European Cooperation in the field of Scientific and Technical Research
- COST -

Brussels, 14 November 2014

COST 088/14

MEMORANDUM OF UNDERSTANDING

Subject :	Memorandum of Understanding for the implementation of a European Concerted Research Action designated as COST Action CM1405: Molecules in motion (MOLIM)

Delegations will find attached the Memorandum of Understanding for COST Action CM1405 as approved by the COST Committee of Senior Officials (CSO) at its 191th meeting on 12-13 November 2014.

MEMORANDUM OF UNDERSTANDING

For the implementation of a European Concerted Research Action designated as

COST Action CM1405
MOLECULES IN MOTION (MOLIM)

The Parties to this Memorandum of Understanding, declaring their common intention to participate in the concerted Action referred to above and described in the technical Annex to the Memorandum, have reached the following understanding:

1. The Action will be carried out in accordance with the provisions of document COST 4114/13 "COST Action Management" and document 4112/13 "Rules for Participation in and Implementation of COST Activities", or in any new document amending or replacing them, the contents of which the Parties are fully aware of.

2. The main objective of the Action is to establish a network of theorists and experimentalists to develop set of tools aimed to address complex molecular systems via novel experiments and simulations of the nuclear motion and educating the next generation of users of the next generation of chemistry tools.

3. 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 2014 prices.

4. The Memorandum of Understanding will take effect on being accepted by at least five Parties.

5. The Memorandum of Understanding will remain in force for a period of 4 years, calculated from the date of the first meeting of the Management Committee, unless the duration of the Action is modified according to the provisions of Section *2. Changes to a COST Action* in the document COST 4114/13.

A. ABSTRACT

Interpretation of sophisticated experiments often requires advanced theories. A consistent set of user-friendly tools for an elaborate treatment of nuclear motions of microscopic and macroscopic systems does not yet exist. Development of the armoury of first-principles nuclear motion theory, via the advancement of theories, algorithms, and codes, is the major goal of this Action, with special emphasis on quantum effects involving electrons as well as nuclei. Molecular scientists, modellers and engineers will all benefit from the new methods and codes. The developments cover quantum chemical, quantum dynamical, semi-classical, and advanced classical treatments. Access to most of the source codes developed within the Action is provided to the scientific community free of charge. Multifaceted collaborative efforts with experimentalists applying the pilot versions of the new tools is considered to be vital to the success of the Action. MOLIM is a platform for (a) development of a network of theorists and experimentalists; (b) quick dissemination of important results to a large and growing scientific community; and (c) establishment of long-lasting European-wide conferences and training schools, educating the next generation of users of the next generation of chemistry tools.

Keywords: nuclear motion theory, first principles quantum chemistry, surfaces and interfaces, new spectroscopic techniques, Born-Oppenheimer separation

B. BACKGROUND

B.1 General background

The 2013 Nobel Prize in chemistry was awarded for advancing the theoretical study of biomolecules, naturally complex systems, via approximate numerical computations. The starting point of this Action is that many molecular systems and processes are complex when studied in sufficient detail. A relevant example is the nuclear motion of even small molecular systems investigated under high resolution in either the frequency or the time domains. Participants of this Action are especially interested in complex features which can only be understood if the quantum nature of the atomic nuclei is considered and in developments urgently needed for modelling and engineering applications of outstanding importance.

Quantum chemistry has two important subfields: electronic structure and nuclear motion theories. They cannot be separated in the sense that only one of them should be preferred. The time and

