

Assessing the Coordinated Call with India 'Computational Material Science'

Report on workshop



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**Assessing the
Coordinated Call with India
'Computational Material Science'**

REPORT ON WORKSHOP

Edited by

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Industrial Technologies
Material Unit

2011

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Acronyms

CMS	Computational Material Science
DFT	Density Functional Theory
DG RTD	Directorate General for Research and Innovation, EU
DST	Department of Science and Technology, India
S/T	Science and Technology

Contents

1. SUMMARY	4
2. INTRODUCTION	5
3. COMPUTATIONAL MATERIAL SCIENCE	7
4. RESPONSES TO THE QUESTIONNAIRE	8
5. CONCLUSIONS	14

Annexes

ANNEX I. AGENDA OF THE WORKSHOP	16
ANNEX II. LIST OF PARTICIPANTS	17
ANNEX III. QUESTIONNAIRE	18
ANNEX IV. SHORT DESCRIPTION OF THE 6 PROJECTS	19
ANNEX V. THE CALL TEXT	25

1. Summary

In 2008 there was an EU-India coordinated call on Computational Material Science. Since the projects are half way through it was considered a good time to receive feedback from them on how this new type of call has been received by the scientific community and how in their opinion DG RTD and DST have handled the call, proposals and projects in order to improve on potential calls and handling of the projects. There are 6 projects with a total of 5M€ Euro in max EU contribution and Rs 19 crores funding from DST.

Overall the call was perceived to have been well focussed and transparent. The evaluation criteria and joint evaluation procedure were very clear up front. The crux came at the point of negotiation when the proposal effectively was divided into two quasi-independent consortia, EU and India, respectively. This created some differences in starting dates within most projects, and some confusion due to differences in reporting requirements for the EU and India half of the projects. In spite of these issues the coordinators agreed that it has been a very satisfactory first experience, with collaboration improving progressively in medium sized consortia.

The coordinators made some suggestions including requests for simpler coordinated reporting rules, use of fewer legally binding documents to avoid potential conflict between them i.e. only one grant agreement and one coordination agreement, and if there will be a repeat of CMS, the topic could be kept reasonably wide, e.g. **multi-scale computational design of functional materials**, and finally to learn from the French-India research collaboration scheme involving one central agency in Delhi.

The specific added value of EU-Indian collaboration projects was summed up as:

- Better exchange of and access to bright students
- Complementary expertise
- Promotion of research ambassadors
- Nucleation points for other research collaborations between EU and India

2. Introduction

Overall the aim of the exercise was to:

- Assess the methodology of the cooperation
- Identify synergies and bottlenecks.
- Receive recommendations on how to handle this new type of call.
- Promote networking both within and between EU-Indian projects.

Since the projects from this call are now halfway through, this is the moment to learn lessons from this specific and new type of call. A workshop for all the coordinator back to back with the EU-India S/T agreement steering committee would streamline resources and facilitate the attendance of the Indian counterparts. A summary of the lessons learnt and recommendations from the coordinators were presented by representatives of DG RTD and for DST the next day (April 1) at the meeting of the EU-India S/T agreement steering committee.

The assessment was done in two stages. First a questionnaire was devised to highlight the main requested input from the projects. The responses were collated and sent out again to the projects as preparation for the workshop in the second step. The responses to the questionnaire were presented at the workshop to form the basis for the discussion on both EU-India networking and handling of EU-India calls.

The workshop included a half day session to present the projects, and thus also for the projects to discover commonalities and the possibility for synergies between them. Overall there was great interest in the presented topics which can be expected to act as a seed for future collaborations.

Also a DG RTD representative gave an overview of the EU-India S/T collaboration over the last decade to put the workshop in an overall setting. A short history of the EU-Agreement S/T was presented. The presentation highlighted the specificities of the S/T agreement such as it being an overall framework of EU-India S&T cooperation based on mutual benefit, shared priority, and investment of resources to implement joint activities: e.g. coordinated calls for proposals and joint workshops.

The second day included a half day scientific session to promote exchange of experiences on computational materials science, more on the tools of the trade rather than specific output from the projects. Some results from the projects were mentioned as a way of highlighting the current best practises in Computational Materials Science. It was noted that the scale and objectives of a project might differ thus also their computational approach. Indeed, all the 6 projects are framed in the context of specific industrial applications. Despite these differences there was a constructive discussion on strategies for choosing an appropriate modelling approach and the relative advantages/disadvantages between approaches. Overall Computational Materials Science should strive to shift focus from explaining behaviours to being a predictive tool to drive both materials research and development of novel and/or improved applications, thus facilitating market take up of novel technologies and materials.

