EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Brussels, 4 June 2019

COST 051/19

DECISION

Subject: **Memorandum of Understanding for the implementation of the COST Action "Computational materials sciences for efficient water splitting with nanocrystals from abundant elements" (CompNanoEnergy) CA18234**

The COST Member Countries and/or the COST Cooperating State will find attached the Memorandum of Understanding for the COST Action Computational materials sciences for efficient water splitting with nanocrystals from abundant elements approved by the Committee of Senior Officials through written procedure on 4 June 2019.

MEMORANDUM OF UNDERSTANDING

For the implementation of a COST Action designated as

COST Action CA18234
COMPUTATIONAL MATERIALS SCIENCES FOR EFFICIENT WATER SPLITTING WITH NANOCRYSTALS FROM ABUNDANT ELEMENTS (CompNanoEnergy)

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 generate a multiscale modelling platform that will be used world-wide for conducting state-of-the-art multi-scale property prediction of materials and tackle the ambitious task of developing renewable energy technologies. 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 72 million in 2018.

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

Modern society in Europe needs a source of energy that is generated without harming the environment. The efficiency of renewable energy converting devices such as water splitting with electrochemical cells based on nano-scaled oxides relies on a sensible choice of material components. However, larger scale material and device properties such as interface segregation, grain boundary movement, ionic diffusion through porous materials, and mechanical loading also strongly impact performance, making the theoretical simulation of realistic devices a challenging multi-scale problem. Although the scientific community has developed expertise in the individual modelling fields, much less effort has been devoted to integrating and combining the scales toward a multi-scale approach. The ultimate central challenge will be to generate a multiscale modelling platform that will be used world-wide for conducting state-of-the-art multi-scale property prediction of materials.

This COST Action intends to focus on bridging the knowledge gaps between different theoretical methods and computer codes in order to facilitate the discovery of novel materials for energy conversion. The objectives of this challenge include building an organized network of European scientists working on achieving greater scientific understanding of water splitting and developing approaches for reliable and realistic multi-scale modelling of nano-oxides material architectures.

This COST Action will also develop initiatives to train young scientists, as well as inform computational users throughout the development and production. The longer term outcome will be the faster achievement of more environmentally friendly energy technologies which has an immeasurably large impact and benefit for society.

Areas of Expertise Relevant for the Action	Keywords
● Chemical sciences: Theoretical and computational chemistry ● Materials engineering: New materials: oxides, alloys, composite, organic-inorganic hybrid ● Nano-technology: Databases, data mining, data curation, computational modelling	● Density Functional Theory ● Water splitting ● Computational materials science ● Energy conversion

Specific Objectives

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

Research Coordination

● Review the current and upcoming methods/protocols/codes for developing novel materials for improving solar energy conversion efficiency, including their applications and advantages and weaknesses.
● Organize a network of European scientists working on achieving greater scientific understanding of energy conversion mechanisms and developing approaches for reliable and realistic multi-scale modelling of material architectures.
● Determine specific material requirements for the assessment of efficient energy conversion. Here the needs for specific energy conversion devices, including photovoltaic cells and photoelectrochemical cells, will be determined.
● Develop existing and new field method centres in several European countries in order to test the efficiency and method applicability and transferability.
● Establish consultation services (technical) and recommendations to end-user groups.
● Strengthen collaboration of theoretical groups with experimental groups in order to receive experimental feedback on the proposed new materials and verify the theoretical hypothesis.

Capacity Building

● Set up a process for assembling scientific information on material properties for solar energy conversion and build a respective reliable and efficient modelling methodology.
● Establish data collections on methodologies currently in use and under development.
● Evaluate the accuracy of these methods and recommend changes to protocols where appropriate.
● Establish a network of existing and new method oriented centres where the new method developments and integration can be tested and demonstrated.
● Provide a platform to train young scientists through STSMs targeted at selected high-impact topics, mentoring programmes and training workshops.
● Promote collaboration among European and international interested parties.
● Encourage the development of new relevant research consortia and programmes within Europe and cooperate with existing related initiatives.
● Establish a communications platform for academia, industry, and the public.
● Foster and create role models with network opportunities for early career scientists and female scientists.

TECHNICAL ANNEX

1 S&T EXCELLENCE

1.1 SOUNDNESS OF THE CHALLENGE

1.1.1 DESCRIPTION OF THE STATE-OF-THE-ART

Computational Materials Science – Overview.