effort invested by the scientific community into developing electronic structure techniques is enormous. Consequently, there are splendid tools to understand accurately the electronic motion in molecules, on surfaces, and in the solid state. Nuclear motion theory lags behind in scope, generality, and accessibility. Treatment of nuclear dynamics has been developed in parallel mostly by spectroscopists studying molecular states and researchers using molecular scattering to study reactivity and related phenomena. Spectroscopists in general start from phenomenological Hamiltonians, while scattering theory uses general Hamiltonians with appropriate potential energy surfaces (PES). The PESs and other property surfaces can be obtained with tools of electronic structure theory. Spectroscopic computations can treat many-atom systems, but the models widely employed are often based on poorly controlled approximations: rotors are often semi-rigid and oscillations are harmonic or only weakly anharmonic. These approximations are the starting points for useful simplifications only for relatively rigid systems, or when the vibrational motion is barely excited, and fail when high spectral resolution is considered. Quantum reactive scattering theory, in contrast, treats the full range of motions accurately, but it is in general restricted to 3- and 4-atom systems. Furthermore, elementary chemical processes are generally not described as the evolution of a wavepacket, while there is growing evidence that a significant number of chemical reactions are impacted by strong quantum-mechanical effects involving not only the electrons but also the nuclei. The spectroscopic, dynamics, and scattering communities have in recent years started to merge, driven not the least by the demands formulated when using time-resolved spectroscopy. This Action places great emphasis on accelerating the merging process and ensuring that researchers in the different fields understand each other better and use the best practices existing within each field. European scientists have played a vital and pioneering role in developing the theory of nuclear motions. Some 90 years ago the modern theory of quantum mechanics (QM) was formulated and worked out by European physicists and molecular physics, and the application of QM to chemistry, *i.e.*, quantum chemistry, has also been pioneered within Europe. Theory has been strong both in the Western and Eastern parts of Europe.

B.2 Current state of knowledge

Molecular spectroscopy, including rotational, vibrational, electronic, and photoelectron spectroscopies, is built around high-end analytical tools developed to obtain detailed information about complex natural systems. These systems include the earth's atmosphere, where spectroscopy helps us to understand the greenhouse effect, and astronomical bodies of our universe, where spectroscopy helps to answer principal questions related to the structure of the universe and the

appropriate conditions for the existence of life. Important applications of modern high-sensitivity experiments include medical research such as linking breath analysis to human health, making combustion more effective and environment friendly, understanding atmospheric chemistry, including (surface) photochemistry, where a complete treatment of even the simple photo-reaction (desorption) has yet to be achieved, and interpretating astronomical spectroscopic observations (*e.g.*, exoplanet research).
Reaching the next level of understanding of complex molecular motions requires reliance on sophisticated and often complex theories, significant team efforts to integrate different competences, and validation and verification of enormous datasets. This Action, via its design of a strong collaboration between leading theorists and experimentalists, will help to fulfil these expectations.

B.3 Reasons for the Action

This Actions will contribute that Europe will regain and maintain its leading role in the development and application of quantum theory to complex molecular systems. Many of the codes applied today in nuclear dynamics are products of European teams, it is enough to mention here the MCTDH (Multi Configuration Time Dependent Hartree) suite of codes. The background knowledge acquired by developers of these codes based in different laboratories must be transferred in a systematic way to the next generation of developers and users. One of the principal aims of this Action, namely the development of "black-box-type" nuclear motion codes, can only be achieved if a network of experts is assembled for a long enough time providing the necessary forum for joint method and code development, if cooperative efforts are emphasized, and if longer-lasting Training Schools as well as symposia and workshops are established for knowledge transfer.
While there is enormous demand for accurate nuclear motion computations to provide a bridge between experiments and *ab initio* (first principles) data to achieve scientific and technological advances, there are few codes that are capable of meeting the stringent standards set by the wide range of experiments and experimental conditions. Furthermore, the otherwise outstanding nuclear-motion codes written so far are often not designed for a general, non-specialist user. This Action plans to integrate European theoreticians working in the field of nuclear dynamics and come up with new theories, algorithms, and preferably widely accessible black-box codes, while reaching out to researchers working in the field of electronic structure theory as well as to experimentalists.

Spectroscopy is an obvious testing ground for quantum mechanics and quantum mechanical, including quantum chemical, computations. There are several relevant directions which will be pursued during this Action.

It is considered that the hallmark of good science is that theory and experiment progress hand in hand, the development of innovative experimental, including spectroscopic, techniques is equally important for the Action. It is noted in this respect that new laboratory or synchrotron radiation sources have pushed forward the development of unprecedented high resolution and high sensitivity instruments. In the VUV (Vacuum Ultraviolet) spectral range, the interplay of spectroscopy and photochemistry will lead to the study of elementary photoreactions below and above the ionization threshold. The related reaction branching ratios will be determined both experimentally and quantum chemically. VUV spectroscopy also leads to important photodynamic studies of interest for planetology and astrophysics. In the infrared and far-infrared (THz) range, the combination of high resolution experiments and theory developed within the Action will lead to the first recording of rotational-vibrational bands related to large amplitude (or hydrogen-bonding) motions.