The workshop ended with a presentation of the collated responses to the questionnaire. A constructive discussion ensued based on their experiences to highlight both what in their view had been handled well and what could be improved for future calls i.e. to define lessons learnt. See section 4 for a summary of the responses. The content of this report is aimed to reflect the feedback from the projects via the questionnaire and the discussion at the workshop.

Projects	Funding (max)		Start dates		Difference (days)
	€	Lahks	EU	India	
AMCOS	520000	242	2009-05-01	2009-05-01	0
ATHENA	849998	126	2009-06-01	2009-04-14	48
DYNAMAG	899936	169	2009-06-01	2009-03-01	92
HYPOMAP	899958	205	2009-06-01	2009-06-01	0
MONAMI	930000	423	2009-07-07	2009-08-18	-48
SIMUGLASS	899994	727	2010-01-01	2010-04-01	-90

Table 1. Summary of the level of funding and starting dates. The duration of all projects is 3 years except the EU part of SIMUGLASS that is 4 years.

3. Computational Material Science

Computational Material Science is a growing field that aims to model, simulate and/or predict properties of materials and structures. These computer simulations can be used to accelerate understanding and discovery in materials science, with the potential to speed up the development of innovations based on material science.

Topics that are covered by Computation Material Science can include areas such as quantum mechanics of superconductors, molecular scale models of interactions between organic polymers, and finite element methods to analyse macroscopic mechanical stresses in bridges. Obviously the field is very varied and requires a number of very different computational tools and methods. One common issue is how to best assess these models with respect to real life observations since quite often there are indeed differences between the mathematical models and the experimental results, partly explained by how they were performed. These comparisons in turn are used to

improve both the computational tools and the mathematical models of materials and their mechanical, physical and chemical properties.

Recent advances have led to computational simulations with wider ranges in both time and lengths, thus trying to combine the results of simulations at atomistic and macroscopic scale, typically via intermediate levels. Thus the electronic structure of atoms/molecules could be linked to micro scale structures via fractures and interfaces up to the overall shape of an object that could be a photovoltaic cell or a new design of an electric generator including its magnet. These advances are also part of the current goal to gear Computational Material Science to be used more as a reliable predictive tool. This is done with the aim to support a more systematic and speedier development of new resource efficient, economically viable and environmentally friendly materials, processing and products.

4. Responses to the Questionnaire

Quantitative part of the questionnaire

On average 8 PhD students and 5 PostDocs are involved, at least part-time, in each project. They have had 3 EU-India meetings. Apart from these meetings there have been some exchanges of staff and students. Those that travel normally stay for a few weeks at the host institutions, PhD students averaging 2-4 weeks, and PostDocs or Profs 4-6 weeks. There is no discernible pattern to indicate that Indians or Europeans travel more, albeit some would have liked to see more and longer exchanges.

Already half way through the projects they show good publication records, ca 18 publications per project. They have around 10% joint manuscripts, i.e. at least one author organisation from both EU and India. Those organisations that already have a

history of collaboration probably are more advanced with the others catching up as the level of collaboration develops during the projects' life. Notably, at least 2 patent applications have been filed. Most projects have also contributed to and/or have made a number of software, codes and databases publically available, some as GPL. Apart from presentations at scientific conferences some projects have also more pro-actively promoted the project and its partners via press releases.

It is difficult to draw clear cut conclusions from the data that was provided since the European projects started over a 7 month period, and the starting date differed plus/minus 3 months in relation to the respective Indian consortium (see Table 1). One should also note that these inputs were given at roughly half way through the projects and considering the normal time to publication in peer review journals. Overall the projects would seem to be on par with projects with similar size, scale and scope.

Comments on the call and its scheme.

In general it was thought to be an interesting initiative, useful and well thought through call and they would like it to continue in the future taking into consideration the lessons learnt from this exercise. The coordinators believe that bilateral cooperation initiatives like this one help in establishing durable scientific relations between Europe and India, in particular across communities with traditionally different background. The call for the project was very clear and transparent. Evaluation procedures were already known while preparing the proposal.