Computational Materials Science is the computer-based employment of modeling and simulation following the laws of physics (from quantum to continuum mechanics depending on the scale) to understand and predict materials behavior either regarding their physical properties or their chemical reactivity. The modeling and simulation of materials is challenging, largely because of the extreme range of length and time scales that govern materials response. Length scales may span from nanometers (involving atoms and their interactions) to meters of engineered structures (where properties can be derived from continuum mechanics). Similarly, important time scales range from femtoseconds of atomic vibrations, again involving description at the quantum mechanical level, to the decades of the use of materials products where the simulation is in terms of classical mechanics likely involving a coarse graining description. The broad conditions of time and length scales required for a complete description of the materials of interest imply that no single technique is able to provide the required information at all scales. Thus, methods have been developed each focused on a specific set of physical phenomena and appropriate for a given range of lengths and times with a few attempts to bridge the gap between the different scales. These include methods mixing quantum mechanics and classical molecular dynamics, Monte Carlo simulation at various scales with different models for the interacton and, finally, continuum modeling. In the following we give a brief overview of the main types of methods focusing on the time and length scale of application.

Quantum Mechanics Methods.

The behavior of a material can be related to the types of bonding between the atoms, such as ionic, covalent, or metallic. A fundamental description of bonding requires the calculation of electronic distributions. The class of methods that yield such information are called electronic structure methods whose basis is the time independent Schroedinger equation. There are classes of methods that assume an approximate solutions for the wave function and find variational solutions (Hartree-Fock and explicitly correlated methods), but a much more common and efficient framework for characterizing materials is provided by Density Functional Theory (DFT) based methods that use the electronic density as a fundamental variable. DFT has become mainstream likely due to its ability to predict material properties with reasonable accuracy at a reasonable computational expense. Yet, several families of DFT methods exist providing increased accuracy at the expenses of using a more sophisticated, and hence more computationally expensive, exchange-correlations potentials. This type of methods can nowadays handle explicitly up 1000-2000 atoms and efficient parallel codes exist than can be run on powerful computers involving thousands of cores. Nevertheless, due to the difficulty to access to supercomputers for long enough runs, most of the calculations carried out world wide rarely involve more than 100-200 atoms. Here, it is worth mentioning the so-called QM/MM approaches where the system of interest is divided into two parts, one treated fully quantum mechanically and the rest treated more approximately (molecular mechanics or lower level quantum mechanical). The QM/MM can be regarded as a starting point for multi-scale modeling which is the main aim of the present COST Action.

Molecular Dynamics.

The molecular dynamics method is one of the most used for gaining information about structure and dynamics at the atomic scale including temperature effects by coupling the system to the appropriate thermostat. The molecular dynamics method was one of the first computer-based techniques for studying properties of materials during the 1950s. The basic idea behind the molecular dynamics theory is that forces are calculated and Newton's equations are solved to determine how atoms move. Here, the main problem lies precisely in determining the forces, these are rigorously provided by the potential energy surface which is obtained from a quantum mechanical electronic structure method. The resulting methods are usually described by an Ab Initio Molecular Dynamics (AIMD) with the famous Carr-Parrinello formalism being an efficient way to carry out the simulations. Here, the cost of computing the forces is the main bottleneck and the simulations are constrained to a few tens of atoms and had run to a few picoseconds at most. To solve the problem of the computational cost associated at obtaining the forces on the atoms, several force fields have been developed either using ab initio data or experiments. The use of force fields allows for simulations with thousands of atoms and up to milliseconds but are restrited to problems where bonds are not made or broken which requires a full quantum mechanical description. Yet, some reactive force fields have been proposed to overcome this problem. Mixing the two description as in static QM/MM is a possibility that needs to be explored to reach the objective of true multiscale modeling. For even larger systems involving lengths at the mesoscale, coarse graining molecular dynamics methods have been developed where groups of atoms constitute different types of objects (coarse grains) which are subject to the forces driving the dynamics. Ideally, mixing quantum mechanics, atomistic force fields and coarse grained methods would lead to a powerful multiscale framework for the research envisaged in this COST Action.

Monte Carlo Methods.

The Monte Carlo method is a powerful approach for providing thermodynamic information. The method was developed in the 1940s to solve multidimensional integrals. The method is used while directly evaluating an ensemble average without dynamical information. The method is based on statistical sampling. In many aspects, these methods are similar to molecular mechanics and a model for the interaction (forces) is needed. Here, the time evolution is substituted by a sufficiently large statistical sampling which is carried out following the Metropolis-Hastings algorithm. With appropriate force fields, including coarse graining, Monte Carlo techniques allow obtaining thermodymical properties under different conditions and for different types of ensembles (microcanonic, canonic or grand canonic). Time and length scales for this type of simulations are as in molecular dynamics (see above) and is strongly dependent on the type of interactions included. Monte Carlo schemes can be used for simulation of reactive systems (Kinetic Monte Carlo), for force field optimization, and for thermal properties in terms of heat and flow.

Continuum Models (incl. microscale models).

Continuum models are used to analyse the kinematics of mechanical behavior of materials on long time and length scales. These models were first formulated in the 19th century. Materials are modeled as a continuous mass rather than a discrete particle and the properties and time evolutions are governed by laws of classical mechanics. Hence, modeling an object as a continuum assumes that the substance is completely filled and ignores that matter is made of atoms. Obviously, these models are aimed at describing properties where individual atoms do not count except than in providing an averaged value. However, microscale continuum models can be applied to microscopic length and time scales to account for geometry and properties of individual constituents, and predict the macroscopic response of heterogenous materials.

