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Supramolecular Aggregation and Nanostructural Transport SANTRAN CEEX 2005

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Abstract SANTRAN aims at developing original and proprietary research on supramolecular aggregation of atomic clusters and nanostructures and functionalizing their transport properties. SANTRAN concentrates efforts of a complex consortium consisting of cca 25 relevant experts in four national institutes of research and a university, integrates itself perfectly in the major objectives of the European Research Area and aims at a major strategic objective both at national and European level - the basic knowledge in physics at nanoscopic level. SANTRAN is based on an original method of supramolecular aggregation, which is an alternative to current methods, like ab-initio wavefunction method, density functional or molecular dynamics. The method originates in developing the quasi-classical description of interacting ions-electrons ensembles, and is grounded on a new solution of the Hartree-Fock equations, corresponding to weak local variations of electronic density. The superiority of the method is seen by the derivation of ion-ion effective interaction potentials from first principles, as based on this new solution to Hartree-Fock equation, and on the consistent application of the quasi-classical description, as expressed by the linearization of the equations of motion of the chemical potential at equlibrium. The effective potentials SANTRAN is based upon are novel, derived from first principles, ensure the existence of bound states and allow for a consistent treatment of the correlations, the later point being an important advance in comparison with traditional methods. SANTRAN envisages to include the quantum corrections in the next step of computational iteration, leading this way to a complete, unitary and self-consistent picture of aggregation of the condensed matter. In addition SANTRAN code allows for computing the elementary excitations, both one-particle and collective, thus extending the applications to the spectroscopy of supramolecular aggregates and to nanostructural transport phenomena. At the present stage SANTRAN aims at describing as fully as possible metallic clusters, including those deposited on solid substrate, hetero-atomic clusters, consisting at least of two different chemical species, cluster liquefaction, complex nano-magnetic states, spin transport in ferromagnet-superconductor nano-junctions, and pulsed nano-tunneling transport. SANTRAN integrates itself fully in the Programme of Excellence's thematic areas 11 (Basic Sciences, Physics) and the European Research area of Nanoscience and Nanotechnology.

PRESENTATION OF NATIONAL AND INTERNATIONAL CONTEXT WITHIN THE MENTIONED THEMATIC FIELDS: SANTRAN continues a remarkable tradition of scientific activity and results, developed at national level in the last five years. This activity is first worth of noting due to a fundamental advance in the basic research in theoretical physics of condensed matter, implemented as a new original, proprietary, method for analyzing the cohesion of nanostructures, their spectroscopic and transport properties, a method which is superior in comparison with traditional procedures like ab-initio wavefunction calculations or density functional calculations. The obvious superiority of the method follows at once from the possibility of computing the ground-state and isomeric states for clusters consisting of hundreds or thousands of atoms, with computing resources and means which are relatively standard for this stage, as compared with traditional methods which seldom go beyond 20 atoms, for instance. At the same time, the method computes new nanoscopic structures, like sheets of atoms, layered nanostructures, atomic nano-wires, with one wall or multiple-walled, nano-structures deposited on surfaces, nanostructural diffusion and, by this means, surfaces, interfaces, contacts and junctions on a nanoscopic scale. All these elements are constitutive for decisive advances in describing the matter aggregation, providing answers to questions formulated as early as 1930 in this field of scientific investigation of theoretical physics of condensed matter. For illustrating the superiority of the method one simple instance at least is to be noted, that of the cohesion of the heavy atoms. This problem was posed and solved approximately in 1928, and the fundamental result was obtained in 1982, by computations which represent a tour de force indeed, based on asymptotic series, and which raise several issues. In this context, the method employed here allowed for a quick and improved solution for the cohesion energy and the correlation energy of the heavy atoms, in a very simple and transparent manner, which opened up the way to new applications concerning the fine structure of these results, like the ionization potential, chemical affinity, the spectroscopy of excited states, etc, etc. Such computations were one of several definite tests which demonstrated the superiority of this computation method. Beside, the method distinguishes itself by the richness of results regarding complex nano-aggregates, like clusters deposited on surfaces, interfaces, contacts and junctions, nanoscopic diffusion and quantum transport. Such results are associated with numerous scientific publications, books dedicated to the subject, communications, electronic means of disseminating results which are specifically graphical, or animated, web sites, etc, promoted by the scientific activity discussed herein, which SANTRAN aims at further developing. At the national level there exist numerous research groups, both in national institutes or in universities, with noteworthy results in synthesis, characterization and functional applications of nanostructures. At this level, the research is directed toward developing ultra-miniatural electronic and optical applications of such aggregates at nanoscopic scale, toward developing biological and biomedical applications, life sciences applications, environmental applications (like aerosol assessing and control), and last but not least, to applications in dyes, textiles, cosmetical products industries, as well as for superior materials. This scientific research activity which SANTRAN aims to continue on a superior scale, is well-known by cultivating and promoting a permanent dialog with experimentalists and applicationists, both in the institutes of research and universities, or in private companies, as seen from the general seminar of condensed matter and related problems, beside the special seminar of theory of condensed matter and mathematical physics, run permanently by SANTRAN.

