Brussels, 13 April 2018

COST 037/18

DECISION

Subject: **Memorandum of Understanding for the implementation of the COST Action "Towards understanding and modelling intense electronic excitation" (TUMIEE) CA17126**

The COST Member Countries and/or the COST Cooperating State will find attached the Memorandum of Understanding for the COST Action Towards understanding and modelling intense electronic excitation approved by the Committee of Senior Officials through written procedure on 13 April 2018.

MEMORANDUM OF UNDERSTANDING

For the implementation of a COST Action designated as

COST Action CA17126
TOWARDS UNDERSTANDING AND MODELLING INTENSE ELECTRONIC EXCITATION (TUMIEE)

The COST Member Countries and/or the COST Cooperating State, accepting the present Memorandum of Understanding (MoU) wish to undertake joint activities of mutual interest and declare their common intention to participate in the COST Action (the Action), referred to above and described in the Technical Annex of this MoU.

The Action will be carried out in accordance with the set of COST Implementation Rules approved by the Committee of Senior Officials (CSO), or any new document amending or replacing them:

a. "Rules for Participation in and Implementation of COST Activities" (COST 132/14 REV2);
b. "COST Action Proposal Submission, Evaluation, Selection and Approval" (COST 133/14 REV);
c. "COST Action Management, Monitoring and Final Assessment" (COST 134/14 REV2);
d. "COST International Cooperation and Specific Organisations Participation" (COST 135/14 REV).

The main aim and objective of the Action is to develop and experimentally validate a computational methodology to simulate the physical phenomena and the resulting effects that occur upon materials irradiation in intense electronic excitation conditions, paying special attention to smart strategies to combine solutions for restricted scopes (timescales) into a functional multiscale formalism. This will be achieved through the specific objectives detailed in the Technical Annex.

The economic dimension of the activities carried out under the Action has been estimated, on the basis of information available during the planning of the Action, at EUR 64 million in 2017.

The MoU will enter into force once at least seven (7) COST Member Countries and/or COST Cooperating State have accepted it, and the corresponding Management Committee Members have been appointed, as described in the CSO Decision COST 134/14 REV2.

The COST Action will start from the date of the first Management Committee meeting and shall be implemented for a period of four (4) years, unless an extension is approved by the CSO following the procedure described in the CSO Decision COST 134/14 REV2.

OVERVIEW

Summary

Electronic excitation reaching high energy density is central in many different applications, from materials processing to medical treatments. It emerges when intense radiation arising from sources such as lasers, swift ions, or high-flux X-ray or electron pulses, interact with matter. In general, only partial aspects related to the excitation produced by this type of sources are treated. The lack of a systematic methodology to face the simulation of the underlying phenomena makes it essential to involve scientists from different fields, theoreticians, simulators, and experimentalists. A successful methodology will require smart strategies to make existing solutions, which are appropriate within restricted scopes, work together within a multiscale formalism. The proposed COST Action will tackle this challenge through the following approach

1.Identify and propose experiments to validate simulations as an optimal way to generate progress in the field of intense electronic excitation.

2. Identify the specific role of different radiation sources on electronic excitation-induced effects. This will allow us to connect distinct communities that explore similar effects in parallel.

3. Identify strategies to connect computational methods on different timescales. This will be a central point of the project, since most methods operate reasonably well within their scope of applicability but their coupling to other approaches is not straightforward.

4. Transfer the newly acquired knowledge to industry and societal applications by taking advantage of COST networking tools.

This Action aims at creating a network of research groups with expertise in the different parts of the challenge tackled and a common research objective.

Areas of Expertise Relevant for the Action	**Keywords**
● Physical Sciences: Electronic properties of materials and transport (theory) ● Physical Sciences: Gas and plasma physics (theory) ● Physical Sciences: Atomic, molecular and chemical physics ● Materials engineering: Transport properties of condensed matter for materials engineering applications ● Materials engineering: Thermal properties of condensed matter for materials engineering applications	● Intense electronic excitation ● Intense irradiation sources ● Multiscale modelling

Specific Objectives

To achieve the main objective described in this MoU, the following specific objectives shall be accomplished:

Research Coordination

● Identify a number of cases of interest amenable to detailed, time- and space-resolved experimental investigation. These cases will be selected according to scientific and/or industrial relevance.

● Establish and optimize interfaces between the computational methods already in use for every timescale. Design validation strategies with appropriate experiments to establish the pros and cons of the different interfacing methods in terms of accuracy and computational performance. Apply the methods to study physical phenomena within their scope of application.

● Identify the most appropriate strategies to tackle cases of interest. Find the most appropriate methods for every scale and the most promising strategies to couple them. The strategy must unavoidably involve the design of appropriate experiments.

● Once the implemented strategy has been validated for a specific application, take advantage of such an achievement and extend it to address other applications.

● Transfer knowledge to industry mainly through software transfer and consultancy and promoting the integration of ECIs in industrial partners.
● Disseminate the achievements. Develop standard open source codes in open repositories to fix standards and keep control of future developments based on this work. Maximize impact by vigorously publicizing the material available in the repositories, by organizing tutorials, and by transferring the methodologies via STSM.

Capacity Building
● Create a network of research groups with expertise in the different parts of the challenge tackled and a common research objective. The Action will promote the network expansion towards ITC groups not included yet. ITC scientists will be given priority to access leadership positions.
● Foster the exchange of researchers and knowledge between groups using the mechanisms available in the Action.
● Merge different fields laying in the fuzzy border between timescales and models in order to fully tackle the multiscale problem.
● Bring together research, industry and society agents to find common points of interest and possible applications of this Action's results.
● Events in ITCs will be prioritised as a way to promote their involvement in the Action. At the end of the Action, the percentage of events organized in ITCs shall be larger than ITC representation percentage.
● The Action will mitigate gender imbalance as much as possible, first, attracting new members and second, ensuring a percentage of female researchers in leadership positions and participation in events larger than the female representation percentage in the Action.
● The Action will support ECIs by fostering their mobility, giving them the leader position of some tasks and ensuring a percentage of ECIs in events larger than the ECI representation percentage in the Action.

TECHNICAL ANNEX

1. S&T EXCELLENCE

1.1. CHALLENGE

1.1.1. DESCRIPTION OF THE CHALLENGE (MAIN AIM)

Electronic excitation reaching high energy density is central in many different applications, from materials processing to medical treatments. It emerges when intense radiation arising from sources such as lasers, swift ions, or high-flux X-ray or electron pulses, interact with matter. In general, only partial aspects related to the excitation produced by this type of sources are treated. The lack of a systematic methodology to face the simulation of the underlying phenomena makes it essential to involve scientists from different fields, theoreticians, simulators, and experimentalists. A successful methodology will require smart strategies to make existing solutions, which are appropriate *within restricted scopes,* work together within a multiscale formalism (Figure 1). The present COST Action will tackle this challenge through the following approach:

1. Identify and propose experiments to validate simulations as an optimal way to generate progress in the field. This is not obvious because effects that depend on whether various processes are consecutive or coexistent (e.g. electron-electron and electron-phonon collisions), require dedicated time-resolved experiments to assess their role and the degree of coupling among them. Moreover, laser-matter interaction strongly depends on the structure of the target at the nanoscale.