The call and its scheme were to consolidate the efforts of computational materials science across EU and India. This is particularly well thought of as scientists in EU and India have their respective strengths in developments and applications of computational methods in materials science. Computational material science is almost

exclusively aiming at novel materials, which in turn mean more efficient use of resources, the possibility to use alternative materials without critical raw materials, and the use of renewable energies due to new materials to harvest, store and process renewable energy sources. The call has opened a new vista in the way knowledge and expertise in Europe and India can be synergistically exploited to address theoretical and applied research in materials science and engineering with the help of numerical computation at various length scales. In all fields, direct impact on India's and Europe's economy and/or energy policy is expected to have a positive global effect.

The drive to become a knowledge-based society strongly favours computational and theoretical projects, suggesting the appropriateness of calls in the field of theoretical sciences in support of industrial applications.

What are your recommendations for new calls and/or schemes?

An increase in the budget would improve the mutual mobility for exchange of researchers, which could also be achieved using a dedicated budget.

Simplified reporting requirements would be welcome. They thought it would be helpful to have simplified common DG RTD : DST guidelines for co-ordination agreements. A single common contact point during the entire call and project cycle would be very helpful. This would also help to synchronise the differences in the funding cycles for the two funding agencies.

They thought it would be very helpful if a joint office for both DG RTD and DST can be temporarily established to act as a central representative for both funding agencies at least during the negotiation phase. It would be desirable to have a clear and simplified

reporting structure, possibly coordinated by a single research body. Compare with the India-French research collaboration scheme.

A networking event prior to the close of future EU-India calls would be helpful to improve partner seeking for proposers.

Overall it was noted that future calls with wide topics would be welcome, especially if they include a link between simulation and experimental skills, which could benefit EU and India, and perhaps be fairly open in scope as to address some grand challenges which necessitate bridging multiple length (and time) scales. Thus **predictive multi-scale material modelling** was mentioned as a more open-ended stand-alone topic, that also could be included as part of the possible solution for more specific call topics.

What is the main advantage of an EU-India project over a purely EU or India funded project?

In their opinion a joint EU-India project would allow them to access a larger range of complementary expertises and ideas. A great advantage is that it brings together highly qualified groups of people from both sides, to communicate ideas and techniques towards common actions against major scientific and technological problems. Interaction with groups with complementary expertise is important, and was easier to identify in an EU-Indian environment than it would have been in a pure EU or Indian environment. In a sense, the participants could be seen as ambassadors promoting potential research collaborations between EU and Indian researchers.

It provides a stronger motivation for collaboration between EU and India partners. The research possibilities became mutually familiar to both partners, which is a true benefit for collaboration.

It is also important to note that the barrier to visit Indian/European partner institutes has been lowered due to the exchanges taking place during the projects. It has opened the door to a wider scientific market. Exchange of students motivates the young researchers to pursue challenging problems as their Ph. D topic.

There is also an element of cultural diversity, which is more difficult to quantify, but certainly equally important.

What has been the main weakness/problem with the EU-India project & call?

The main identified weakness of the initiative was the lack of clarity on how the two networks (the EU and the Indian one) should operate with respect to each other and in particular how they should report to their funding bodies, a problem which still affects the execution of their projects. The request to – essentially – run two independent consortia is counterproductive to the aim to strengthen collaboration; while it surely simplifies administration for the funding agencies it implied an apparent duplication of the administrative load for the projects. Another consequence of this problem was also the many changes during negotiation of the starting date, including up to 3 months difference for the start date of the EU and Indian consortia respectively, which will lead to problems for the reimbursement of a common final meeting.

Difficulty to pay Indians visiting EU partner, i.e. board and lodging as stated in the call text. There are differences in how this is classified by the host organisations, there are issues with national employment laws, e.g. it might be considered as a stipend and/or salary depending on country and/or host organisation. They proposed two solutions: DG RTD pays directly to Indian partners that send persons to EU partners; or each partner pay both board and lodging for their own personnel and students.

Practical problems also included:

- obtaining visas for bilateral visits: difficult to get multiple entry visa for the duration of the project; Often max 6 months, by default only for one entry.
- collaboration over long distances,
- an unusually large proportion of the budget is for travels for project meetings
- cultural differences in understanding of co-authorship and associated issues
- differences in the academic years put some hindrance on opportunities for exchange travels
- how to include PhD students for 3 years in a project that lasts for 3 years.

Which impacts do you expect from your project?