Multiscaling Approach. The ultimate goal of materials science and engineering is the discovery and development of new materials. Historically, materials development has involved numerous trials and errors. This process is slow and creates limitations for the timely development and applications of new materials. Reducing the time and cost of materials development is thus a major goal.

Multiscaling is an integration of the different types of modeling and simulation described above and offers a path to accelerate materials development, specifically for renewable energy technologies. QM/MM methods provide a first step towards multiscale modeling, ab initio embedding theories provide an interesting alternative but a consistent integration of these different approaches including also existing databases and big data analytics methods is needed to reach the point where new materials for energy conversion could be discovered. There are strong indications that improving material design through computational modeling will involve directly the product design process and benefit companies.

Extending and improving the existing methods so as to increase length and time scales of simulations is, however, an urgent need for a successful outcome.

1.1.2 DESCRIPTION OF THE CHALLENGE (MAIN AIM)

Modern societies needs an inexpensive source of energy generation with minimal environmental impact. Europe cannot be a mere spectator in this endeavour and has the responsibility to contribute to the global goal of searching for alternative energy solutions. Indeed, the European commission has announced a mission to accelerate global clean energy innovation (http://europa.eu/rapid/press-release_IP-16-2063_en.htm). Currently, the major source of Europe's energy usage comes from fossil fuel combustion which is tremendously polluting, damaging our health, and destroying our planet. There are numerous examples of promising emerging technologies such as seasonal heat storage(heat battery) to improve the applicability of solar energy for providing thermal comfort in the building sector, thermochemical materials which store solar energy in form of chemical energy via a hydration-dehydration cycle and phase change materials which store the thermal energy during the process of melting and freezing. Novel designed materials can be developed having high energy density storage and fast kinetics able to store and release the heat when needed. Several promising solutions for solar energy conversion are being intensively studied based on solar energy conversion, including photovoltaic cells and photo-electrochemical cells. The purpose of solar cells and photo-electrochemical cells is to convert solar energy into useful energy, such as electricity and fuel. The efficiency of such energy converting devices relies on a sensible choice of material components. In particularly, a good material must match several criteria, including being inexpensive, non-toxic, electronically conductive, light absorbing, and chemically active for catalysis. Known existing materials do not meet all of these demands and this is severly limiting the implementation and usefulness of these technologiesin industry. Therefore novel multifunctional materials must be developed.

- This COST Action proposes to identify new designer materials for renewable energy technologies

Integrating several research and development methods to tackle this ambitious task of developing renewable energy technologies is of great importance to society world wide and especially in the highly industrialized European countries. The science behind photovoltaic cells and photo-electrochemical cells are based on phenomena that occurs at the smallest scale (atoms and molecules) up to full system operation. The composition at the atomic scale can affect band-to-band solar energy absorption efficiency as well as atom-to-atom electron transport and conductivity. However, larger scale material and device properties such as interface segregation, grain boundary movement, ionic diffusion through porous materials, and mechanical loading also strongly impact performance, making the theoretical simulation of realistic devices a challenging multi-scale and multi-physics problem.

- We will develop a theoretical framework for multi-scale material modelling

First-principles based multiscale methods that are able to predict material properties have been shown to be promising. Although our scientific community has developed expertise in the individual modelling fields, much less effort has been devoted to integrating and combining the scales toward a multi-scale approach. Multi-scale modelling is a field of solving problems which have important features at multiple scales. In physics and chemistry, multiscale modelling is aimed at predicting materials properties using information or models from different levels. The following levels are usually distinguished: quantum mechanical models (information from electronic structure at the atomic level), molecular dynamics models (information about time evolution of atoms under realistic conditions of pressure and temperature), coarse-grained and nano-level methods (information about parts of the system made from particular groups of atoms), and continuum models (information at the device scale). Each level addresses a phenomena over a specific range of length and time scales. Multiscale modelling is important in integrated computational materials science and engineering since it allows prediction of material properties and device performance based on knowledge of structure-process-property relationships. Since multiscale modelling relies on expertise at different levels and involves multidisciplinary activity, collaboration is mandatory.
Thus the most important challenges for the development of this interdisciplinary strategy that will be coordinated by this COST Action are the following:
a) Evaluating and benchmarking different methods/codes on the micro-nano-scale for predicting specific material properties related to energy converting devices, including materials structure, energetics, mechanical properties, optical, magnetic and electronic properties.

b) Examination of the specificity of selected materials based on existing databases and available experimental information for energy conversion processes exploiting the massive information available at different repositories (e.g. The Novel Materials Discovery (NOMAD) Center of Excellence, the Materials Project and aflowlib). These prototypes will be used for validating theoretical methods.
c) Development of specific schemes for integrating theoretical methods at different levels towards a useful multiscaling approach.
d) Providing a basis for discussion and bridging between different fields.