2. Identify the specific role of different radiation sources on electronic excitation-induced effects. This requires connecting distinct communities that explore similar effects (e.g., intense laser irradiation and swift ion irradiation) and will contribute to a better understanding of the general picture. This requires the participation of experimentalists and theoreticians from different fields.

3. Identify strategies to connect computational methods on different timescales (Figure 1). This is particularly important when the different methods do not run consecutively but simultaneously, overlapping over a certain period of time. This will be a central point of the Action, since most methods operate reasonably well within their scope of applicability but their coupling to other approaches is not straightforward (e.g. Molecular Dynamics and Boltzmann transport equation).

4. Transfer the newly acquired knowledge to industry and societal applications.

1.1.2. RELEVANCE AND TIMELINESS

A better understanding of phenomena induced by an intense initial electronic excitation is of interest for a broad range of disciplines: Solid-State Physics, Plasma Physics, Chemistry, Materials Engineering, Computational Science, Electronics, Photonics, Medicine, Astrophysics. The following are examples of straightforward applications that will benefit from progress in understanding intense electronic excitation: plume formation by intense laser irradiation, laser-generated particle beams, planet and star core studies, medical applications such as hadron and X-ray therapies, generation of high order harmonics, detectors in general, transducers, materials processing with swift ions, intense lasers and plasma discharges, materials and devices for nuclear and space environments.

The field of intense electronic excitation turns out to have some peculiarities with respect to others. It is necessary to understand them to anticipate how the field will progress in the coming years.

i. Multi-scale simulations of highly excited matter require the coupling of different methods (Figure 1), which typically cover different time and space scales. The methods are relatively mature and have shown success when utilized within their natural scope of application. The major difficulty arises when trying to couple them.

ii. A general solution is not expected. The goal is to apply multi-scale modelling to selected cases of interest.

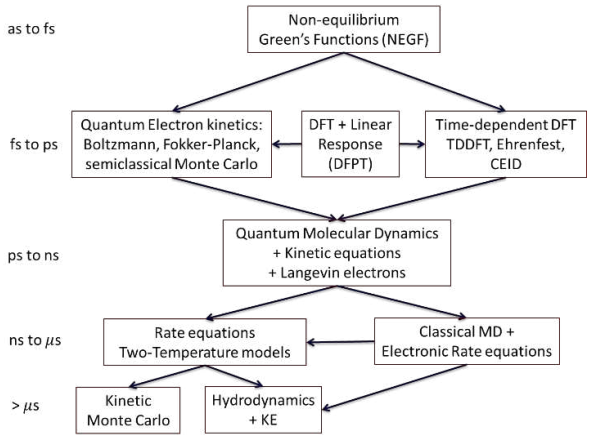


Figure 1. *Schematic representation of the multi-scale paradigm applied to intense electronic excitation of materials. The boxes represent different methods applied to the study of highly excited systems. The lines connecting boxes constitute the essence of the multi-scale approach since they represent strategies to extend the capabilities of one particular method by coupling it to another method. The time scales are indicative, and in many cases they overlap. These are the most challenging cases from the modelling angle.*

Taking into account these points, one can realize that progress will be fast in some of the selected areas, but not in all of them. When the solution to a problem depends on different coupled codes that only slightly overlap in time and space (weak coupling), then the probability of success greatly increases. That is, when the fine details of the physical evolution at a particular time scale do not have a strong influence on the time scale of interest, then the development of a multi-scale approach is easier. In general, the fewer the number of involved codes the easier the implementation and, vice versa, the larger the number of involved codes and the stronger the coupling between methods, the harder the implementation.

Let us consider the example of a three-dimensional diamond detector such as those utilized in the Large Hadron Collider, but which are also useful as detectors for any type of ionizing radiation like ions, electrons, gamma, and even indirectly ionizing radiation such as neutrons. An advantage of monolithic systems like this, is that the electrodes for collecting the charges can be engraved into the bulk in the form of conducting graphitic wires, by focusing a high-power laser that produces a local phase transition leading to non-thermal graphitization. The resistivity of these conducting channels depends on the irradiation details. A first aspect of interest for this system is to understand how these electrodes are created, and hence to gain control over their properties, i.e. resistivity, diameter, length, etc., by optimizing the pulse parameters. The process starts with the electronic excitation by the laser field in the sub-femtosecond timescale. While the laser pulse is still on, excited electrons will experience collisions between themselves (e-e interactions), concurrently absorbing more energy from the field and producing additional excited electrons via collisional ionization. The description of this phenomenon at the fundamental level can be achieved via ***many-body non-equilibrium Green's function techniques (NEGF)***. In the femto- to picosecond timescale, excited electrons start exchanging energy with lattice vibrations (e-ph interactions) and charged defects. These processes can start while the electrons are still far from (electronic) thermal equilibrium. Apart from the intrinsic possibility that the e-e timescale be similar or longer than the e-ph timescale, there is an obvious influence of the duration of the excitation process. At this scale, NEGF techniques become computationally very expensive, and simplified treatments are required. There are two clear ways forward. One is to use a mean-field approach like ***time-dependent density functional theory (TD-DFT)***, supplemented with electron-nuclear correlations like in the ***Correlated Electron-Ion Dynamics approach (CEID)***, and possibly also with some e-e collisions term, possibly of a stochastic nature. A second possibility is to use quantum kinetic equations like **Boltzmann** or **Fokker-Planck**. Both approaches require the determination of electron-phonon interaction strengths and timescales, which can be computed in linear response via ***density functional perturbation theory*** Another strategy is to use **semi-classical Monte Carlo methods**. *These actions will be treated in Working Groups WG2 and WG3. A vigorous interaction between these two WGs will be required in addition to the obvious collaboration with WG1.* Graphitization requires

changes in the bonding characteristics of the material (sp^3 to sp^2) driven by the motion of the C atoms following irradiation. This phenomenon occurs in the pico- to nanosecond timescale, accessible to the methods in the previous timescale. ***Ehrenfest molecular dynamics (MD)***, which involves electronic excitations, can hardly reach the ps. ***Ground state ab initio MD*** can access the sub-nanosecond scale, but will not include electronic excitations. Therefore, a methodology is required that includes electronic excitations within a framework of classical force fields. This can be achieved through ***Langevin dynamics*** for the atoms coupled to a diffusion equation for the electronic temperature, ***Two-Temperature Models (TTM)*** coupled to MD, assuming that electrons are always in thermal equilibrium. Moreover, this can be supplemented with electronic temperature-dependent force fields that take into account that electronic excitations weaken interatomic bonds. If the laser field is intense enough (over 50 TW/cm^2), it will generate a large density of highly excited electrons that will develop into a plasma. Further interaction of intense laser with the plasma can be modelled using **Particle in Cell** (PIC) codes. This plasma will evolve in the nano- to microsecond timescale following ***hydrodynamic equations***. This evolution is driven by the kinetic energy stored in the electron fluid, but part of this energy is also used to heat the lattice. Therefore, there is again a superposition of time scales, requiring a description where *plasma and lattice evolution may not be separable*. This also involves spatial scales far larger than before, in the order of the micrometres. **Classical MD** simulations can reach up to a billion atoms, i.e. about 100 nm as a linear dimension. Therefore, again simpler models are required. One possibility is two-temperature models, which describe the coupled evolution of the two continuous temperature fields, electronic and nuclear, in time. Any of these models, ***PIC, hydrodynamics, TTM, or kinetic Monte Carlo***, will require input from WG2, in the form of equations of state, transport coefficients, as well as a through validation against explicit MD methodologies. *These actions will be treated in WG3 and WG4. Substantial interaction between these two WGs will be required in addition to the obvious collaboration with WG1*