For the wider society the projects are expected to deliver tools that by means of computer based simulation (individual simulation methods ranging from Quantum Mechanics, ab initio and density-functional theory, to atomistic simulations over Finite Element Methods to continuum models, with multi-scale techniques applied to bridge these scales, and inclusion of proper statistics) that can predict material properties decreasing the need for experimental input, thus aiding to speed up the development of new materials with industrial application, and to equip both EU and Indian industries with guidelines to improve their process (e.g. yield) and reduce cost of production.

For the scientific community the projects are expected to create a strong collaboration between EU and Indian partners, also after the projects have ended.

The generated knowledge would be delivered as high impact scientific publications and software (code and database) for distribution. A few patents applications have already been filed.

5. Conclusions

The coordinators thought that the scope of the call was well targeted. Overall the good sized consortia are progressing well both in their collaboration and scientific output. Both the scope and transparency of the procedures for the call and the evaluation were perceived as strong points. Much of the perceived difficulties started at the point of negotiation as then the projects were essentially split into two consortia, one EU and one Indian. In spite of the challenges that arose from this it has been an overall positive experience. But for the future it would also be important to keep in mind the importance of nurturing and growing of this field by networking with a long-term view, clustering of projects and benchmarking of strengths.

The coordinators gave some general hints on where improvements could be made

- It would be helpful to avoid multiple legally binding documents that potentially might contradict each other, thus one grant agreement and one consortium (or coordination) agreement, the latter to cover IPR and exploitation etc.
- A harmonised template for the coordination agreement would be helpful
- The reciprocity rule of board and lodging is not easy to comply with in Europe because of different national employment laws
- Future topics, if repeat of CMS, could be kept reasonably wide, e.g. [multi-scale computational design of functional materials](#)
- Compare with the scheme set up for the Indian French S/T agreement with one central point (Indian French centre in Delhi) for administration of calls
- Streamlined reporting guidelines would also be helpful

The coordinators summarised the strongest reasons for the added value of EU-India coordinated calls as follows:

- Better exchange of and access to bright students
- Complementary expertise
- Creation of research ambassadors (sherpas)
- Nucleation point for other research collaborations between EU and India

ANNEXES

- Annex I. Agenda of the workshop
- Annex II. List of participants
- Annex III. Questionnaire
- Annex IV. Short description of the 6 projects
- Annex V. The call text

Annex I. Agenda of the workshop

Workshop on assessing the call

NMP-2008-2.6-2 Computational Material Science - Coordinated Call with India

DATE : 30-31 March 2011

VENUE AND PLACE: SDME 2F, Brussels, Belgium

DAY 1 : 30 March

13:30	Reception opens	DG RTD
14:00	Welcome	DG RTD / DST
14:15	EU-India S/T relations	DG RTD D1
14:30	Round Table	DG RTD/ DST
15:00	Project presentations	Coordinators
	Timing (10 + 5 minutes for each project)	
	EU and India coordinators together present their projects	
16:30	Break	All
17:00	Summary of the RTD part of the questionnaire	DG RTD
17:30	Discussion on possible synergies and networking	All
19:30	Voluntary get-together	

DAY 2 : 31 March

09:00	Session on computational materials science	Coordinators
10:30	Break	All
11:00	Session on computational materials science	Coordinators
12:30	Lunch	All
13:30	Summary of MGT part of the questionnaire	DG RTD
14:00	Discussion incl. learnt lessons	All
15:00	Suggestions for improvements	Coordinators
15:30	Discussion on possible synergies	All
16:00	Conclusion	All
16:30	End of workshop	

Annex II. List of participants

Projects	EU	India
AMCOS	George K Papadopoulos	Rajesh B. Biniwale
ATHENA	Stefano Sanvito	Priya Mahadevan
DYNAMAG	Volodymyr Kruglyak	Arti Kashyap
HYPOMAP	Thomas Heine	Sourav Pal
MONAMI	Olle Eriksson	Indra Das Gupta
SIMUGLASS	Fei Wang	Dipayan Sanyal

Directorate General for Research and Innovation (DG RTD)

Jean-Michel Sers

Johan Veiga Benesch

Martin Gieb

Patrice Millet

Pilar Aguar

Susanne Becker

Department of Science and Technology (DST)

Arvind Kumar, on behalf of DST

Annex III. Questionnaire

Questionnaire : EU-India call topic and projects : Assessment of call

NMP-2008-2.6-2 Computational Material Science - Coordinated Call with India

Note : Only 1 questionnaire per project, i.e. include both EU and India consortia.

