Chemistry, Materials, Petrolchemistry, Pharmacy and Physics. The students of the doctorate are meant to become expert in the use of distributed High Performance (HPC) and High Throughput (HTC) Computing for ab initio Molecular Simulations. The specific research line carried out in Perugia is "Networked computing for ab initio modeling the chemical storage of alternative energy" in which distributed workflows are used to ab initio compute electronic structure, nuclei dynamics and efficiency of energy and mass exchanges intervening in the storage of energy from renewable sources. In particular, the reduction of carbon dioxide to methane is investigated and an industrial prototype apparatus is being built to produce carbon neutral methane in collaboration with the spinoff Master-up srl and Enea. The storage of hydrogen by adsorption on graphene is also being investigated. University of Perugia participates to TCCM with the Department of Chemistry, Biology and Biotechnology.