The degree of maturity of the methods described in this section is unquestionable. The next step, which is addressed by this COST Action, is to combine different sophisticated codes by means of smart coupling strategies with solid experimental support to apply the developed methodology to a number of relevant cases in different disciplines. Notice that, deliberately, mention is made to methods and not to specific codes to avoid being prescriptive in the nature of the coupling methodologies. The aim is to be completely open and encourage colleagues in possession of useful tools or ideas to join the effort. This can only be done through a multidisciplinary network as proposed in this Action. Efforts carried out by isolated groups with access to a limited (though sophisticated) number of methods would be futile to achieve overall progress in the complex landscape unfolded by an intense electronic excitation. Instead, *this Action is envisaged to be an important and timely progress in the field as a result of the networking effort described here*.

1.2. OBJECTIVES

1.2.1. RESEARCH COORDINATION OBJECTIVES

In order to be concise, a case of relevance was described in Section 1.1.2 by means of an example. The necessity of interaction between experts from different fields turns out essential to describe and optimize the fabrication process. Depending on the level of detail required, different approaches can be adopted. Since no universal solution will be applicable, every selected case will have to be studied and tackled using different strategies. With these ideas in mind, the objectives of this COST Action are summarized next:

1. Identify a number of cases of interest amenable to detailed, time- and space-resolved experimental investigation. These cases will be selected according to scientific and/or industrial relevance.

2. Establish and optimize interfaces between the computational methods already in use for every timescale. Design validation strategies with appropriate experiments to establish the pros and cons of the different interfacing methods in terms of accuracy and computational performance. Apply the methods to study the physical phenomena occurring within their limited scope of application.

3. Identify the most appropriate strategies to tackle cases of interest. Find the most appropriate methods for every scale and the most promising strategies to couple the various scales. Experimental validation is of paramount importance. Therefore, the strategy must unavoidably involve the design of appropriate experiments. Coordinate the common work involving different working groups, in particular between experimentalists, simulators and theorists.

4. Once the implemented strategy has been validated for a specific application, take advantage of such an achievement and extend it to address other applications.

5. Transfer knowledge to industry. The involved companies will benefit from this effort and it is expected that other industrial partners will join and benefit with adequate dissemination strategies.

6. Disseminate the achievements. Develop standard open source codes in open repositories to fix standards and keep control of future developments based on this work. Simultaneously, incorporate these methodologies into commercial software through the companies participating in the Action. Maximize impact by vigorously publicizing the material available in the repositories, by organizing tutorials, and by transferring the methodologies via Short-Term Scientific Missions (STSMs).

1.2.2. CAPACITY-BUILDING OBJECTIVES

This COST Action is intended to tackle a multidisciplinary, multi-scale problem, as shown in figure 1. One group alone cannot succeed in this problem. Moreover, as stated before, the challenge lies in the fuzzy border between different timescales and physical models. Advances in the field must be driven by a network of complementary research groups collaborating tightly. Thus, this Action will contribute to boost the European Research Area by creating the conditions needed to build a wide network of research groups that work together in this problem, and consolidate it during and after the end of this Action. The objectives of this Action towards the aforementioned goal are:

1. Create a network of research groups with expertise in the different parts of the challenge tackled and a common research objective.

2. Foster the exchange of researchers and knowledge between groups using the mechanisms available in the Action (i.e. short term scientific missions – STSM).

3. Merge different fields laying in the fuzzy border between timescales and models in order to fully tackle the multiscale problem.

4. Bring together research, industry and society agents to find common points of interest and possible applications of this Action's results.

1.3. PROGRESS BEYOND THE STATE-OF-THE-ART AND INNOVATION POTENTIAL

1.3.1. DESCRIPTION OF THE STATE-OF-THE-ART

An overwhelmingly large fraction of the theoretical work aimed at describing the properties of materials makes use of the Born-Oppenheimer (adiabatic) approximation. It assumes that electrons follow a “slave” dynamics dictated by the motion of the nuclei, where transitions between electronic states are not allowed. The treatment of non-adiabatic effects, i.e. electronic excitation and decay, requires a different approach. In recent times, various methodologies have been developed and applied to study interesting phenomena. Perhaps the simplest one is Time-Dependent Density Functional Theory (TD-DFT) [1] combined with the Ehrenfest approximation for the nuclei [2]. While electronic excitation processes are captured correctly by this approach [3], the mean-field character of Ehrenfest distorts the characteristics of energy transfer from electrons to phonons, e.g. Ehrenfest cannot describe properly ubiquitous phenomena like Joule heating [4]. A second limitation is related to the exchange-correlation approximations used in TD-DFT. In most cases, these are semi-local in space and local in time. Therefore, memory effects in the electronic evolution are ignored, thus leading to another host of pathologies, mainly related to the lack of electronic decoherence (no electron-electron collisions term) [5,6]. In addition, incoherent electron-phonon scattering by ionic vibrations, which are not explicitly represented in classical molecular dynamics, are not accounted for in TD-DFT calculations [7]. While Ehrenfest dynamics is straightforward to implement and computationally efficient, it is not trivial to go beyond it.

To improve on the electron-nuclear correlation, a possibility that has attracted interest amongst chemists is “surface hopping” [8]. In this method the forces on the nuclei are determined from single electronic potential energy surfaces (PES) but hops between surfaces are allowed to include non-adiabatic effects. Surface hopping works reasonably well when non-adiabatic transitions occur between a small number

of PES [9], but not for a dense manifold of excited states. Perhaps the most sophisticated way to go beyond Ehrenfest in a controlled manner is the Correlated electron-ion dynamics approach (CEID) [10]. CEID relies on expansions of the quantum Liouville equation for the electron-nuclear system, with different formulations proposed in the limits of weak [11] and strong [12] electron-nuclear coupling. It has also been implemented in a similar spirit to quantum chemistry methods in electronic structure.

On the electronic front, a possible way forward is to start from the very general equations of non-equilibrium quantum statistical mechanics, e.g. the Balescu-Resibois formalism [13] or the time-dependent non-equilibrium Green's functions approach (NEGF) [14-16]. When applied to intense laser irradiation of matter, this ambitious program may in principle describe both the coherent and incoherent interaction of electrons with sub-picosecond optical pulses as well as spatially inhomogeneous particle (e.g. ion) irradiation. Calculating the sub-picosecond kinetics of observable quantities entails the solution of the Green's function (Kadanoff-Baym) equations of motion and leads to extremely arduous numerical computations when correlations and screening are included [17].