Qualitative

- Comments on the call and its scheme.
- What are your recommendations for new calls and/or schemes?
- What is the main advantage of an EU-India project over a purely EU or India funded project?
- What has been the main weakness/problem with the EU-India project & call?
- Which impacts do you expect from your project?

RTD : Quantitative

- No. of Indian and EU PhD students whose thesis (work) is/was based on the project
- No. of Indian and EU postdocs whose research is/was focused on the project
- Person weeks that EU PhD students spent in India
- Person weeks that Indian PhD students spent in EU
- Person weeks EU postdocs or Professors spent in India
- Person weeks Indian postdocs or Professors spent in EU
- Total number of peer reviewed publications from the project
- Number of EU-India meetings
- Number of refereed publications with at least one Indian and one EU author
- Any other quantitative output, e.g. patents, databases, DFTs, press releases etc

Annex IV. Short description of the 6 projects

Project: **AMCOS**

Advanced materials as CO₂ removers: A computational study of CO₂ sorption thermodynamics and kinetics

<http://comse.chemeng.ntua.gr/amcos/>

Coordinators

George K Papadopoulos

National Technical University of Athens

Rajesh B. Biniwale

National Environmental Engineering Res. Inst.

Abstract

The proposed work aims at developing the tools required for the intelligent choosing and tuning of nano-porous materials with respect to a specific application. For this purpose, a combined computational theoretical and experimental study is envisaged in order to digitally reconstruct the porous matrix of selected advanced materials, mainly for applications involving sorption of carbon dioxide and methane by employing advanced Statistical Mechanics based computer simulation methods, both, in atomistic (Monte Carlo, ab initio and equilibrium and non-equilibrium Molecular Dynamics) and mesoscopic level (Kinetic Monte Carlo and Lattice Gas Cellular Automata).

The reasoning behind this strategy is that the structure of materials spans a wide range of length scales, making thus sorption and transport phenomena depend upon length and time scale.

As a consequence, the proposed computational methodology consists of many levels in order to address properly these phenomena. Moreover, a complementary approach to computer simulations is provided through direct comparison of two highly sophisticated methods for measuring motion of guest molecules inside porous materials, namely, quasi-elastic neutron scattering (QENS) and pulsed field gradient nuclear magnetic resonance (PFG NMR), carried out by the groups of Lyon and Leipzig respectively.

This type of combined studies can be perfectly utilized through the proposed work towards a fascinating insight of the relation of the material interior to the sorption and transport mechanisms of sorbates such as carbon dioxide and methane, both involved in the so-called greenhouse effect.

Project: ATHENA

Advanced theories for functional oxides: new routes to handle the devices of the future

<http://www.athenacomp.eu/>

Coordinators

Stefano Sanvito

Trinity College Dublin

Priya Mahadevan

S N Bose National Centre for Basic Science

Abstract

Transition metal oxides are the building blocks of future microelectronics, due to outstanding properties such as, e.g. colossal magnetoresistivity and electroresistivity. Envisioned applications are countless, from spintronic devices to multiferroics, to non-volatile magnetic memories.

Despite the huge amount of work already accomplished, a deep and complete understanding of these systems is still lacking. This is due on the one hand to the complexity inherent to the physics of strong-correlated electrons, which includes a plethora of fascinating but overtly complex phenomena (e.g. charge and orbital ordering, polaronic formation, spin-charge separation, non-Fermi liquid behavior, to name just few). On the other hand, there is an unquestionable lack of coordinated effort devoted to share, integrate, and develop the most advanced and powerful computational techniques nowadays available.

With the present project we aim to close this gap by gathering in a synergic collaboration some of the most experienced groups in the subject, equipped with the most advanced methodologies for the theoretical study of strong-correlated phenomena in transition metal oxides. Specifically, the European units assemble a vast competence on methodologies that are at the developmental forefront of First-Principles methodologies, whereas the Indian partners are worldwide recognized experts on both First-Principles and model many-body (e.g. Hubbard Hamiltonian (HH)) techniques.

In the project we plan to develop an unprecedented fusion of these two different but complementary viewpoints, applied to the study of the most fascinating and technologically promising class of systems candidates to be employed in the devices of the future.

