The Antiphysical Review

Founded and Edited by M. Apostol **102** (2004)

ISSN 1453-4436

Enhancing Nanostructures Computations and Materials Characterization A European Research Project

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Objectives

1. Upgrade of computing facilities for refining and enhancing the capabilities of computational models and tools, such as to enable us to reach large nanostructures computations, up to thousands of assembled atoms

2. Approaching the space-oriented valence atomic orbitals for semiconducting nanostructures *via* refined software, graphical capabilities, computers farm, databases, archiving, storage and communication links

3. Strenghtening the local computing and information technology tools for implementing the comparison with standard ab-initio and density functional computing techniques

4. Enable a regional jobshop at Magurele-Bucharest for focused - oriented computations of particular, customized nanostructures of interest

5. Create and enhance the infrastructure for high-quality, value-adding research in computational nanostructures science

Description of work

The major need of understanding the behaviour of complex and new materials, as well as new processes and devices related to materials science, is a salient feature of the contemporary scientific research, both in fundamental and applicative aspects. The modern society developed an immense potential for characterizing and harnessing complex atomic systems at the condensed matter level, in order to both understand and design and control new capabilities generated by new forms of matter aggregation. The advance in this huge area of science, development and innovation is guaranteed by new physical and chemical models and large-scale computational activities. Structural computation is a newly emerging field which governs the solid-state physics, condensed matter physics, soft matter physics, matter under extreme conditions, and, not in the least, the huge area of nanostructures, supermolecules, atomic aggregates and nano-objects. The advanced materials include, beside new forms of metals, insulators or semiconductors, glasses, ceramics, composites and superalloys; as well as liquid crystals, plastics, polymers and biomaterials; all possessing a multitude of new properties, or amenable to a variety of new processes and devices; and everything is greatly enhanced and put onto a new scale by nanostructures microfabrication. Apart from displaying new phenomena, like exotic superconductivity and magnetism, fractional Hall efect or Bose-Einstein condensation, all these new atomic structures exhibit a great potential of new and efficient applications The major route towards understanding, designining and controlling their new properties and potentialities is provided by the computational science of nanostructures.

For a few years, the N**anome - Mapping the Nanoworld - Project** is pursued actively at Magurele-Bucharest, as a high priority research project in the science of the nanostructures. **Nanome** aims at characterizing the physical and chemical properties of any possible nanostructure, producing a comprehensive recording sheet for each. The list includes structural properties like form, shape, atomic positions and vibration spectrum; cohesion properties like binding energy and isomers; and the electronic properties like one-particle electron spectrum, ionization potential and chemical affinity. The computations are based on an original model of quasiclassical description of matter aggregation and chemical bonding, developed at Magurele-Bucharest, which provides, within an iterative scheme, the major structural and electronic properties of the nanostructures. By employing this procedure we are currently producing atomic clusters, both homo-atomic and hetero-atomic, exotic nanostructures, like atomic two-dimensional sheets, nanowires, collection of interacting clusters, ultraminiatural solids. One of the big achievement of **Nanome** is the production of clusters deposited on surfaces, which opens the way toward studying surfaces, interfaces, contacts and junctions. All this is achieved by specific algorithms, computational software, medium-scale computations, the results being recorded and archived in incipient databases. One of the end target of the **Nanome** Project is to offer information services on the physical and chemical properties of the nanostructures, to be used as input data for designing nanostructures with specific electronic, chemical and biological functionalities.

The Nanome Project is to be developed in several directions:

1. Refining and enhancing the capabilities of the computational models and tools, such as to enable us to reach large nanostructures computations, up to thousands of assembled atoms. The world limit today is about 20 Au atoms from ab-initio methods. By including the atomic degrees of freedom of the upper shells valence orbitals and their coupling to the extended orbitals, within the new, original model developed at Magurele-Bucharest, the limit is pushed up to hundreds of atoms, and thousands of like atoms. Upgrade of hardware, including high-speed and large memory computers, is needed in order to test the method extension, as well as a large manpower, in order to collect enough data and set up sufficiently large statistical ensembles. Milestone 1, by first semester.