None of these approaches is capable, with present day computers and algorithms, of reaching time scales beyond a few femtoseconds (maybe up to picoseconds if using simplified electronic structure methods like tight-binding), since the time step (typically around an attosecond) is dictated by the time-dependent electronic Schrödinger equation. The electron dynamics following electronic excitation, however, develops in a longer time scale where processes like electron-hole recombination, electron-phonon interactions and diffusion become significant. These time scales require a different theoretical approach. This is the realm of kinetic models, where one starts from Boltzmann-like kinetic equations and develops complex, yet tractable numerical schemes. Kinetic models like the Master and Boltzmann's equations can be formally derived from the theory of non-equilibrium Green's functions above, within the framework of the so-called quasi-particle approximation. These, however, are limited to the semi-classical regime, i.e. when the electron-hole plasma dynamics is controlled by collisions (Markovian) rather than by coherent quantum effects [18]. This condition is often satisfied in the sub-picosecond regime, with the mean time-independent collision rates calculated via Fermi's golden rule. Instead of tracing the motion of the individual particles, one follows the time evolution of the particle distribution function in phase space, starting from the Liouville equation. This approach may be useful in describing photo-induced phase transitions, where atomic transformations are driven on a ps timescale [19]. Simplifications of the latter lead to the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy [20], Boltzmann's kinetic equation [21], and the Fokker-Planck equation [22]. When Markovianity is not fulfilled the semi-classical approach no longer applies and a full quantum approach based on the evolution of the density matrix (quantum Liouville equation) should be used [23]. An alternative approach to Boltzmann equations is to describe the semi-classical carrier dynamics according to Langevin equations and then solve them by Monte Carlo methods [24].

Simulations of ion-solid interactions have traditionally been driven by state-of-the-art molecular dynamics (MD) simulations using empirical potentials that have limited realism and accuracy. Electronic energy losses are generally not included, and the effects of electron-hole pair production and charge-density redistributions are ignored. To go forward in this direction and access the ps-ns regime one needs to incorporate electronic energy losses in MD simulations. This has been done based on the Langevin equation, where the electronic losses are taken care of by a friction term and then this energy is redistributed to the atomic system via a random force [25]. The most recent works in this area consider friction forces whose direction and magnitude depend on the local, time-dependent environment [26], or simplified descriptions of the environment in which a structured bath coupled to the nuclear motion via a Generalized Langevin equation [27].

1.3.2. PROGRESS BEYOND THE STATE-OF-THE-ART

The present methodologies (electronic friction, Langevin equation, random forces, etc.) are limited to relatively weak intensities. An aspect that is mostly ignored is that, under intense electronic excitation, the interatomic forces are weakened and thus the empirical potentials should be modified [28]. Therefore, there is a need for improvement in this classical description. Approaches to estimate the electronic stopping power as those in the popular code SRIM (Stopping and Range of Ions in Matter) proved inaccurate when swift heavy ions (e.g. Br) are used to irradiate semiconductors (e.g. SiC) [29]. Connecting the electronic dynamics at the NEGF/TD-DFT and/or kinetic equations' level with the lattice evolution scale is one of the key outstanding problems in the field.

Distribution functions obtained either via kinetic equations or MD simulations can then be used to compute macroscopic observables by means of thermodynamic relations. While equilibrium

thermodynamics is a well-established discipline, its time-dependent non-equilibrium counterpart is still under development. Therefore, extracting thermodynamic relations where neither particles nor their distributions enter the equations is very relevant. In fact, these methods may allow us to trace changes in the experimentally observable values (temperature, pressure, volume) without considering the detailed description of processes occurring with individual particles [30]. The main advantage is the computational cost that can be decisive for many applications of interest.

Finally, methods usually employed in plasma physics, namely, hydrodynamic equations, may turn out advantageous for a number of situations in which long term evolution of highly ionized matter upon certain initial conditions play an important role, e.g. plume production and evolution. This will require putting on firm grounds the connection between kinetic and hydrodynamic equations [31].

The state-of-the-art in modelling intense electronic excitation consists of a variety of computational methods, many of them mature enough to provide accurate results within their scope of application. However, in general the effects produced by this type of electronic excitation extend to different timescales and evolve in large space regions. In order to provide quantitative results, one must develop a multi-scale methodology. Similar multi-scale paradigms have been developed and applied to a number of studies in the irradiation of solids, e.g. within the nuclear materials or the biological or soft matter contexts, using different methods for different scales: DFT, MD, Coarse graining, Kinetic Monte Carlo, Dislocation theory, Continuum theory.

The multi-scale approach has not been fully realized yet in the field of highly excited matter. The difficulty stems from the need to follow the electronic evolution of the highly perturbed, non-equilibrium system, and to propagate this information to other scales by coupling various methodologies designed for different goals. Therefore, any such coupling strategy is unique and beyond state-of-the-art. This is precisely the remit of this COST Action, where a large effort will be carried out to couple different computational methods involving highly excited electrons, with the aim of solving relevant problems, of scientific or industrial impact. More specifically, this Action will provide significant progress as a result of a successful combination of computational methods (properly coupled) and validation experiments. In this sense, progress beyond the state-of-the-art will be measured by the successful developments to couple methods, usually, with the aim of studying certain relevant application.

As an example to facilitate the understanding on the important role of coupling, some strategies are considered to tackle the laser-irradiated diamond case described above going beyond the state-of-the-art by the development of **interfaces** between codes. Quantum mechanical effects are essential for the correct description of early stages of photoionization and photoexcitation on a femtosecond time scale beyond the conventional Keldysh approach. They can be incorporated via ab initio approaches (TDSE, TD-DFT). The coherent connection between the generated charged carriers and the irradiating laser field is given by the laser-induced polarization. The dephasing of the polarization is caused by interband electron-electron interaction (leading to impact ionization and Auger recombination) and by electron-phonon scattering. These processes can be described by **interfacing** the TDSE with Boltzmann quantum kinetic equation by solving them self-consistently. The photoionization term from the first principles calculation can be substituted into the kinetic equation containing the collision integrals. Depending on the pulse duration a non-thermal melting of the material can take place in which the energy absorbed into the generated electron-hole pairs will not cause thermal effects but rather change the bonding strength of the lattice ions due to high density of the generated carriers. For longer pulse durations or after the end of the pulse the energy deposited into the electron system will be transferred to the phonon modes of the lattice via electron-phonon interaction thus affecting the lattice temperature. The time evolution of the thermal energy deposition in the lattice and the space distribution of the lattice temperature can be modeled by **interfacing** Boltzmann quantum kinetic equation with Molecular Dynamics simulation. This requires to consider all the energy transfer channels to the lattice (not only electron-phonon coupling) and a way to include the transferred energy as lattice energy in MD. A continuous feedback from MD (temperature, atomic density, defect structure) must be passed back in each iteration step to the Boltzmann code. This way the structural changes in the material due to dissipation of the absorbed energy that causes changes into the lattice bonding through a thermal mechanism can be modeled.

1.3.3. INNOVATION IN TACKLING THE CHALLENGE

The particularities of COST Actions will allow us to use novel and innovative strategies to tackle the challenge of developing a multi-scale methodology to study highly excited electronic systems. Both top-down and bottom-up approaches will be used during this COST Action.