Project: DYNAMAG

Advanced computational studies of dynamic phenomena in magnetic nano-materials
<http://www.dynamag.eu/>

Coordinators

Volodymyr Kruglyak University of Exeter
Anjan Barman S. N. Bose National Centre for Basic Sciences

Abstract

The opportunity to modify the excitation spectra in materials with modulated properties has stimulated striving research activity in the area of artificial nanostructures with novel functionalities - so called metamaterials. Magnetic materials with modulated properties also possess properties that cannot be reduced to those of their constituents. The best example is the phenomenon of giant magneto-resistance (GMR), the discovery of which was marked by the Nobel Prize in Physics last year. The spectrum of magnons (spin waves) in periodic magnetic nano-materials shows a tailored band structure. The latter consists of bands of allowed magnon states and band gaps in which there are no allowed magnon states. By analogy to studies of other band-gap materials, the field of research is called magnonics.

Further development and application of magnetic nano-structures requires a thorough understanding of the relation between their physical and chemical structure and useful magnetic functionalities. The ability to accurately predict properties of fabricated magnetic nano-structures and complete devices theoretically would generate huge savings of resources, but remains illusive at present.

The goal of this project is to consolidate efforts of European and Indian researchers with a broad range of leading expertise to create, to validate and to implement a flexible computational framework for modelling of dynamics in realistic magnetic nano-materials and complete devices. The framework will be validated via comparison of computational results against those obtained experimentally or using analytical theories. We will model magnetic dynamics in topologically complex nanostructures, in view of applying them in design of realistic devices. This project will provide a computational foundation for creation of not only novel high speed magnetic technologies but also of those at interfaces with photonics, plasmonics, phononics, and electronics.

Project: HYPOMAP

New materials for hydrogen powered mobile applications

<http://ses.jacobs-university.de/ses/theine/projects/HYPOMAP>

Coordinators

Thomas Heine

Jacobs Uni, Bremen

Sourav Pal

National Chemical Laboratory Pune (NCL)

Abstract

Emission-free energy generation in mobile applications is one of the major challenges to science to reduce global warming. A particularly promising approach is the electrochemical oxidation of hydrogen in fuel cells.

Two challenging questions have to be solved to achieve this goal: Hydrogen has to be stored at reasonable volumetric and gravimetric storage capacities in materials which allow efficient, energy-neutral loading and unloading. The released hydrogen must be oxidized electrochemically to produce electric power and water, the only by-product of this process. We will investigate various strategies to store hydrogen in nanoporous materials and by chemisorption in various hydrides. Special emphasis is given to the mechanism of adsorption, the thermodynamics of the ad- and desorption process, tuning of the materials etc. For studies on chemisorption, materials shall be searched with a suitable energy balance between hydride and dehydrogenated species.

The reaction mechanisms will be studied in detail and tuning of reaction barriers by advanced catalysts shall be investigated. The studies include various known and advanced materials such as carbon nanostructures, metal organic framework materials (MOFs), covalent organic framework materials (COFs), boron nitrides, clathrate hydrates and metal clusters. While present fuel cell technologies are more advanced than hydrogen storage devices, there is still room for significant improvements.

We will investigate new proton conducting materials for high- and low-temperature fuel cells, based on perovskites and new inorganic nanomaterials like imogolite derivatives (HT) and organic substances (LT). Investigations will include a wide range of theoretical approaches, including ab initio quantum chemistry, density-functional theory, quantum-liquid density functional theory for hydrogen, molecular dynamics and Grand-Canonical Monte-Carlo simulations.

Project: MONAMI

Modeling of nano-scaled advanced materials intelligently

<http://www.iacs.res.in/monami/>

Coordinators

Olle Eriksson

Uppsala Universitet

Indra Das Gupta

Indian Association for Cultivation of Science

Abstract

The proposed consortium focuses on a collaborative effort of developing novel techniques and paradigms concerning theoretical modelling of nano-scale advanced materials. The objectives are to identify novel methodologies and to identify appropriate approximations to successfully undertake simulations of the materials which are to be used in our future society.

An important aspect here is to be able to carry out this development all the way from idea and concept to working computer soft-wares. In addition to this technical development we will focus on establishing knowledge concerning an emerging class of materials; nano-scaled materials with potential for tailored properties and potential for novel functionality. Training of younger scientists forms a natural aspect of this ambition, and is a strategically relevant outcome of our planned efforts. Finally, it is envisaged that the collaboration will enable an intensified collaboration between European and Indian research laboratories and universities.