The ultimate central challenge will be to generate a multiscale modelling platform that will be used world-wide for conducting state-of-the-art multi-scale property prediction of materials.

1.2 PROGRESS BEYOND THE STATE-OF-THE-ART

1.2.1 APPROACH TO THE CHALLENGE AND PROGRESS BEYOND THE STATE-OF-THE-ART

There are many challenges that remain to be overcome before the multiscaling approach will become a user friendly approach. One of the great challenges is how to connect between the different theoretical regimes. In fact, the QM/MM type of approaches discussed above are also applicable in special cases, for instance when the bonds that are broken can be saturated by hydrogen atoms or when the outer part of the material of interest is made of discrete parts as in the case of molecular based materials. Another challenge is how to import information from the small scale to the larger scale theory (and vice versa). For example, the larger scale Molecular dynamics can use Quantum Mechanical information for building potentials of atomic interactions (for example, through the ReaxFF approach), but many potential energies have not yet been derived for exotic materials such as nano-structures. This issue is significant for developing renewable energy materials since nanostructures have a large surface area and are able to absorb solar energy. The COST Action presented here will be aimed at integrating all available knowledge on potential parameters that can be transferred from one scale to another in the most possible general way so that one could reach a full system design.

This COST Action will create synergies at the scientific level (at European and International levels) to produce new computational tools, enhance research productivity and come up with results of interest likely to be brought to experimental test. This COST Action will also develop initiatives to train young scientists, as well as inform computational users throughout the development and production.

The interconnection between chemistry and computer science is ever increasing in developing new materials for various applications. Our expertise and experiences in chemistry and programming needs to be combined and expanded in order to achieve breakthroughs in efficiently developing new and advanced materials. Multiscale modelling techniques such as ab initio molecular dynamics or force field based calculations still suffer from the limitation of the number of atoms that can be simulated even with the biggest super computers in the world. In this context, novel approaches such as machine learning offers a potential pathway to develop new computational modelling techniques in atomic and molecular simulations. In addition, better ways to parameterize complex force fields will also need to be explored for faster and accurate modelling of chemical processes.

The innovative character lies both in methodology, simulation and material properties investigation and development. GCMC studies have been conducted previously to model for instance sorption in multi-component systems. These studies cannot be applied however to model bulk reaction (e.g. oxidation) because the transition from pure metal to bulk metal oxide requires significant material rearrangement. A hybrid Grand Canonical Monte Carlo and MD method to simulate systems like on crystal level (e.g. the hydration/dehydration conditions for sorption materials) and the effect of the crystal defects and dislocations on larger scale. These methods are applied for a larger class of applications: solar cells, photo-electrochemical cells, etc.

1.2.2 OBJECTIVES

1.2.2.1 Research Coordination Objectives

To help maximize the benefits of different levels of materials science, this COST Action will collate and disseminate available information on theory integration. This will facilitate research and exploitation of this methodology, identify information gaps and research needs, allow it to develop new research targets

and identify gaps that need further development. In addition, computational materials scientists will be made aware of the resulting methodology and of its potential to contribute to the scientific and technological community. They will be informed about the potential benefits and limitations and engaged in discussions.
The main objectives and deliverables of this COST Action include:
1. A review of the current and upcoming methods/protocols/codes for developing novel materials for improving solar energy conversion efficiency, including their applications and advantages and weaknesses.
2. An organized network of European scientists working on achieving greater scientific understanding of energy conversion mechanisms and developing approaches for reliable and realistic multi-scale modelling of material architectures.
3. Determining specific material requirements for the assessment of efficient energy conversion. Here the needs for specific energy conversion devices, including photovoltaic cells and photoelectrochemical cells, will be determined.
4. Developing existing and new field method centres in several European countries in order to test the efficiency and method applicability and transferability. Such efforts could be implemented at computational facilities across Europe, such as PRACE.
5. Establishing consultation services (technical) and recommendations to end-user groups.
6. Mentoring, organizing workshops, certified training programmes and computer and staff exchange to improve researcher to end-user efficacy. Where practical this will be done in association with other related international symposia and conferences.
7. Encouraging and publishing research reports by scientists involved in multiscale and theoretical related studies.
8. Strengthening collaboration of theoretical groups with experimental groups in order to receive experimental feedback on the proposed new materials and verify the theoretical hypothesis.

1.2.2.2 Capacity-building Objectives

This COST Action will establish:
• An international research consortium of scientists based in Europe and national research programmes on theoretical multiscale modelling, who will be able to exchange knowledge with the worldwide science community.
• An international consortium for materials design aimed at solar energy conversion devices and their products to provide scientific support for technological development and regulatory authorities in EU and elsewhere.
• Overall, this COST Action will result in a network oriented scientific platform for discussions and public outreach on the solar energy conversion technology.