Another central question of this Action is how to control chemical reactivity and selectivity.

Another important aim of this Action is to lay down the framework of long-lasting European-wide international conferences and Training Schools in the area of nuclear motion theory and nuclear dynamics.

The Action will provide prominent leadership for European scientists in the field of nuclear motion theory and nuclear dynamics, in computational and certain parts of experimental spectroscopy (*e.g.*, ultrafast and time-resolved spectroscopies), in handling coupled electronic and nuclear motions (including Born-Oppenheimer breakdown cases), in further development of all these fields, and their application in atmospheric, interstellar and industrial contexts. As such this multifaceted network will be unique in the world and developing chemistry further really needs a strong collaboration among scientists with different expertise and computational and experimental facilities, among algorithm developers and code writers, among theorists and experimentalists.

B.4 Complementarity with other research programmes

It is not known any other European-supported programs in the field of molecular nuclear motion theory. This Action should complement very effectively the efforts of theoretical, computational, and experimental groups and should help to define European research in the field of nuclear motion theory.

C. OBJECTIVES AND BENEFITS

C.1 Aim

The main objective of the Action is to develop computational tools for molecular sciences including determination of properties of complex non- and quasi-periodic systems, for the coupling of electronic and nuclear motions, for the application of the new tools to experimental problems of an outstanding nature, and it will become the ground for the emergence of the next generation of chemists who will be users of the next generation of chemistry tools.

C.2 Objectives

This Action plans to achieve what is required and expected from cutting-edge theoretical research and plans to accomplish this via close and enhanced interactions and collaborations in the following directions: (a) develop new theoretical formalisms and efficient codes based on them; (b) advance approximation techniques and test them via comparison with other techniques and/or experiment, mostly focusing on directly measurable quantities; (c) provide benchmark, fundamentally relevant results which help to further advance science; (d) explain experimental phenomena which previously remained unexplained due to insufficient theoretical knowledge and thus help to push experiments further or provide enhanced control; (e) propose novel experimental approaches as well as new experimental setups requiring sophisticated theory and simulations; (f) validate and verify experimental findings and help to transfer data into knowledge so that they can be used safely by modellers and engineers; and (g) provide recommendations to the scientific community and international organizations. Only collaborative efforts emphasized within the Action and a mutual understanding of scientists working in interdisciplinary fields (mathematics, physics, and chemistry, as well as programming), obtained via attending a set of dedicated conferences and workshops, will help to accomplish the stated ambitious goals of the Action. Finally, a principal educational objective of the Action is the development of a set of conferences, workshops, training schools, and training materials which help to ensure that the stated scientific objectives can be achieved and which will remain in the focus of the collaborating European research laboratories long after the Action finished its activities. Moreover, this Action will promote collaborations between different regions of Europe

C.3 How networking within the Action will yield the objectives?

Development of the field of nuclear motion theory clearly calls for enhanced collaboration which must be catalysed. The expertise and the often expensive equipment readily available to some of the Action participants already constitute one of the strengths of the Action. Participants of the Action will benefit from the extensive networking made possible by the COST framework, since the scientific meetings and the Short-Term Scientific Missions (STSMs) will help to define as well as to overcome the scientific bottlenecks.

Specific networking ideas the Action has are as follows: (a) Coordination of research projects including preparation of trans-national collaborative research proposals between the groups participating in the Action. (b) Establishment of annual conferences and training schools which would outlast the Action. This includes organization of workshops bringing together experimental and theoretical experts on specific topics which are also marked as scientific objectives of this Action (*e.g.*, the theoretical modelling of helium-mediated deposition of nanoparticles with tailored optical-electro-magnetic properties on technologically relevant surfaces). (c) Dissemination of the results of the Action to the community of end users. The organization of Training Schools will play a key role in this respect. Most of the trainers at the Training Schools will be senior participants in the Action but outside experts will also be involved. This will help to further strengthen the Action and maintain its global influence. (d) Mobility of Early-Stage Researchers (ESRs) will be promoted through a large number of STSMs. Exchanges between experimental and theoretical groups and between groups having complementary expertise will be particularly encouraged in order to ensure that ESRs will be trained in several areas. (e) Assessment, validation, verification, quantification, and standardization of data must involve a large number of groups and expertise. Networking within the Action should help to develop novel information systems and improve existing ones which modellers and engineers consider as canonical sources of information.