2. Computing the semiconducting nanostructures and exotic nano-aggregates, geometric constraints including, by implementing adequate software for angular-dependent valence orbitals. This step opens the way toward ones of the most interesting nanostructures, with a great applicative potential, consisting of C, N, B, Ga, As, O, Al atoms. the computations are now enhanced by an N^3 factor at least, as due to the added rotational degrees of freedom. consequently, new, optimized algorithms are to be developed, which, in turn, require very large scale integrated computational techniques, pictorial and graphical softs and large data storage in order to identify the ground-states and characterize individually the great number of isomers. Milestone 2, by second semester

3. Assess the validity of the computations by comparing them with standard ab-initio and density functional computing techniques. An essential prerequisite test-bed, enabling the estimation of the accuracy, error marges, various accuracy levels of the algorithmic recipees, computation procedures and protocols, and finally the relevance and quality of the output. It completes the specific activity and procedures tables of the computing jobs. Milestone 3, by the third semester

4. Enable a regional jobshop at Magurele-Bucharest, for focused - oriented computations of particular, customized nanostructures of interest, as performed by scientific researchers on a temporary basis in order to respond to the increasing need of computing one's own nanostructure and fully characterizing it, for specific needs, customer - taylored job place, procedures, programme and schedule. Milestone 4, by the fifth semester

5. Create and enhance the infrastructure for high-quality, value-adding research in computational nanostructures science and characterization of materials. Evaluating the output, reviewing the activities patterns, the relevance, valorisation, disssemination, platform for next developments, table of new project subjects. End of the project.

A particular by-target we are recently focusing on is to develop the source system for accelerating beams of nanostructures in the Tandem accelerator in operation at Magurele-Bucharest. The major aim of this project is to determine the patterns of nanoclusters interaction with matter. Tandem accelerator needs a specific upgrade in view of this project, regarding stabilization of its accelerating power, improving the vacuum system, enhancing the data acquisition and processing systems and enhancing control over its operation safety. The source system, which is essential for performing nanostructure acceleration, is designed on the basis of a furnace with a cold wall, where nanoaggregation occurs in a flow of noble gas, a module of ionization and separation of the nanoclusters, and collimation and injection modules. Ionization potentials, as well as electronic properties as produced by **Nanome** Project are relevant in this aspect. Of relevance is also the behaviour of a low density classical gas of nanostructures under variable pressure and temperature conditions, another objective of nanostructures accelerating project. As a by-product outcome, an improved understanding of cluster interaction with surfaces, interfaces, contacts and junctions is obtained. The complex set of interdisciplinary objectives of this project workpackage is performed by an articulated local team of scientific researchers and technical staff, involving materials scientists, nuclear researchers, electronics and accelerated beams experts and oriented theoretists.

Deliverables

Computer farm, local links and network, information technology communication tools for new, highly efficient algorithms and numerical codes for computing large metalic nanstructures of up to thousands of atoms.

A booklet of data sheets, structural and electronic properties data, an scientific movie, website, CDs archive

Dedicated software for space-oriented valence orbitals in matter aggregation, semiconducting and exotic nanostructures, publications, scientific movie, report booklet

Manual of input data, procedures and protocols for computing nannostructures, implementation of the comparison with ab-initio and density functional computations, specific softwares and adequate computing high speed and data storage.

Report booklet.

Seting up the jobshop with specific job procedures and protocols for computing customized, customer - taylored nanoaggregate.

Conferences, talks, meetings, popularization and vulgarisation public presentations, video recording, scientific movies, booklets, scientific pamphlets.

Milestones and expected results

Milestones:

Computers farm hardware, its functional configuration for developing, refining and enhancing the capabilities of the computational models and tools for very large metallic nanostructures, by 1st semester.

Approaching the angle-dependent valence orbitals for semiconducting and exotic nanostructures through adequate algorithms and computing codes, producing new nanoaggregates, by 2nd semester.

Implementation of computing high speed large memories software for comparison with traditional, currently - employed, ab-initio wavefunction method and density functional computing technique, by 3rd semester.

Regional jobshop at Magurele-Bucharest, for focused - oriented computations of particular, customized nanostructures, by 5th semester.