The capacity building objectives of this COST Action are to:
1. Set up a process for assembling scientific information on material properties for solar energy conversion and build a respective reliable and efficient modelling methodology.
2. Establish data collections on methodologies currently in use and under development. To this end strong collaboration with the NOMAD Center of Excellence (https://nomad-coe.eu/) and open quantum materials database is envisaged (http://oqmd.org/).
3. Evaluate the accuracy of these methods and recommend changes to protocols where appropriate.
4. Establish a network of existing and new method oriented centres where the new method developments and integration can be tested and demonstrated.
5. Provide a platform to train young scientists through STSMs targeted at selected high-impact topics, mentoring programmes and training workshops, building on existing training networks (e.g. CECAM, Materials Modeling Council: https://emmc.info).
7. Promote collaboration among European and international interested parties.
8. Encourage the development of new relevant research consortia and programmes within Europe and cooperate with existing related initiatives.
9. Establish a communications platform for academia, industry, and the public.
10. Fostering and creating role models with network opportunities for early career scientists and female scientists. The members at proposal stage include a balanced blend of senior/junior and male/female ratio.

2 NETWORKING EXCELLENCE

2.1 ADDED VALUE OF NETWORKING IN S&T EXCELLENCE

2.1.1 ADDED VALUE IN RELATION TO EXISTING EFFORTS AT EUROPEAN AND/OR INTERNATIONAL LEVEL

The Action will facilitate the incorporation of state of the art scientific information to be available in an open access (open source code) manner to the European scientific community and encourage software companies to envoke the Action developments. This will enable incorporation of the Action ideas into broad usage in a user-friendly platform. The Action will establish a strong collaboration with existing related efforts, including NOMAD Center of Excellence, CECAM Network, Psik Netwrok, Materials Modeling Council, etc, since members of the action are associated with these groups. Considering energy supply aspects in parallel with the development of new methodologies will streamline usage of such products significantly. This COST Action will encourage the introduction of computational technology into the mix of new technologies that will support the EU economy initiatives in H2020 and beyond. In addition, it will support worldwide initiatives (e.g., the global initiative for clean energy declared in 2016) for developing sustainable energy production and providing energy security.

2.2 ADDED VALUE OF NETWORKING IN IMPACT

2.2.1 SECURING THE CRITICAL MASS AND EXPERTISE

The Action will promote scientific exchange and communication on the science and will promote the development of a theoretical and computational machinery for characterizing a wide range of materials that are being researched and developed worldwide. Specific material compositions include bulk semiconductors, solvated surfaces, and metal/semiconductor interfaces and heterojunctions; all of these components are used in energy converting devices.

The benefit of the networking on all these topics will be the increased synergy created between scientists, which will stimulate exchanges of knowledge, ideas, methods and computational codes, and therefore enhance their productivity and optimize the use of resources and maximize research output and impact. Networking is specifically important since there is the need to bridge disciplines which usually do not interact. Young scientists will benefit from the larger pool of shared knowledge and experience and be able to work in laboratories with different expertise and experience and this will help ensure continued ongoing synergy into the future. In addition, there will be networking with industry (including software developers of scientific codes), which will enhance knowledge and facilitate shared experiences with the users of the technology. Understanding the ultimate requirements of end users will help efficiently align the research agenda with the practically required technology. As a result, the research programs will have greater relevance to the real needs of the user-community. The training programs will be able to exploit this combined network of knowledge and expertise to provide training which is beyond the state of the art.

2.2.2 INVOLVEMENT OF STAKEHOLDERS

As already stated, the Action aims to bring together researchers from most European and many other countries. These will include scientific leaders in their fields and advanced developers of the technology. The Action will identify the leaders by creating a database of scientists that are experts in each topic of the WGs and will interest them by organizing international conferences in Europe (see "Technology and know how transfer plan" in the work plan). These funded platforms will attract and interest the different groups. Hence, the scientific consortium will reflect the state of the art and development of the new technology. The Action will organize events specifically targeted at the different theory level types and multidisciplinary events to allow interchange between the different specialties. These will include:

• Scientists, scientific institutions, organizations, scientific academies and societies e.g. ECS,

E-MRS, Royal Society of Chemistry, Research Institutes for Energy Research (ECN), etc.

• Industrial organizations of code development.

• Public organizations, media, journalists, politicians from the Energy and Environmental Ministry offices of each country.

• Decision makers at political and scientific level for funding and support of research, determination of research priorities.