C.4 Potential impact of the Action

There are a large number of reasons why scientists from different COST countries decided to form this Action. One particularly important reason is that it is shared the feeling that significant advancement of the field of nuclear motion theory requires large-scale networking. For collaborative efforts and knowledge transfer COST provides an ideal framework.

A large number of different bodies will benefit from the Action results, including international scientific communities (theoretical chemists, molecular physicists, experimental chemists,

spectroscopists, astrochemists and astrophysicists, atmospheric scientists, and biophysicists). Those who study molecular interactions, H-bonding dynamics will also benefit from the research results, as well as applied/industrial research (as specified elsewhere), users of current and future large European research facilities (synchrotrons, ELI), and all the users of the new codes.

C.5 Target groups/end users

As the topic covered by this Action is of fundamental nature, its results will help to increase the general knowledge of molecular processes and as such the whole community will be able to exploit them. A considerable number of physicists and chemists have been involved in the preparation of this Action. The target groups and the end users are scientists, engineers, and database managers.

D. SCIENTIFIC PROGRAMME

D.1 Scientific focus

The Action focuses on the science of complex molecular motion investigated theoretically, computationally, as well as experimentally for species in the gas and in condensed phases, as well as on surfaces and at interfaces. In the future investigations almost all possible target conditions will be included, such as very low and very high temperatures, very low and very high pressures, etc. This is made possible because both electronic and nuclear motions together have been considered, as is absolutely necessary when dealing with many molecular phenomena, including those considered to be extreme at present. As emphasized above, participants of the Action will be engaged in hand in hand theoretical and experimental method development. The most important research tasks (RT), providing the scientific focus of the Action, are summarized as follows:
RT1: Development of new time-dependent and energy-domain (time-independent) theoretical models and approaches for solving nuclear-motion quantum-mechanical equations for increasingly complex molecular systems of non- and (quasi-)periodic nature, including semiclassical, quantum, and so-called mixed approaches, in a form readily accessible for non-experts. An essential part of the theoretical method development will seek to integrate new numerical, mathematical, and computational methods into nuclear motion theory, including vibrational coupled cluster theory, tensor decomposition, automatic differentiation, and automatic code generation techniques. Time-domain methodologies are important for many aspects of chemical kinetics and dynamics and can be combined with classical or semiclassical technologies, such as QM/MM (quantum

mechanics/molecular mechanics), *ab initio* dynamics, and the many variants of Car-Parrinello techniques. New treatments for highly accurate time-dependent quantum dynamics will be searched for, including adapting approximate time-independent techniques to time-dependent wave packet propagation.

RT2: Spectroscopic treatments of large systems require special attention. In electronic spectroscopy a common approach is computing simply the vertical energies from the equilibrium configuration of the complex and then "dress" the absorption line with some function, Gaussian, Lorentzian, etc., whose parameters depend on the local slope of the potential. Going beyond this simple approximation is a challenge and one of the goals of the Action. In some intermediate systems it is possible to use the MCTDH approach to study the spectroscopy. The problem then is the representation of the potential energy surface in many dimensions. Though progress has been achieved by participants of the Action, this approach is still restricted to relatively small systems. One possibility to overcome the dimensionality problem is to use on-the-fly computation of the potential. This, however, requires the use of dynamical methods which depend locally on the potential, such as quasi-classical trajectories (QCT). In this regard there are many promising semi-classical methods which need to be tested and developed as part of the Action, such as those based on path-integral (PI) formalisms (ring polymer, molecular dynamics PI, centroid dynamics, quantum trajectories, etc.). Another technique which has been receiving increasing attention is multiscale modelling, including QM/MM or similar methods. These approaches divide the total system into subsystems, connecting them with so-called embedding potentials, which account for the mutual interaction between the subsystems. Lot more research is needed to understand how to develop embedding potentials for the study of quantum (sub)systems. This research will help to study the spectroscopy of chromophores embedded in large systems. As to photoreactivity, a specific objective is to bridge the description of collective electronic excitations within the material with the photodynamical description of the adsorbate-surface molecular complex.