Create and enhance the infrastructure for high-quality, value-adding research in computational science of the nanostructuires, end of the project

Expected results:

Large metallic nanostructures, new, large semiconducting and exotic nanostructures, procedures and protocols in the computing nanoscience, regional jobshop for functional nanostructures, nanostructures phyiscal and chemical information archived data.

Implementation Plan

The existant, proprietary algorithms and numerical codes for nanostructures computing will be restructured as to enlarge their capabilities up to thousands of metallic atoms, in accordance with the enhanced computing power. New extension, compatibility, communication and security protocols will be devised and implemented as to take advantage of the new computing facilities and upgrading, including the computer farm, enhanced local networking, high speed processing and great storage facilities, communication links and electronic dissemination tools. Advanced graphical capabilities and data processing will be used to implement new codes for computing more demanding nanostructures, as the semiconducting and exotic ones, with directional degrees of freedom in the valence orbitals. Procedures and protocols will be established and incorporated in a computing job manul from bed testing in comparison with, and against the performances of the current ab-initio wavefunction method and density fuunctional technique. The manual will be used as the central documentary element for seting up the regional jobshop for computing customized, customer - taylored functional nanostructures. Routinizing nanostructures computation and responding to specific functional demands of personalized nanoaggregates will be the ultimate philosophy and the steering vision of the workpackage. Databases and service providing facility for computing nanostructures and characterization of advanced materials will be produced. Dissemination, valorisation and infrastructured research will improve our basic knowledge and advance our value-added attractivity on the European scientific market.

Relevance to the objectives of the Integrating and Strengthening the ERA (European Reserach Area)

Areas concerned: 2 Knowledge-based Multifunctional Materials, 2.1 Development of fundamental knowledge by: providing the basis for developing novel materials with predefined physical characteristics: nanostructured materials. 3 3.41-3.4.1.1 Long-term interdisciplinary research into understanding phenomena, mastering processes and developing research tools providing new tools based on IT (Information Technology) for computing customized functional nanostructures. Contribution to objectives of IT-ERA: It will be increased the reorientation toward European priorities by improved model-calculations methods for nanostructures, following and completed by new developments of algorithms and numerical codes, regional jobshop for computing nanostructures will be developed to assist the preparation of European Enhancement of the Research Area

Potential impact

The optimal use of the results of the project will include also: further development of customized nanostructures computing.

The proposed work will be based on the existant original model, algorithms and numerical codes for computing nanostructures, in order to improve, strenghten and enhance our knowledge of new processes, materials and devices, and to design new atomic structures with electronic, chemical or biological functionalities. The ultimate use of the project will result in optimally routinizing nanostructures computing so as to establish a regional jobshop for such customized, taylored computations, as based on a set of coherent, self-containing and complete computing procedures and protocols incorporated in a nanostructures computing manual.

The added-value in carrying out the work at a European level will include also: The model calculations carried out by means of the both point-like ionic cores for metallic atoms, as well as the exotic structures like metallic nanowires, two-dimensional atomic sheets, interacting clusters, heavy atoms calculations, clusters deposited on surfaces, incipient interfaces, contacts and junctions, will be largely used for extending the application to space-oriented valence orbitals in semiconductig nanostructures, for incorporating advanced computing power, for attempting the production of clusters as large as possible, toward the bulk limits. Quantum corrections will be incorporated for electronic, optical and magnetic properties, and the resulting Regional Jobshop of Computing Nanostructures (RWCN) will get on the European scene of scientific production and science marketing.

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The project workpackage resources

To the completion of the workpackage the following full group with additional personnel resources/skills: Condensed Matter and Theoretical Physics at NIPNE-HH- apoma laboratory-http://www.theory.nipne.ro/CMP: the code METALLIC, proprietary Cluster ARCHIVE (http://www.theory.nipne.ro/~apoma) model calculations for point-like ionic cores of metallic atoms

Dissemination Conferences, Talks, Meetings, Websites, CDs, Scientific Movies, Booklets, Scientific Pamphlets, Popularization and Vulgarisation Public Presentations

Activities Enhancing Infrastructure, Networking, Create Jobs, Create Methodology and Procedures Protocols for doing Scientific Research in Nanostructures Computations, in Characterisation of the Nanostructures and Materials, Valorisation of results, Formulating new proposals for European projects, Writing up project proposals seeds.