1. The full multi-scale problem is divided in a top-down way (Figure 1). Several time-scales and physical models have been identified. Thus, rather than a universal multi-scale model, a broad selection of relevant applications will be made, and strategies to study them will be developed.

2. The strategies the Action will use to evaluate models and couple them between timescales are based on selected cases of interest (i.e. bottom-up, from industrial applications to a full multi-scale model). The intended strong presence of industrial and technology transfer partners in this Action along with the multidisciplinary background of its members will allow the Action to involve researchers from different fields to identify and work on the best strategies for coupling different methods and applications. Specific tools as STSM and workshop will be used to foster the collaboration between industry and academy.

3. Experiments will play a fundamental role in this Action, and for this reason there is a dedicated experimental WG. Carefully selected experiments will be used to challenge and validate the scope of application of existing computational methods. The predictive capability of the resulting coupled models will be tested against experiments.

4. Benchmarked, multi-scale models will be used to display cases of interest for both basic research and industrial applications. In this way, the developed models will drive new experiments and applications to be attacked during the action or even pursued afterwards. The Action will make the most of the methodology, pushing forward its expansion and novel applications.

The only way to tackle a multi-scale, multidisciplinary challenge involving research groups, enterprises and society, such as this one, is to use innovative methods and policies. This Action will take advantage of its strengths (stakeholders from a huge variety of research fields and industries, strong know-how of specific applications) to implement innovative top-down and bottom-up strategies to ensure the success of the Action.

1.4. ADDED VALUE OF NETWORKING

1.4.1. IN RELATION TO THE CHALLENGE

A multi-scale problem such as the modelling of matter under intense electronic excitation requires a multidisciplinary approach. While significant progress in this field has taken place in the past decades, the efforts conducting towards the multi-scale computational development described in this document are still lacking. Such a development requires a high degree of cooperation between different experimental and theoretical groups, from the condensed matter, materials and plasma communities. The only way to tackle this challenge is to create a multidisciplinary network encompassing researchers from different fields and relevant industrial stakeholders.

In this COST Action all these different communities will meet and formulate strategies to develop a better understanding of the propagation of intense electronic excitation through the scales, using multi-scale modelling. In addition, new applications in different fields will arise naturally and stimulated by the contact among diverse communities thanks to the transversality built into the Action, and boosted by the presence of industrial partners.

1.4.2. IN RELATION TO EXISTING EFFORTS AT EUROPEAN AND/OR INTERNATIONAL LEVEL

Multi-scale modelling as a tool to address phenomena occurring across space and time scales has been under development for a few decades now. Being a central problem in Materials Science and Biology, there is a significant level of activity in the field, both in Europe and internationally, which can be judged by the number of Workshops, Schools, and collaborative initiatives. Less transited is the road that involves electronic excitations and how these propagate across scales. Probably the first time this topic was specifically addressed, was in a CECAM (Centre Européen de Calcul Atomique et Moléculaire) workshop held in Dublin in June 2015, entitled Multi-scale modelling of matter under extreme irradiation. A related CECAM activity was the workshop Systems far from equilibrium: from solid state physics to warm dense matter (Paris, 17-19/6/2014). On the multi-scale modelling front, there were several CECAM Workshops: Multiscale modelling of materials with atomic scale resolution using phase-field methods (Lausanne, 21-23/5, 2014), Multi-scale simulation methods for soft matter systems (Mainz, 6-8/10, 2014), Computational plasmonics: an ab initio and multiscale perspective (Lausanne, 2-4/11, 2015), Understanding function of proteins in membrane by atomistic and multiscale simulation (Lugano, 6-12/11, 2015), Multi-scale simulation: from materials to industrial usage (Dublin, 5-7/9, 2016), amongst

others. Another partially overlapping theme is charge transport, where there were CECAM Workshops on: Charge transport in organic materials (Bremen, 31/3-4/4, 2014), High performance models for charge transport in large scale materials systems (Bremen, 6-10/10, 2014), Electron dynamics on Surfaces and nanostructures (Zaragoza, 5-7/11, 2014); and Interactions and transport of charged species in bulk and at interfaces (Vienna, 4-7/7, 2016). Finally, there were CECAM activities on electron dynamics at the attosecond scale, such as the 6th TD-DFT workshop (Bensaque, 14-17/1, 2014), Recent progress in non-adiabatic methods in quantum dynamics (Lausanne, 12-15/5, 2014), Electron-vibration coupling: theoretical and numerical challenges (Lausanne, 27-29/5, 2015), Exploration of ultra-fast time scales using TD-DFT and quantum optimal control theory (Lausanne, 28/9-2/10, 2015), Ultra-fast phenomena in quantum physics: a challenge for theory and experiment (Lausanne, 11-15/4, 2016). In terms of networks, there are four COST Actions that partially cover topics discussed here: MP-1208 entitled “Developing the Physics and the Scientific community for Inertial Confinement Fusion at the time of NIF ignition”, MP-1203 entitled “Advanced X-ray spatial and temporal metrology”, CM-1204 entitled “XUV/X-ray light and fast ions for ultrafast chemistry (XLIC)”, and MP-1002 entitled “Nanoscale insights in ion beam cancer therapy (Nano-IBCT)”. The overlap of other initiatives with this COST Action is partial. The distinctive aspect is that this Action will focus on the multiscale modelling of intense electronic excitation itself, while other initiatives address the issue of structural modifications (radiation damage or processing) or different aspects of intense irradiation, or specific areas of application. The pertinence of this COST Action is related to the increasingly important necessity of accurate simulation results of intense electronic excitation for technological applications. Such simulations can only be developed through a communal effort as the one proposed here.

2. IMPACT

2.1. EXPECTED IMPACT

2.1.1. SHORT-TERM AND LONG-TERM SCIENTIFIC, TECHNOLOGICAL, AND/OR SOCIOECONOMIC IMPACTS

The present COST Action has been designed with the objective of making a quantifiable impact related to fields such as laser processing of materials, ion implementation, medical radiotherapies and radiation resistant materials. All these impacts have technological, socioeconomic and scientific aspects. The present Action emerged as a multi-sided need:

1. Firstly, there is an increasingly large number of industrial processes and biomedical applications that involve highly excited electronic initial states, such as laser-processing of materials, ion implantation, medical radiotherapies, and radiation resistant materials. Connecting the initial and final states will harness and optimize the practical use of such tools.

2. Secondly, there is a need for understanding the effects of unintentional irradiation, such as sunlight, cosmic rays, highly radioactive environments such as nuclear power plants and nuclear waste repositories, medical dosimeters, in order to prevent undesirable outcomes like secondary cancers due to poorly planned radiotherapies, the failure of electronic devices in space and other aggressive environments, or excessive radiation dose due to inaccurate dosimeter calibrations.

3. Finally, there is an intrinsic fundamental interest in understanding how a strong initial electronic perturbation propagates across the scales, changes the physical and/or chemical properties of the sample, and in many cases results in macroscopic modifications of the irradiated material.