RT3: Development of open and modular software tools and of interfaces between the existing and the new codes, exploiting unique features of highly efficient electronic structure and nuclear motion codes, and connecting pure, first-principles theory and the semiempirical tools traditionally employed by many experimentalists. Large-scale parallelization of the codes with attractive scaling with system size and applications based on resources provided by the European network of supercomputers. This is an important aim to take advantage of the next generation of HPC.

RT4: Novel platforms for applications in the fields of atmospheric, combustion, material, and astrochemistry, as well as femto- and attochemistry. Identification of new and exotic molecular species, probing new chemical mechanisms and reaction pathways, especially at short timescales.

The application to different types of complex molecular systems and environments requires the adaption of codes for the treatment of symmetry properties, large-amplitude motions (LAM) and electronic and rovibronic structures, as required for handling isolated species, van der Waals systems, and condensed phases. Most of the complex systems, especially atomic and molecular clusters, have structures that cannot be obtained efficiently by “hand”. Here the use of global search algorithms will be highly useful for the efficient location of the proper nuclear configurations. Aimed at correctly describing LAM, emphasis will be put on methods under development by Action members such as the Nuclear Orbital (NO) approach, as well as the existing Diffusion Monte Carlo (DMC) or PI treatments.

RT5: Development of innovative (quantum-consistent) nuclear-density-based embedding for dynamical and spectroscopy simulations by linking nuclear TDDFT (time-dependent density functional theory) with wave-packet propagation techniques. Density-based embedding is a topic well developed within the framework of electronic structure theory. In the case of nuclei, it would be possible to take advantage of the orbital-free DFT formulations (*e.g.*, the Orsai-Trento functional for the case of He nuclei).

RT6: Fully controlling the nuclear motions either by lasers or by other external fields is an important goal of the current research of several Action participants. It has potentially far-reaching applications in the development of quantum information and quantum computation using molecular systems. This is an important test of the ability to understand and predict the interaction between light and molecules. Simulations of control experiments are extremely computationally demanding and new algorithms are being developed to tackle this (*e.g.*, the SHARC methodology). The interaction of the shaped laser field with the system has to be treated quantum mechanically because the essence of control is in the (constructive or destructive) interference of the laser pulse phase with the quantum mechanical phase of the matter.

RT7: Some of the information-system-related developments will be based on the principle of active databases and novel ways to estimate uncertainties exemplified by the "Unified Monte Carlo" (UMC) approach to uncertainty estimates and uncertainty covariances. The latter uses the language of Bayesian analysis and may proceed as follows. Use a parameterized PES as the unknown vector and derive a model prior distribution from some plausible estimates of the accuracy of a best fitted PES. For any parameterized PES one can run variational nuclear motion computations to get a calculated rovibrational spectrum. That then gives the *a posteriori* likelihood via Metropolis sampling. For diatomic molecules, of interest to IAEA (International Atomic Energy Agency), the fitting and the solution of the nuclear Schrödinger equation is not an issue but coupling the electronic excitation spectrum to the rovibrational motion is.

RT8: Development of laboratory or synchrotron experiments and tools combining *ab initio* or QM/MM methods with molecular dynamics simulations to study PESs far from equilibrium, excited electronic states, and to reveal the photodynamics and reaction paths for molecules or ions as well as radicals playing a special role in atmospheres and/or in the interstellar medium.
RT9: The key required features of state-of-the-art spectroscopic experiments probing nuclear motions are very high sensitivity, wide spectral coverage, high time and frequency resolutions, and instrumental simplicity. Dual laser comb spectrometers with slightly different repetition rates in the comb built for the mid- and far-infrared regions will offer an outstanding possibility to tackle a large number of vibrational and rotational, as well as basic and applied, research problems in the gas, liquid, and solid phases and at interfaces.
RT10: Computation of rovibrational contributions to molecular properties is an area where nuclear motion theories in relatively simple, but computationally demanding, forms can have a broad impact. Response theory for vibrational contribution to linear and non-linear optical properties will be developed to higher order, both in accuracy and for new properties, and related to new spectroscopic techniques and measurements.