Project: SIMUGLASS

Development of a synergistic computational tool for material modeling, process simulation and optimization of optical glass molding

<http://www.simuglass.com/>

Coordinators

Olaf Dambon

Fraunhofer

Dipayan Sanyal

Central Glass and Ceramic Research Institute

Abstract

For the production of complex optical components precision glass moulding is fast emerging as a powerful and economically viable technology, where the novel mouldable optical glass is directly deformed at high temperature. To improve the efficiency, the complex shrinkage behaviour of the glass material during the cooling step has to be understood and thus predicted by means of innovative collaboration between material science and computational modelling. The overall objective of is the development of a powerful synergistic computational FEM-tool (Finite Element Modelling) for material modelling, process simulation and optimisation of optical glass moulding for optical glass moulding. Based on this ambitious goal, the following scientific and technological objectives have to be realised:

- Scientific analysis of the relevant thermal, mechanical, rheological and optical glass material properties and their dependence on the moulding parameters (forming velocity, temperature, force, etc.)
- Development of powerful computational material models able to describe and predict glass material behaviour
- Implementation of the developed glass material models into a computational framework based on FEM
- Computational modelling of the glass moulding process including the radiative heating and viscous flow of glass and the thermal and mechanical properties of other relevant components
- Validation of the developed FEM-tool in real glass moulding experiments on an industrial glass moulding machine for theoretical model optimization.

These objectives finally lead to the development of a computational-based FEM-tool, in which the complex behaviour of the glass material during the moulding process is implemented. The basis for the development is the multidisciplinary approach between European and Indian researchers, which is essential for the material understanding.

Annex V. The call text

NMP-2008-2.6-2 Computational Material Science - Coordinated Call with India

Technical content/scope: In the framework of the EU-India S&T Cooperation Agreement, the European Commission representing the European Community (EC) and the Department of Science and Technology (DST) of the Government of India are working together to enhance opportunities for coordinated activities in materials research between European and Indian teams. Computational modelling has become a major tool to understand materials properties, as well as in their design and industrial use. Multidisciplinary efforts using the powerful computational tools of materials modelling are essential for the understanding of the complex behaviour of new knowledge based materials. Numerous methods are now available, ranging from ab-initio calculations and molecular dynamics to the macroscopic level.

The proposals for coordinated projects must be clearly relevant to computational materials science at the frontier of knowledge. The expected coordinated projects should focus on the understanding and modelling of materials properties, processing and performance. Various computational approaches can be considered, including ab-initio theories, model Hamiltonian methods, atomic simulation tools such as MC and MD, FEM, DEM, Quasi continuum approaches and, with a particular emphasis, multi-scale simulation methods which take into account scale integration covering from the atomic level to continuum approaches. The links between simulation, theory, experiment, validation and use should be taken into account.

Areas of computational materials science covered include, but are not limited to, modelling of nanomaterials, metallic materials, ferroic materials, ceramics, polymers, composites, nature mimicking materials, biomaterials, green solvents, alloys, clusters, interfaces, size-dependent effects, dislocations, diffusion, electronic and optical

properties, as well as different aspects of the thermal and mechanical behaviour of materials.

Funding scheme: Small or medium-scale focused research projects, carried out in coordination with DST (India).

Additional eligibility criteria

For each project, the maximum EC funding requested must not exceed EUR 1 million. Proposals which do not include coordination with an Indian project will be considered ineligible. Therefore, the EC proposals must include a detailed explanation about the coordinated Indian proposal to be submitted to the DST.

Special features: To ensure a project implementation that reflects a genuine EU-India cooperation, priority in evaluation will be given to proposals showing a balanced effort between the two coordinated projects and where the research plan involves properly coordinated research activities between Europe and India. The proposals should also take into account the exchange of researchers, so that any accommodation (board and lodging) of the Indian researchers in Europe should be paid by the European host institution, whereas that of the European researchers in India should be paid by the Indian host institution.

Additional selection criterion: Proposals will only be selected on the condition that the corresponding coordinated project is also selected for funding by the DST.

Expected impact: An EU-India Materials Science partnership, supplemented by two-way mobility of researchers, can help create the critical mass of human resources and competence to achieve success in generating new knowledge beyond the state-of-the-art to contribute to industrial innovation for the benefit of European and Indian societies. Reinforcement of the international dimension of European Research within the 7th Framework Programme and of Indian Research. Validated predictive models should contribute to the development of new materials, including newly emerging

nanostructured materials, for the flexible production of knowledge-based products leading to industrial competitiveness.