In the short to medium term, it is expected to deliver technological impact in relation to the specific cases of interest identified in this Action, which include detectors, electronic devices, and materials processing. Directly or indirectly, all these are also potentially beneficial from the economic and societal points of view. In addition, other interesting and useful applications will emerge during the course of this Action. The deliberately inclusive structure of the Action along with the broad range of expertise in the consortium including academia and industry (see 3.3. Network as a whole) will allow for these new applications to be incorporated into the programme and tackled using the tools already developed or by developing new tools if necessary. Socioeconomic impacts related to these technological advances are expected in the longer term.

Scientific impact, i.e. understanding the effects of intense electronic excitation across the scales based on the multi-scale methodology, probably translates into longer-term impacts. A short to medium-term

expected scientific impact is the establishment of new international research groups behind each workgroup and across the working groups. It is important to mention that being this an initiative mainly led by European groups, the exploitation of the results will certainly benefit Europe. Clear synergies with other COST Actions will enhance the scientific, technological and socio-economic impact. In particular, Actions focused on biomedical applications will benefit from the unique work proposed in this Action to understand and model the role of intense electronic excitation. To illustrate this, consider the example of intense electronic excitation in biomedical applications. Modelling the electronic excitation induced in biological material will help a user company to control undesired outcomes related to external or internal irradiation and to improve dosimeter calibration. In particular, tomography techniques that require the introduction of radionuclides in the body will benefit from a better understanding of radiation effects. Laser acceleration with different medical applications (e.g., radionuclide production) is considered a good alternative to conventional particle accelerators. In collaboration with industry, particle production will be optimized, in particular, through optimized targets properly designed with the aid of modelling. Therapy methods will be also considered in collaboration with industry. For example, photothermal therapy is a very promising therapy for non-invasive cancer treatment. It is based on the introduction of plasmonic nanoparticles in tumour cells and the subsequent laser irradiation at the localized surface plasmon resonance (tuned to be in the biological spectral window, 700-900 nm) producing local massive electronic excitation and eventually cell death. Nanoparticles can be also used in theranostics (therapy + diagnostics) [32]. Theranostic agents constitute a new generation of therapeutic agents that induce contrast for imaging techniques and sensitize cells to ionizing radiation by improving dose efficacy (radiosensitization). This combination of technologies for a single image-guided treatment holds clear potential for improved clinical outcome. Since many aspects related to intense electronic excitation remain poorly understood, the contribution of this Action will be very beneficial for our industrial partners. Finally, the development of dosimeters (example of diamond detector in Section 1.1.2) will have applications in the field of radiotherapy.

Several companies will participate in two ways: Firstly, by helping identify a specific system and process to model that is of interest. Secondly, by providing (or guiding) the Action with the materials and instruments necessary to carry out the validation experiments in WG1. Careful arrangements and non-disclosure agreements will have to be in place to protect intellectual property and encourage industrial participation.

A second way in which industry will get involved is through dissemination. In this sense it is remarkable the role of software companies, who will incorporate the technical developments of the Action, e.g. coupling methodologies between scales, into their commercial or academic software packages, thus enabling manufacturing companies to use this enhanced software to improve their products and processes, e.g. the industrial applications discussed above. Interestingly, there is an opportunity for direct interaction between companies from the three different sectors.

2.2. MEASURES TO MAXIMISE IMPACT

2.2.1. PLAN FOR INVOLVING THE MOST RELEVANT STAKEHOLDERS

Each specific application is, in a sense, unique, as it depends on the characteristics of the initial excitation (intensity, pulse duration, radiation nature, etc.) and on those of the material (type, size, and environment). Therefore, modelling strategies will be application-dependent rather than general.

- To maximize the technological impact, the Action has involved a number of companies focused on laser technology, coating fabrication, target fabrication and medical imaging.

- To maximise the socioeconomic impact, the Action has involved partners who work in challenges with high societal impact, like the application of radiation in medicine (e.g., production of radioisotopes for medical imaging and development of new dosimeters).

- To maximise the scientific impact, the Action has involved software companies interested in incorporating the methodologies developed under this Action into their modelling software packages.

A fundamental aspect to ensure higher impact of the Action is the participation of experimentalists. The combination of codes that work in different regimes is quite delicate. It necessarily involves approximations that depend on the case. The ultimate test for a scale-bridging strategy is then its

validation against experimental data. In the absence of this, the predictions are less reliable and thus limit the impact as end users will be reluctant to adopt approaches not properly validated.

Explicit actions will be taken in order to ensure that the entrepreneurial skills of interested researchers, are identified, fostered and developed. STSMs between research and industrial partners along with mixed workshops will be explicitly fostered by the Management Committee (MC). These STSMs will make possible to make *in-situ* case studies of interest for industrial partners. The exchange between industry and research will be fostered through webinars.

Finally, the spirit of this COST Action is to bring together researchers from different fields to raise awareness about the goals and needs of each other, to facilitate communication and to identify relevant problems and routes to solve them. Actually, this collaboration has already started by involving the relevant actors since the beginning of the submission phase of this COST Action, by starting to identify relevant cases and strategies, and by contacting local industries.

Further actions will be pursued to seek funding for case-oriented research projects, e.g. to develop detectors for high-energy particles, novel medical therapies, highly controlled dosimetry for medical image, novel nanostructuring methods. For example, the diamond detector used as an example in section 1.1.2 has applications in high energy physics and in the radio therapeutic use of photon beams. These applications will promote the exchange between Industry and Academia through this Action. The working groups will be stimulated to apply for funding to exploit their achievements. The Action participants will endeavour, as far as possible, to participate in EU Science committees to ensure that the field of intense electronic excitation forms part of the research portfolio.

2.2.2. DISSEMINATION AND/OR EXPLOITATION PLAN

The targets of the dissemination activities of this COST Action are:

- Other academic researchers and potential new members of the action. Being the nature of this Action multidisciplinary, this group is vast. They are an important target since, when new physics or requirements for the models are identified during the Action, they can give invaluable input, join the Action and start further collaborations after the end of the Action.

- Industrial partners, since increasing their number and involvement is one of the objectives of the dissemination plan. Technology-transfer, training and collaboration between academic and industrial partnerships are outcomes expected from this Action.

- National and European policy makers are also a target of dissemination activities. It is crucial to make policy makers realize the importance of research on intense electronic excitation (both basic and applied) and the possible applications and benefit of it.

- The laymen will also be a target of the Action's dissemination policies. It is central to explain the importance of research to Society.

Dissemination and exploitation of the Action's results play a major role in the success of the Action. Thus, a Working Group (WG5) is fully dedicated to this task. Dissemination will be done at all levels through the Action website, mailing lists, social networks and the communication departments of the institutions involved in the Action. The specific media used will depend on the specific target of the dissemination activity. For example, some specific dissemination actions will be:

- WG meetings and training schools will be widely advertised through the webpage and mailing lists to rise attention about the Action and attract collaborations/partners.

- Scientific results will be published in international peer reviewed journals, acknowledging the COST Action. This policy will be actively encouraged and verified once a year by WG5.