D.2 Scientific work plan methods and means

Most of the science is done in the individual research groups taking part in the Action; these groups will secure funding from their own national or regional agencies. The Action will support scientific research by funding a large number of STSMs. Naturally, the scientific conferences and workshops organized within the Action are very important, providing outstanding opportunities to present new science done in the individual research groups and their focused discussion. They also provide excellent platforms for scientific discussions which can lead to new collaborations, new scientific ideas, and even to new major breakthroughs. The Action workshops primarily intended for early-stage researchers are also important in addition to the arguments presented above as they provide an opportunity to young researchers to interact with and learn from the most experienced workers in the field.
There are several ways that the Action will try to ensure that the research tasks of the Action listed above will be achieved. Part of the plan is to strengthen well-established and time-proven collaborations between European and non-European partners. Furthermore, development of new computer codes connecting pure, first-principles theory and the semiempirical tools traditionally employed by experimentalists will improve understanding of the relevance of the theoretical determination of "effective" experimental quantities. Providing training of the next generation of

molecular scientists, modellers, and engineers will ensure that bringing closer certain scientific subfields, another stated goal of the Action, will have a lasting effect. Organization of formal meetings and STSMs between the ESRs of this Action for presenting and promoting the works performed in each institution should also help in this respect. The related STSMs should allow the discussion of ongoing projects and help for solving problems. All these activities will enhance the transfer of knowledge and of techniques between the participants of the Action.

A large number of Action participants have been involved in methodology developments within their own institutions, a special aim of the Action is to achieve synergy among these research efforts via networking and capacity-building activities.

The aim of this Action is to study quantum effects in molecules, bridging chemistry with molecular quantum physics, and tackling new and yet unresolved challenges in molecular sciences, some of which were raised during scientific meetings organized by some of the Action participants. The Action will allow researchers to discuss the new approaches in order to overcome the difficulties associated with the numerical treatment of nuclear motions in complex molecular systems and developing probes via novel experimental techniques. New strategies should arise through the combination of approaches that go much beyond the harmonic approximation, the Franck–Condon principle, or even the Born-Oppenheimer separation of electronic and nuclear motions. The further developments emphasized within the Action should help in the analysis and interpretation of recent experimental studies of highly excited molecular systems and astrophysical observations of interstellar and stellar as well as planetary and atmospheric media.

The Working Groups are organized in a way to maximize the interaction within a given field. Nevertheless, the Action plans to integrate the different fields and thus most major achievements will be the result of strong interaction between members of different WGs.

E. ORGANISATION

E.1 Coordination and organisation

The Action will be organized according to relevant COST regulations. The Management Committee (MC) will be in charge of the coordination, implementation and management of the Action's activities and it will be responsible for budget planning and allocation of funds. The first MC meeting will be organized to appoint: (a) the Action Chair (AC) and the Vice-Chair (VC); (b) the Working Group Leaders (WG); (c) the Webmaster (WM); (d) the Schools Coordinator (SC); (e) the STSM Manager (SM); and (f) the Dissemination Manager (DM). The MC will meet regularly to

ensure smooth progress of the Action. The SC will be responsible for the smooth running of Training Schools. Since the Action participants plan to continue the Training Schools beyond the existence of the Action, the role of the SC is crucial. The DM will be trusted to organize and oversee the publication policy of the Action, finding opportunities to come up with Special and Themed Issues in high-profile international scientific journals, and multi-author textbooks on nuclear motion theory based on the lectures given at the Training Schools. The DM is also responsible for making the Training School lectures publicly available. Following the first MC meeting, the MC will organize the first scientific meeting within 2-3 months to start the scientific work of the Action.
Each year there should be at least one large conference dedicated to the aims of the Action. Each year at least 10 STSMs are planned but it would be ideal to have about 15 STSMs per year. If the resources allocated to the Action allow, additional Working Group meetings will also be organized by the WGs.