2.2.3 MUTUAL BENEFITS OF THE INVOLVEMENT OF SECONDARY PROPOSERS FROM NEAR NEIGHBOUR OR INTERNATIONAL PARTNER COUNTRIES OR INTERNATIONAL ORGANISATIONS

The Action will facilitate the incorporation of state of the art scientific information to be available in an open access (open source code) manner to the European scientific community and encourage software companies to envoke the Action developments. This will enable incorporation of the Action ideas into broad usage in a user-friendly platform. The Action will establish a strong collaboration with existing related efforts, including NOMAD Center of Excellence, CECAM Network, Psik Netwrok, Materials Modeling Council, etc. Considering energy supply aspects in parallel with the development of new methodologies will streamline usage of such products significantly. This Action will encourage the introduction of computational technology into the mix of new technologies that will support the EU economy initiatives in H2020 and beyond. In addition, it will support worldwide initiatives (e.g., the global initiative for clean energy declared in 2016) for developing sustainable energy production and providing energy security.

3 IMPACT

3.1 IMPACT TO SCIENCE, SOCIETY AND COMPETITIVENESS, AND POTENTIAL FOR INNOVATION/BREAK-THROUGHS

3.1.1 SCIENTIFIC, TECHNOLOGICAL, AND/OR SOCIOECONOMIC IMPACTS (INCLUDING POTENTIAL INNOVATIONS AND/OR BREAKTHROUGHS)

Developing and exploiting multiscale methods in computational material science is a relatively new technology which has huge potential to progress beyond the state-of-the-art as described in Section 1. This COST Action will bring together many of the key players involved in researching and developing this technology and assessing its potential for material characterization, which will enhance the likelihood of both scientific innovation and new breakthroughs toward material design and discovery. The Action will promote efforts to increase awareness of the importance to invest in research and development on novel materials via computational approaches. The Action will establish links and invite to workshops research funding organizations such as DFG, ISF, National Ministry of Sciences, H2020, National research councils and scientific academies, other international and national funding organizations and industry. Many scientists have expressed interest in this COST Action, and it is foreseen an accelerated amount of members joining at the first year. The return trade-off is significant for both fundamental science development and application to society's needs.

3.2 MEASURES TO MAXIMISE IMPACT

3.2.1 KNOWLEDGE CREATION, TRANSFER OF KNOWLEDGE AND CAREER DEVELOPMENT

The COST conferences and workshops will be linked if possible to other national or international meetings/conferences on computational modeling related topics, e.g. those organized by CECAM, NOMAD Center of Excellence, Psi-k, MRS, EU, scientific societies and organizations etc. One MC member will be specifically in charge of the dissemination through the different media. In addition, participants in this COST Action will also promote the activities of the COST Action in meetings and workshops around the world organized by other scientific organizations. Other Communication activities: In year 1 an open access Webpage will be established with news and articles on multiscaling developments and information on the COST Action events and activities. This will be linked to Facebook, twitter, LinkedIn and provide podcasts and/or reports of all meetings, workshops etc. There will also be an intranet site for COST Action members to communicate news, activities, products, reports etc. within the Action. There will be some constraints associated with intellectual property rights and confidential

business information associated with some new developments and the Action will examine ways to protect these while enabling as much sharing of information as possible. The Action will encourage efforts of intellectual property submissions for patents when novel materials are discovered.

3.2.2 PLAN FOR DISSEMINATION AND/OR EXPLOITATION AND DIALOGUE WITH THE GENERAL PUBLIC OR POLICY

The Action will organize events specifically targeted at the different theory level types and multidisciplinary events to allow interchange between the different specialties. These will include:

• Public organizations, media, journalists, politicians from the Energy and Environmental Ministry offices of each country.

• Decision makers at political and scientific level for funding and support of research, determination of research priorities.

4 IMPLEMENTATION

4.1 COHERENCE AND EFFECTIVENESS OF THE WORK PLAN

4.1.1 DESCRIPTION OF WORKING GROUPS, TASKS AND ACTIVITIES

The objectives of this COST Action will be achieved through the systematic organization, the effective functioning of the selected group of researchers and, most importantly, the interactive character of the individuals, as described in detail below. It should be emphasized that the consortium and its working groups (WGs) are set up in such a way that the contributions of its members form an integral part of the main focus of this COST Action. Through the Action, regular meetings, workshops and reports will be organized for the consortium to exchange updated data and information.

WG1: Quantum Mechanics Theory

Objectives: Compare state-of-the-art electronic structure methods (from the many different flavors of density functional theory to quantum-chemical approaches (coupled cluster etc.) with respect to their usability in the development of functional materials for photovoltaic and electrochemical cells.

Tasks, Deliverables:

1. Review existing knowledge and state of the art to provide a solid background for new developments, applications and research information. Identify knowledge and data gaps.

2. Define relevant quantum mechanical observables related to material functionality for energy storage that can be parametrized and transferred to multiscaling in WG2.

Deliverable: Develop a data base of references and relevant documents.

3. Review and study materials systems that have been and are being developed and commercialised. Itentify specific material properties and criteria needed to match highly efficient photovoltaic and photoelectrochemical technology. Compare approaches, determine advantages and disadvantages, specificity, etc.

Deliverable: a review of the methods of quantum mechanics in modeling materials for renewable energy applications.