European Commission

Assessing the Coordinated Call with India NMP-2008-2.6-2 Computational Material Science - Report on Midterm Workshop

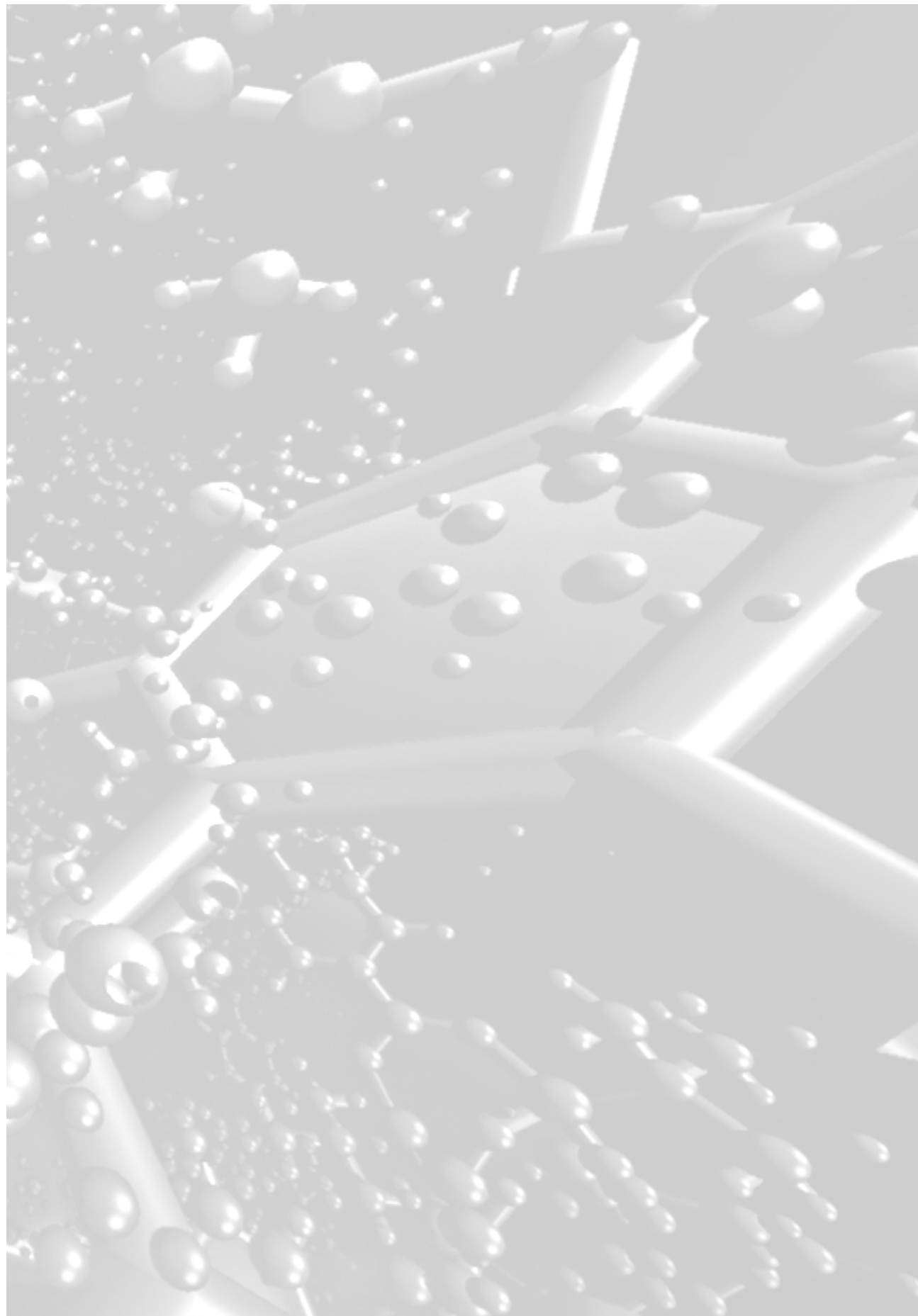
2011 - 32 pages - B5

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In 2008 there was an EU-India coordinated call on Computational Material Science. Since the projects are half way through it was considered a good time to receive feedback from them on how this new type of call has been received by the scientific community and how in their opinion DG RTD and DST have handled the call, proposals and projects in order to improve on potential calls and handling of the projects. There are 6 projects with a total of 5M€ Euro in max EU contribution and Rs 19 crores funding from DST.

The specific added value of EU-Indian collaboration projects was summed up by the coordinators as:

- Better exchange of and access to bright students
- Complementary expertise
- Promotion of research ambassadors
- Nucleation points for other research collaborations between EU and India