The TCCM-EJD project aims at applying computational modelling to strongly interdisciplinary problems demanded by the industry and with high societal impact, namely Materials with special properties, Biomolecules for new therapies and Energy storage. In the first area photo-induced isomerization processes and the design of new materials with specific nanoelectronic or nanomagnetic properties, as well as the design of graphene-based gas detectors are considered. The second includes the design of photosensitizers for cancer phototherapy, the production of photostable drugs, the characterization of drug metabolites, Aluminum Chelation Therapy, and hadron-therapy. The third is focused on the design of efficient components of photovoltaic organic cells, and energy storage. These studies require to go beyond the conventional electronic structure methods, by exploring ground and excited states. This goal can only be achieved by the joint effort of several groups with different, but complementary expertise. Consistently, the Consortium of this project is integrated by 12 European Universities and 14 partners, including 7 industrial companies.

The TCCM programme puts the emphasis in common training, including 3 Schools on High Performance Computing, and 3 Tutorials, on very used computer codes, namely ADF and SHARC and a third one to be decided. It also included a Core Course devoted to providing the ESRs with transferable skills on communication techniques, group working, and Entrepreneurship, among others. Career development opportunities are enhanced. Three annual International Workshops, the first one already held in Paris in 2016, in which the 15 ESRs discuse the research carried out with a group of worldwide recognized experts from outside the Consortium, are also mandatory.

The overall objective of the Joint Doctorate is to prepare future research leaders, able to develop and...
use multidisciplinary computational techniques (methods and software), with solid communication skills, with many contacts established through an intensive relationship with worldwide leading researchers in the field.

**Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far**

The activities of the ITN begun with a two-weeks Core Course, (Madrid, Sept. 28-Oct. 9, 2015) focused to improve the ESRs’ background on transferable skills, namely, i) communication in science, ii) formulation of work plans, iii) searching of scientific information, iv) group working, v) preparation of progress reports, vi) Entrepreneurship, vii) how to publish in Science. The Young Research Forum as a platform to the dissemination to non-experts was also created.

One School on Parallel Computing (Barcelona Supercomputing Center), and two tutorials, the first one on ADF (Amsterdam Density Functional Code) (18-22 April 2016, Software for Science and Materials (SCM), Amsterdam), and the second one on the SHARC code (Univ. of Vienna 3-7 Oct., 2016) have been organized already.

The 18-20 July 2016 took place in Paris the First Annual Workshop organized by the UPMC and Paris-Saclay. In this Workshop the 15 ESRs presented oral communications on the research carried out so far, which was evaluated by an ensemble of external experts. Discussion sessions of the ESRs and their supervisors with the external experts were also included.

During this period the ESRs progressed significantly in their research projects, as reflected in 21 publications in peer-review journals and in outreach platforms, and a total of 51 communications in different Conferences. They have participated also in different outreach activities, such as the Passion for Knowledge (Sept. 27- Oct. 1, 2016) organized by the DIPC in Spain, where they had meetings with Nobel Laureates in Chemistry, encounters with secondary school students, and published dissemination papers in the Mapping Ignorance blog (http://mappingignorance.org/). Some of them also participated in local outreach activities such as Science Weeks or nights of researchers. They also launched the Young Research Forum (YRF) creating, at the same time, two communication media, a Newsletter (https://tccm-alumni.qui.uam.es/?page_id=1930 and a Facebook forum.

**Progress beyond the state of the art and expected potential impact (including the socio-economic impact and the wider societal implications of the project so far)**

As far as the design of new materials with special properties and the analysis of their behavior under external stimulus are concerned, during this first period the study of the photoinduced isomerization of Ru complexes carried out by ESR6 was completed, whereas also significant progress was achieved in the study of materials with nanoelectronic or nanomagnetic properties, as in the work developed by ESR11 on titania nanoclusters and by ESR12 on the bistability in molecule-based magnets. The last project in this area, by ESR15, designed absorption potentials of different gases on Graphene with strong technological implications in the design of gas sensors.

The modeling of biomolecules is the main objective of four of the projects, those of ESR7, ESR8, ESR10...
and ESR14. These four projects are focused more specifically, i) on the design and characterization of photosensitizers for cancer phototherapies by analyzing the properties of bodipys, ii) on the production of photo-stable drugs by analyzing the photo-toxicity and stability of pharmaceutical excipients, iii) on the improvement of methods for the structural characterization of drug metabolites through the analysis of collisional cross sections, and iv) through the survey of Aluminum Chelation Therapy. A fifth project in this area is focused on the use of state-of-the-art techniques, based on the analysis of highly-charged-heavy ions bombardment process of these complex molecules and their aggregates, in order to gain some insight into their molecular growth processes, a part of modern cancer therapy, usually known as hadron-therapy.

In the chapter of Energy, three projects, those of ESR1, ESR2 and ESR3 are initially focused on the design of more efficient compounds for photovoltaic organic cells, with the final goal of produce more efficient devices for light harvesting. This objective requires unavoidably a good knowledge of the excited states of the systems involved in such processes, and to this goal contributes the research work developed so far by ESR1 and ESR3. The former has been working in the development of analytic Energy Gradients of Excited States within the TDDFT/MMPol framework, and the latter on the application of nonorthogonal configuration interaction techniques to calculate singlet fission efficiencies. Similarly, the research developed so far by ESR2 was focused on the study of the properties of materials with potential application in organic photo-voltaic devices, in particular N-heterocyclic carbenes in Gold (I) complexes. The remaining two projects, those being developed by ESR4 and ESR5, are more focused on energy storage. In this topic, ESR4 made a significant progress in setting up a networked computing for ab initio modeling the chemical storage of alternative energies, which was applied to investigate the methane production from Carbon Dioxide on a Collaborative Research Infrastructure, whereas ESR5 carried out a detailed investigation of the properties of Cyclacenes and on the polyradical character of [n]cyclacenes.
Core Course of the ITN. The first mandatory activity. Madrid, September 2015

Tutorial on SHARC held in Vienna, October 2016.

Tutorial on ADF, third mandatory activity. Held in Amsterdam, April 2016.

Fellows during the Meet Professor event of the Passion for Knowledge held Basque Country, Spain.

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