E.2 Working Groups

WG1 - ENERGY-RESOLVED METHODS: Experimentalists, interested in atmospheric chemistry, astrochemistry, combustion and material chemistry, as well as femto- and attochemistry, and theoreticians working in the energy domain form this WG. High-resolution spectroscopy gives detailed information about the states of a dynamical system. Sophisticated codes to help assign complex spectra and give a molecular picture to what is observed is required. New techniques, including vibrational coupled cluster and sparse matrix techniques for eigenstate solvers, need to be developed. The strong interaction of leading experimentalists with theorists of this WG provides a quick feedback for both communities about the latest developments coming from this Action and from outside sources.

WG2 - TIME-RESOLVED METHOD DEVELOPMENTS: Experimentalists and theoreticians working in the time-domain will form this WG. The experimental basis rests on, but not exclusive to, pump-probe spectroscopy and laser control experiments. Various theory strands such as wave packet dynamics, trajectory surface hoping and density matrix propagation are being developed to model and understand these experiments. Efficient codes are required, much advanced compared to the present to keep up with the experimental advances, especially looking forward to the use of modern facilities which will greatly enhance the capabilities in this field.

WG3 - ALGORITHM DEVELOPMENT AND HIGH-PERFORMANCE COMPUTING: Effective algorithms will be developed to allow the intended end users to deal with ever larger and ever more complex molecular and material systems. Current electronic structure theory is one example showing the way to go. The basis of efficient codes is the use of modern computer architectures, such as GPUs and massively parallel machines, and algorithms need to be developed correctly to take advantage of these computers. WG3 will encourage best practice in coding as well as look for practical solutions to common bottlenecks in computational needs. Parallel codes running efficiently in a wide range of computing environments, including Tier-0 and Tier-1 EU supercomputers are the goal. Standards and open-source modelling software and appropriate interfaces will be developed.

*WG4 - INFORMATION SYSTEMS***:** Modellers and engineers prefer the availability of scientific data in the form of (active) information systems. The complimentary expertise of Action participants will yield appropriate information systems for the benefit of a large community, way beyond the theoretical chemistry core of the Action.

E.3 Liaison and interaction with other research programmes

The COST Action CM1401 “Our Astro-Chemical History" is complementary to this Action. Astrochemistry is an important field considering applications for molecules in motion. Thus, collaboration between these two Actions is envisioned and should strengthen both Actions. By far the most important tool for exploration of low to medium temperature (T < 1000 K) gas in the Universe is molecular spectroscopy. Many of the observed species, including radicals (C_n, hydrides of C and N), radical ions (H_2O^+, C_nH^-, C_nH^+), and molecules which tend to polymerize (HC_nN), are elusive in usual terrestrial environments. Thus, theoretical understanding of their spectroscopy, as well as of the isotopologues and isotopomers, is crucial. This Action could provide the theoretical framework upon which some parts of Action CM1401 would be based. Common workshops and common schools could strengthen both Actions. Two common goals could be: (1) a careful, calibrated way to predict molecular spectroscopy in the 1-2 THz region, recently opened to exploration, thanks to reliable solid-state devices generating those frequencies, and suitable space telescopes, launched or to be launched; (2) spectroscopy of isotopic variants while accounting for nuclear spin statistical effects.

E.4 Gender balance and involvement of early-stage researchers

This COST Action will respect an appropriate gender balance in all its activities and the Management Committee will place this as a standard item on all its MC agendas. The Action will also be committed to considerably involve early-stage researchers. This item will also be placed as a standard item on all MC agendas.

A large number of female ESRs are currently working within the research groups of the participants. ESRs will be involved in the Action, especially as far as the STSMs and the Training Schools are considered.

Additionally, Action members have expressed their intention to cooperate with FemEx (promoting female excellence in theoretical and computational chemistry) to promote female parity.

F. TIMETABLE

The Action will last for four years. Altogether four large international conferences, four Training Schools, eight WG meetings, and 50 STSMs are planned.