- Communication departments of the institutions will help the Action to write and disseminate press releases through the institutional webpages and national press media, in order to reach the general public. In addition to this, the Action will register and maintain, with the help of experts from the institutions, Twitter and Facebook accounts. The possibility of maintaining a YouTube channel will be considered by WG5.

- Open Access and Open Data will be encouraged to maximize the scientific and societal impact.

- At this stage no intellectual protection plan is needed. However, if the need arises, industrial partners of the Action may advise the MC to prepare and implement Intellectual Property Rights policies.

2.3. POTENTIAL FOR INNOVATION VERSUS RISK LEVEL

2.3.1. POTENTIAL FOR SCIENTIFIC, TECHNOLOGICAL AND/OR SOCIOECONOMIC INNOVATION BREAKTHROUGHS

Some gross numbers can help assessing the potential for innovation of this Action. So far, 82 persons belonging to scientific groups and companies from 17 countries have actively participated in the preparation and submission of this Action. Even more persons showed their interest in participating. Most likely, the number of participants in the Action will increase after the kick-off meeting. Such a network of multidisciplinary research groups has the potential of successfully tackling the challenge stated. Moreover, the participation of relevant industrial and technology transfer stakeholders ensures that the research work done will result in technological applications, returning benefits to our society.

The structure of this Action allows for a high innovation potential while keeping the risks at bay. The risk level of the cases of interest in which the WGs will work can be adapted as required. For example, several low risk and one high-risk high-gain application can be selected to ensure a positive balance of success and innovation. Industrial partners will be crucial in this selection since they can identify technological and socioeconomic cases of interest with the required level of risks. Indeed, industrial partners have identified and already proposed some cases of interest for example in biomedical applications and materials tailoring, (e.g., phototherapies, theranostics, particle acceleration to produce radionuclides, dosimetry implications, fabrication of detectors for High Energy Physics…)

Finally, the Action will encourage the use novel policies like Open Access and Open Data. It is safe to affirm that these policies will strongly impact on research and industry, attracting new groups and ideas to this Action.

3. IMPLEMENTATION

3.1. DESCRIPTION OF THE WORK PLAN

3.1.1. DESCRIPTION OF WORKING GROUPS

The challenge that this COST Action will face is to develop quantitative multi-scale computational strategies (Figure 1) to tackle specific problems. In order to succeed, a number of groups from different fields will be put in contact. This will be organized according to the following structure:

Management Committee (MC)

Its main task regarding the implementation will be to supervise and coordinate the activities of the working groups. In this COST Action this task is particularly important since the whole Action is based on the coordination between theorists, experimentalists, simulators, all of them from different fields to tackle specific cases of interest. The MC will also implement gender policies aiming at a balanced representation of women in the MC itself, WG leaders, and STSM amongst others. It will also follow the involvement of Early-Career Investigators in the Action, using available tools to boost their career. Finally, the MC will continually seek new partners, especially from Inclusiveness Target Countries.

Working group 1: Experimental

The main task of WG1 will be to design and carry out experiments aimed at challenging the various computational methods, especially in interface areas where there is overlap of scales (e.g. electronic excitation and electron-phonon interaction). This will be crucial for the validation of methods, but it will also challenge experimentalists to develop new methodologies and instrumentation, both for measurements and for fabrication of targets, e.g. nanostructuring. Photon (lasers) and ion sources used in different regimes (pulsed and continuous) will be explored. Industrial input will be an integral part of this WG to identify specific systems of interest for experimental studies, such as radiation detectors, time-resolved ultra-fast optics methods, *in situ* monitoring of radiation-induced materials modifications. *WG1 will develop and apply advanced time-resolved techniques (e.g., ultrafast photoemission,*

diffraction, and thermoreflectance) to address specific processes in the excited non-equilibrium state to validate the computational approaches.

Working group 2: Electronic excitation

WG2 will focus on the interface between the first two rows in Figure 1. Starting from highly accurate many-body theoretical approaches such as non-equilibrium Green's functions, it will focus on the development and validation of simplified approaches such as TD-DFT and Boltzmann/Fokker-Planck equations for the electronic evolution. More efficient methods will allow us to cover longer time scales and larger sizes. It is expected an intense interaction between researchers with expertise in the various methodologies such as NEGF, TD-DFT, kinetic equations and semi-classical Monte Carlo methods, always under the guidance of experimental work from WG1 for validation, such as ultra-fast optics, plume formation and particle acceleration. It will be important to address the role of the different radiation sources and materials and to develop methodologies based on coupling specific codes. *WG2 will develop strategies to describe the first instants following the electronic excitation.*

Working group 3: Electron-lattice coupling

WG3 will encompass the three middle rows in Figure 1. A highly excited initial electronic distribution has two possible effects: the modification of the interatomic forces, and the transfer of energy to the lattice by different routes, notably by electron-phonon interactions. Both of these translate into the motion of the atoms in the lattice, possibly even melting it. This is the realm of electron-lattice coupling, which occurs in longer time scales. Strategies are needed here to treat non-equilibrium excited electronic distributions that decay into phonons, while the interatomic potentials also depend on the time-evolving electronic distribution. Of course, if electrons equilibrate before they can transfer energy to the lattice, the coupling will be less important. Molecular dynamics methodologies, both quantum and classical, will be central in this WG to follow the atomic motion. The validation of these simplifications will require a strong connection with more accurate theory levels in WG2. There is still scope for simplification by describing the electronic evolution by means of rate equations or even simpler, a space-dependent electronic temperature, as in two-temperature models (TTM). Applications central to this WG include laser processing, irradiated materials evolution (defects), transient temperature variation phenomena, non-radiative decay routes, guided by experiments in WG1. *WG3 will study how the energy stored in the electronic system is transferred to the lattice by different pathways.*

Working group 4: Macroscopic aspects

WG4 will focus on the interface between the last two rows in Figure 1. The goal is to describe permanent modifications in the macroscopic properties of materials, e.g. mechanical stability, embrittlement, phase transitions, refractive index variation and also plasma generation and evolution. Methods developed in WG3 like classical MD and TTM supplemented with electronic information operate in the submicron scale. They are useful to understand the nature of microscopic processes, which can be then used by kinetic Monte Carlo (KMC) methods to study evolution in longer and larger scales. Some information from WG2, in the form of defect energies computed via DFT, is also useful for KMC approaches. An alternative is to resort to continuum methods like dislocation dynamics for solids, or hydrodynamic equations for liquids and plasmas. For the latter one needs constitutive equations, whose parameters can be taken from simulations in WG3 and experiments in WG1. An intriguing possibility is to combine MD with finite elements simulations. Typical applications include materials processing, micro-machining and transducers. *WG4 will study how the energy initially stored in the electronic system and then transferred to the lattice, induces modifications in the physical properties of the material.*

Working group 5: Training, outreach, dissemination, and technology transfer

1. *Training:* This will be organized through collective and individual actions.

    a. *Schools*: two Summer Schools are planned, during the second and the fourth year. The first one will focus on reviewing state-of-the-art and initial steps in coupling methodologies. The second one will focus on reviewing the advances made in various directions and training in new methodologies and experimental tools.

    b. *Short-term scientific missions*: This is an instrument uniquely offered within the framework of COST Actions. This is a crucial component of this Action, and the MC will endeavour to implement a vibrant scheme of STSMs.