4. Explore potential new materials for renewable energy technology.

Deliverable: Review of existing and future materials studied with quantum mechanical methods.

5. Development of a web-page with links to accessible informatics data base on target materials

Deliverable: Review of existing materials informatics data base and needs.

6. Support training, conference and workshop programme. The workshops should include specific tutorials for each pair of WGs, for example WG 1&2, , emphasizing the overlap between groups. If possible, the workshops will be taking place for a duration of five days each year and leaded by a member of the groups at their country. The workshops will be dedicated to disseminate the knowledge gained by partnering at the Action. If possible, someAction conferences will be coupled to regional conference meetings at Europe twice a year, where members for the Action will be recruited, such as the E-MRS. More details described in section 2.2.2.

Milestones

1. Joint meeting with WG 2: Months 12, 24

2. Access to information on methods available for further multiscaling integration studies: Month 24

3. WG meeting: Months 36

WG2. Molecular Dynamics Simulations

Objectives: To determine the state of development of molecular dynamics simulation and factors involved in their development

Tasks, Deliverables:

1. A study of the current situation on the development and application of molecular dynamics simulations worldwide.

Deliverable: A review of current developments of molecular dynamics simulations.

2. The feasibility, methodology and advantages of the different materials systems will be compared and recommendations, including future improvements, of the systems will be made.

Deliverable: A report on various material model systems for molecular dynamics simulations.

3. Develop research and delivery priorities, strategies, and initiatives for developing novel materials and to fill the knowledge gaps. This will enable the Action to communicate to European and national funding agencies the high priority needs for this research.

Deliverable: Research Priorities Report.

4. Support training, conference and workshop programme as described in 2.2.2.

Milestones

1. Joint two meetings with WG 1 & 3: Months 12, 24

2. Development of the scientific data base for the reporting platform developed in WG5 to communicate relevant information: Month 24

3. WG meeting: Months 36

WG3: Monte Carlo Simulations

Objectives::

1. Collect scientific information about material properties aspects linked to molecular dynamics simulations

2. Promote research collaborations in this area in order to enhance certainty about relation between theoretical approaches among other length scales and WGs.

3. Produce protocols to support simulations based on information provided by WG 1 & 2.

Tasks & Deliverables:

1. Compilation of reviews on the available knowledge on aspects of material properties that are essbential for energy conversion processes in relation to monte carlo simulations.

2. Identification of known or new knowledge gaps arising in the area of obtaining parameters from the theme of WG 1 & 2 to the area of theme WG 3.

3. Develop a data base on material targets that can be characterized with monte carlo simulations. This activity will be developed jointly with WG1 and WG2.

4. Develop some case study of materials assessments based on running research activities of current material applications as examples of methodology and outcomes.

Deliverables: Communications of results in reports, workshops and COST Action conferences to interested parties and promote training, workshops, exchange of scientists, etc.

Milestones

1. Joint two meetings with WG 2 & 4: Month 12

2. Choice of relevant case studies: Month 20

3. WG meeting: Months 36

WG4. Microscale and Continuum Modeling

Objectives:

1. Provide analyses and information on the impacts of material properties that can be calculated with continuum modeling.

2. Review applications of microscale models in predicting in-situ and macroscopic physical properties of materials for energy conversion applications, including approaches for determination of input parameters and validation techniques

Tasks & Deliverables:

1. Review the social and economic impacts of material discovery through continuum modeling.

2. Case studies: Perform cost benefit analyses of some existing and future material systems to demonstrate benefits to consumers as well as economic costs.

3. Compare the observables calculated by other WGs.

Deliverables: i) a data-base of study on material properties calculated with continuum modeling. ii) a teaching module for continuum modeling. iii) Reports and communication of results to users at workshops and in training programmes

Milestones:

1. Joint meeting with WG 4: Month 12.

2. Communication of Task results and deliverables to trainees: Month 24

3. Establishment of data base: Month 24

4. WG meeting: Months 36

WG5: Multiscaling Approaches

Objectives: To develop an effective communication strategy and platform for the Action that reaches all interested parties and the general public as well as members of the Action. All of the members will take part in the WG5 since this group will integrate the different threoretical approaches of WGs 1-4 toward a single multiscale approach.

Tasks, Deliverables:

1. A communication and dissemination plan developed in year 1. This will include:

- Organizing the conference and workshop programme together with other WGs.

- Establishing links with a wide range of experts from different countries and organizations (developers and users). Involve them in discussions and workshops on the computational issues.

The dissemination plan will be updated with the scientific progress of the research partners involved in the Action as well the results of its own studies (e.g. on multiscaling) in order to allow rapid dissemination of the most recent developments during the course of the Action.

Deliverable: A communication and dissemination plan.