Action	Year 1	Year 2	Year 3	Year 4
1st scientific Meeting	1, within 2 months			
Action conference	1, within 3-8 months	1, within 3-8 months	1, within 3-8 months	1, within 3-8 months
Training School	1, within 3-10 months	1, within 3-10 months	1, within 3-10 months	1, within 3-10 months
MC meeting	1, within 8-10 months	1, within 3-5 months	1, within 3-5 months	1, within 3-5 months
WG meeting	2	2	2	2
STSM	10	15	10	15

G. ECONOMIC DIMENSION

The following COST countries have actively participated in the preparation of the Action or otherwise indicated their interest: AT, BE, CH, CZ, DE, DK, ES, FI, FR, HR, HU, IT, NL, NO, PL, PT, SK, UK. On the basis of national estimates, the economic dimension of the activities to be carried out under the Action has been estimated at 72 Million € for the total duration of the Action. This estimate is valid under the assumption that all the countries mentioned above but no other countries will participate in the Action. Any departure from this will change the total cost accordingly.

H. DISSEMINATION PLAN

H.1 Who?

The Action targets audiences in several fields related to quantum motions of nuclei: (a) researchers in academic and industrial environments will be the targets of the algorithm and code developments; (b) ESRs in the partner universities and around Europe, who would greatly benefit from their active participation at the Training Schools organized by the Action; (c) international bodies such as IUPAC and IUPAP via specific recommendations formulated by Action participants; (d) national and European networks of specialists, and other national societies and academies; (e) database managers.

H.2 What?

Results from individual research activities within the Action will be the subject of publications in specialized, peer-reviewed, leading international scientific journals. Nevertheless, to promote the output of the Action further steps will also be taken: (a) an effective and fast forum for the dissemination of the results is provided by all the scientific meetings of our Action, including conferences, workshops, Training Schools, and STSMs; (b) the codes developed as part of the Action will be distributed freely, aided by the website of the Action and once they exist in beta version; (c) the main results from the discussion meetings will be put on a public page of the website; (d) the applications of the codes to specific molecular systems will be the subject of specialized publications; (e) the Action plans to publish several review articles, Themed and Special Issues, recommendations to the scientific community, and multi-author textbooks.
As far as the information systems are considered, measures will additionally be adopted and the results will be made available on a password protected page of the website of the Action.

H.3 How?

All information concerning upcoming scientific meetings, training schools and workshops of the Action will be sent by email to all MCs, to all other scientists involved in the Action, and, when appropriate, to news groups such as MOLECULAR-DYNAMICS-NEWS and SPECTROSCOPY-GROUP.

A number of innovative ways, listed below, will be used to disseminate our results:

Website: A website dedicated to the Action will be created. This website will include (i) a general presentation of the aims of the network and its members with specific details provided by Action participants; (ii) the Action newsletters, (iii) information on individual and Action-based training (Training Schools and STSMs); (iv) links to the website of each Action member; (v) all the scientific presentations at the international conferences, workshops, and Training Schools organized within the Action (the format planned for the videos of the scientific lectures at the Training Schools is MOOC, massive open online course, which would allow the inclusion of these lectures in university courses, benefitting everyone); and (vi) links to other relevant websites. The WM will be in charge of the website.

Blog: A blog related to this Action will be created and managed by the WM. This blog will contain initially frequently asked questions (FAQ) and the answers given by leading Action scientists. The blog will be open access. All members will be contributing and making it an easy platform to share ideas on how to solve specific scientific problems associated with the Action.

Mailing-list: A mailing-list will be created and it will be aimed at all participants interested in the achievements of the Action. Each WG Leader will be in charge of contacting the scientists and engineers and those interested in industry.

Publication of results in peer-reviewed international journals: Reviews and articles will be written and published in peer-reviewed journals which provide the most important vehicle for the dissemination of the data and the scientific achievements.

International meetings organized within the Action: To disseminate the output of the research performed within the Action, workshops will be organized each year. At these workshops, the work of each WG will be evaluated and discussed by all Action participants and ESRs. All of them are expected to participate in these meetings and give an oral or poster presentation based on their latest published and especially unpublished research. Besides the discussion of scientific topics, the workshops will include a discussion about the current status of the joint projects. An important part of these meetings will be the discussion of the further strategy to complete ongoing projects.

European and national networks: Creation of networks at the European and national levels.
Training: The results and the methodologies developed within the Action will be incorporated in the training leading toward ESRs. The International meetings and workshops organized within this Action will provide occasions for ESRs to meet leading scientists and also industrial partners.