2. *Outreach and dissemination*: As described in Section 2.2.2.

3. *Technology transfer*: An important task of WG5 will be to coordinate the activities of the WG1-4 with the companies and via technology transfer institutions involved in this Action, to facilitate technology transfer to the industrial sector.

3.1.2. GANTT DIAGRAM

Task 1. *Identification of models and cases of interest*. Within this task, several models will be selected, having in mind their scope and applications of scientific and industrial interest. Validation experiments play an important role. Discussion to select cases of interest must consider the experimental capabilities.

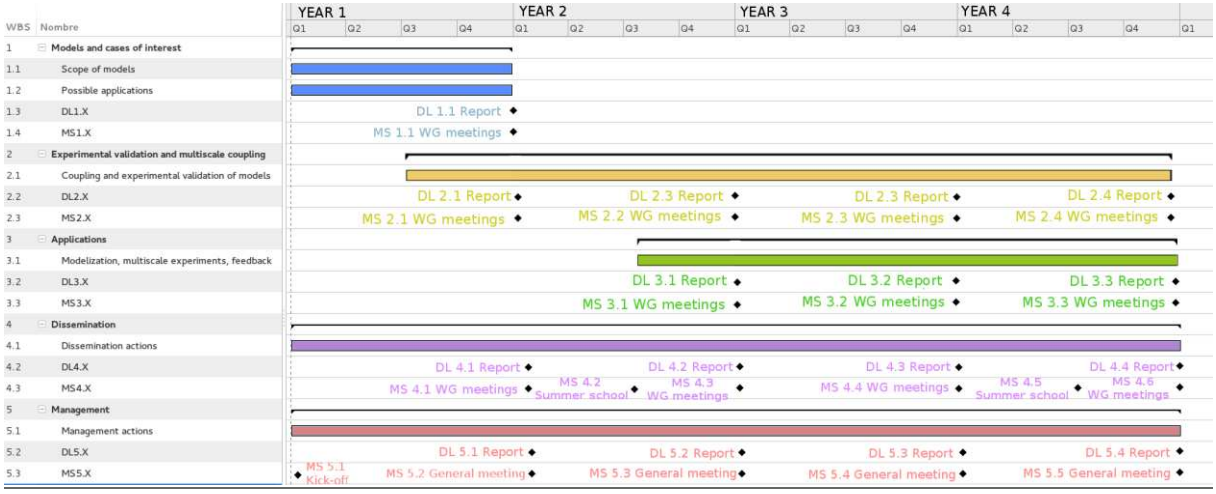
Task 2. *Coupling models and validation*. Strategies for coupling different models and experimental validation will be discussed and agreed within this task. As soon as some coupled models are available, they will be used within task 3.

Task 3. *Applications*. The models developed in task 2 will be used to study applications identified in task 1. Feedback from the results will be given to improve the models within task 2.

Task 4. *Dissemination and outreach*. This task will cover the dissemination and outreach activities in 2.2.2. Two summer schools are planned during the second and fourth year of the action.

Task 5. *Management*. The MC will coordinate the different WGs meetings, status reports of each task and/or WG and of the Action in general. A general meeting will be organized annually.

WG meetings (depicted at the end of each year in the Gantt but taking place all along the Action) will ease the tasks, fostering collaboration between partners. Each year, a final report about the status of the Action and each of the tasks will be spread among the Action members.



3.1.3. PERT CHART (OPTIONAL)

3.1.4. RISK AND CONTINGENCY PLANS

The following risks, which might appear during the course of this Action, have been identified:

- There exists a serious risk in the beginning of this COST Action if too complicated cases are selected. To mitigate this risk, industrially-relevant cases that can be afforded with existing capabilities will be selected. Thus, WGs will start working in so called “weak coupling” applications. Once, progress in a given case is reached, the experience can be extended to more complicated and relevant cases with high probability of success.

- Some coupling strategies between models might be too complicated to implement or computationally expensive for practical uses. There is no way to predict the importance of this risk until WGs have selected several models, applications and coupling strategies. This risk will be

mitigated by selecting a broad spectrum of models so as to ensure that at least one coupling strategy will be successful. The MC committee will be periodically informed, and will look for new partners with the needed expertise to join the Action, if required. The MC may decide not to pursue strategies that are deemed too risky or showing little promise. This risk, however, is constructive as it highlights to the community roads that are not worth transiting.

- There exists a risk that some WGs will not meet with the required regularity (due to agenda problems of WG members, for example) thus delaying the Action. WG leaders and MC will mitigate the risk by ensuring that each WG has enough workforce to deliver results and attend the meetings and, if this is not possible, it will be necessary to attract new members to the Action.

3.2. MANAGEMENT STRUCTURES AND PROCEDURES

The management structure has been designed to enable the efficient coordination of this multidisciplinary Action easing the achievement of its objectives. A Management Committee (MC) will be established to coordinate the organisational and scientific elements of the Action. It will be set accordingly to point 4 and Annex I of the “COST Action Management, Monitoring and Final Assessment” document. WG leaders will also be members of the MC. This will ensure a smooth communication between MC and WGs. In the same spirit, Early-Career Investigators will be involved as members of the MC in order to actively participate in the development of life-long training. In addition, gender balance will be pursued in the composition of the MC. Monitoring of the Action will follow the rules described in point 4 of the same document. The MC will produce the required progress records for the external monitoring. Once the feedback is received, corrective actions will be taken by the MC.

Intellectual property protection and exploitation will be dealt thoroughly and with special care, mainly in the workgroups where industrial partners and/or experimental facilities are involved. Gender issues, development of Early-Career Investigators' career and life-long training are top priorities of this Action. Three people, each in charge of these issues will be elected as representatives in the MC without voting rights. These persons will follow these issues and propose further actions to the MC.

Dissemination is also a key issue for the success of this Action. The dissemination leader will be the WG5 leader in charge of organizing an international conference/workshop and/or dedicated sessions in already existing international conferences and workshops. The workshops organized in this Action will be used to disseminate among workgroups the different potential funding opportunities from national research programmes. In this way, the Action will promote the formation and consolidation of consortia capable of attracting research funding. In addition to workshops/meetings, the participants will interact through other mechanisms like training schools, covering the different working topics of this action and the diverse expertise of the partners (research and industry). The Dissemination leader will also take care of Technology Transfer and relations with industrial partners.

3.3. NETWORK AS A WHOLE

This Action aims at developing a physical multiscale framework to treat intense electronic excitation phenomena. This is a multidisciplinary task due to the extreme spatio-temporal scales involved in the problem and the variety of processes that must be taken into account. A network of research partners, each tackling one part of the problem but collaborating tightly with others is a must to ensure the achievement of the objectives. The pool of researchers participating in the Action covers all the required expertise and backgrounds from the first principles theory to macroscopic modelling including experimental expertise and technology transfer.

Rooted in existing collaboration between several groups, this Action will develop the network through the available mechanisms: Action workshops and meetings, Short Term Scientific Missions, and collaboration between Work Groups. It is expected that a community on intense electronic excitation will emerge through the course of this Action.

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