2. Coordination of Training courses: Training is one of the main objectives of this COST Action. A series of Short-Term Scientific Missions (STSMs) will be offered to young scientists. These STSMs will facilitate transfer of knowledge, training in new techniques, the use of important new codes and modules. Furthermore, young scientists will benefit from a mentoring program, due to the presence of highly qualified scientists in this consortium with extensive mentoring experience and tutoring. This will foster personal connections and provide opportunities for future career development of the early career.investigators Training Schools, with hands-on training, will be designed to provide young scientists with the skills in mutiscaling. If possible, Training Schools linked to existing international conference programs will be organized at the participants' institutes with the respective know-how and expertise. The material from the Training Schools will be available to all participants via the Action web site.

Deliverables: establishment of training programmes, training material available on Action website.

3. Establish and manage On Line Platform and **Web site.** This Action web site will serve as an open-portal for all Action activities providing up-to-date information on Action achievements and contact point for all interesting parties (e.g. SMEs, grower groups, etc.). In addition, it will publish information on Facebook, Linked-in and Twitter with links to the website. The web site will be frequently updated but with major revisions following each management board meeting. Theinformation posted will include:

- General information about COST and this COST Action (objectives, guidelines, achievements, etc.);

- Intranet: a secure portal for Action participants will be made;

- National portals highlighting activities in individual countries;

- Proceedings of meetings (talks and posters from meetings), bulletins and information, pamphlets, and other reports (e.g. STSM reports);

- Videos of useful material (e.g. transformation systems);

- Short-term Scientific Missions STSM Calls (guidelines and application material);

- Job announcements;

- Publications and contact information for Action participants;

- Other relevant news and links (institutes, research groups and EU organizations).

4. Establish a Publications Task Force to consider the desirability and feasibility of publishing a book containing a comprehensive review on multiscaling. The book would need to be of broad scientific

interest as well as a valuable teaching tool for students. If considered desirable, book proposals would be sent to prospective publishers for their reaction.

Milestones

1. Joint meeting with all WGs: month 12

2. Establishment of intranet platform: month 12

3. Establish a Publications Task Force: month 36

4.1.2 DESCRIPTION OF DELIVERABLES AND TIMEFRAME

Outline Plan of meetings and events (subject to revision when the consortium is formed due to possible changes in priority of topics):

Year 1:

• Kick off meeting

• All five WGs joint meeting

- Establishing a web presence to coordinate the Action and distribute News, workshop announcements, research highlights etc. The webpage will be linked to Facebook, twitter, LinkedIn and provide podcasts and reports of all meetings, workshops etc.
- There will also be an intranet site for COST Action members to communicate news, activities, products, reports etc. within the Action.

• 1st Conference: Multiscale Modeling in Computational Materials Science for Energy Applications: Present situation and future research requirements.

• Training School : Theoretical methods of material characterization techniques for energy applications.

Year 2:

• WG meetings.

• Computational Materials Workshop / Participation at international conferences

• 2 Training Schools :

- Computational methods in practice usage
- Material discovery, design, and development

Year 3:

• WG and Small Group meetings.

• 2nd Conference: “Applications of computational materials science for renewable energy applications”. This will be accompanied by workshops and briefings for industry, media, public etc.

•Participation at international conference Training School: Overlap between computational materials at different scales.

Year 4:

• Final Conference: Multiscaling in 2020 (A review of the COST Action activities in relation to scientific knowledge, developments and future prospects), accompanied by workshops and briefings for industry, media, public, etc.

• Final Training Schools: Multiscaling in practice.

4.1.3 RISK ANALYSIS AND CONTINGENCY PLANS

Risks to the conduct of the project include:

i. Attacks on the web site. This will require professional and technical advice from the Security computing team available at Universities on how to protect the web site and have high levels of security for its access and operation.

ii. Disinterest or lack of participation. This risk is more likely to happen when a new member enters the Action and does not yet know what are the topics and requirements. Information will be provided on the COST web site about the activities to avoid unsuitable/uninterested members. All partners will be required to identify substitutes and involve more members from research groups who can take over their roles in the project.

iii. Financial losses. The coordinator/chairman will establish tight financial limitations.

iiii. Specialists work on their time and length scale / method, but that the methods are not connected. In order to avoid this problem adjunct WGs will meet to identify and define interfaces between the methods and transfer data.

4.1.4 GANTT DIAGRAM

Timeline for Action/months	6	12	18	24	30	36	42	48
Management Coordination								
Action kick-off								
Management Committee established								
Executive Committee selected								
WG activities coordinated								
Internet web site in the air								
Web site updates								
MC meetings								
Mid-term/Final reporting to COST								
Working Group Programmes								
Programme planning								
WG scientific meetings								
Reviews of methods and applications								
Proceedings from WG meetings								
Integration and development of multiscaling techniques								
Testcases and development of materials for energy								
Training								
Training Programme organization								
Training workshops								
STSMs								
Technology and Know-how Transfer Plan								
Workshops and conferences								
Delegations of international conferences								
Reports and publications in peer-reviewed journals								