These two forms of interactive, multi-, pluri-, inter- and trans-disciplinary scientific activity allow for delineating, formulating, debating or solving many issues of major scientific interest, in a profitable manner on a large scale, succeeding in creating an effective transfer of knowledge from the fundamental domain of theory to the applicative domain, and viceversa, by bringing to theoreticians' attention many scientific and technical questions of large social interest. One of the major outputs of such an interactive, sustainable collaboration was, and continues to be, attracting a large number of young researchers, graduate, post-graduate, masters and doctoral students, who are exposed systematically and intensively to the newest technical and scientific developments in the field. SANTRAN aims at a continuous development at all the superior levels of this tradition and intense activity of scientific research, of fundamental, applicative and social relevance. The scientific research activity of SANTRAN integrates itself in a complex of international professional relationships, by multiple connections with similar research centers in Europe, USA and Asia. This international standing of SANTRAN is another reason for its opportunity. In fact, one of the major objectives of SANTRAN is including the research and dissemination activities, the scientific results and international participation, in the context of the international scientific research in the field, for adopting on a greater scale the international procedures and practices, for aligning to the competitive professional standards, especially those of the European Union. The international scientific research in the field of condensed matter is dominated at this moment by nanoscience and nanotechnology studies, with major objectives like the electronization of the biology, biomedical, electronic and optical applications, nanoscopic control and command devices, biological informatization, materials sciences. A second major direction adds to the former, regarding the complex systems like the living cell, climate, environment, the planet, where the main investigation means are the electronic simulation and the distribution, administration and manipulation of information at nanoscopic level. Atomic clusters, nanostructures and supramolecular aggregates are the main target of such major research. Important breakthroughs were made recently in this direction, such as the molecular transistor, partially integrated circuits at nanoscopic level, quantum dots, nano-wires and nano-layers, with special optical spectroscopy properties, partial self-assembling of nanoscopic layers, the vectorization of pharmaceuticals agents which are biochemically active at the level of the living cell, magnetic memories with giant magneto-resistance effect, nanoscopic spin valves for ultraminiaturization of the information storage, etc, etc. The fundamental substrate of all these breakthroughs in nanoscience and nanotechnology originates in the aggregation, cohesion and functionalization of the supramolecular aggregates, which is the major theme of the present SANTRAN. As regard the aggregation and cohesion of the nanostructures at the worldwide level it is worth noting at this moment an intense activity, measured by electronic producing or re-producing of a number of atomic clusters as large as possible, with a structure as complex as possible. The top record at this moment is about 20 atoms (Au), with errors of about 5%. In contrast, SANTRAN is able to produce clusters and supramolecular nanostructures consisting of hundreds and thousands of atoms, much quicker and with rather common computing resources, at an accuracy level of cca 15%. This is only the first level of iteration of the computations, the second level raising the accuracy to 3-4%. This accuracy level is a limit, an upper limit, according to the fundamental theories of matter aggregation, originating in the one-particle wavefunctions approximation, and its overpassing would require multiparticle wavefunctions, complex simulation and corresponding computing resources.

At the same time SANTRAN produces the complex picture of nanostructured isomers for each cluster, which provides the data basis for obtaining the information regarding the atomic stability and excitations, optical dynamics and spectroscopy, related to the atomic vibrations and their coupling to electrons. To the next order of the ensemble of fundamental knowledge regarding the nanostructures, the knowledge of the excited states, both electronic and magnetic, is needed, as well as their contribution to the response of the nanostructures to the perturbational action of the external factors, and to transport phenomena. In this respect SANTRAN fits perfectly in the most recent fundamental trends of scientific research in the field of the nanoscience at the worldwide level.

OBJECTIVES: SANTRAN sets up its objectives according to two major requirements. On one hand, the necessity of adding value to the results already obtained, having in view the enhancement of the efficiency of its own activity of scientific research. On the other hand, SANTRAN aims at responding questions of major interest, both at the national and international level, with the view of increasing the international visibility, professional stature, scientific assessment quotas. In another respect, SANTRAN looks for subtle, complex, points of scientific research of virtuosity at the fundamental level, envisaging the advancement of basic knowledge, and, at the same time, tackling also the issues of principle in applicative questions, for attracting interest in its own research and integrating itself more firmly in the international main stream. The activity developed by SANTRAN warrants such strategies and tactics, as seen from the large number of scientific publications, communications, dissemination of scientific research, permanent multiple-interactive seminars, and, not in the least, by the large number of projects and grants funded on a competitive basis, recorded by the scientific activity of SANTRAN. In this context, SANTRAN aims mainly at the following objectives at this stage:

Metallic clusters. This objective aims at developing and extending previous results regarding the construction of nanostructures on the basis of the method and theory of quasi-classical description of the ion-electron interaction in multi-atoms ensembles. The main result of this procedure is getting the effective inter-atomic potentials which lead to cohesion. It is possible thus to compute the ground-sate energy, isomers energy, form and structure of the nano-aggregates, magic numbers and vibration spectra. The method involves a second iterative step, consisting in solving the Hartree-Fock equations for one-particle wavefunctions with the potential derived from the electronic density established in the first step. It is obtained this way the excited states spectrum, ionization potential and chemical affinity, fundamental parameters for the spectroscopies and transport properties of the nanostructures. The method is applicable to nanostructures with a reasonably large number of atoms, i.e. precisely to the most interesting case for nanoscience, and the proper case for nanotechnological investigations. An expedient method of computing the electronic excited states is the approximation of the anisotrop spatial oscillator, known also as the Clemenger-Nilson potential, whose functionality is explained by the quasi-classical description method. Homo-atomic clusters are obtained this way, with a large number of atoms, up to a few hundreds or even thousands, together with their isomers, their own stability islands, vibration spectra, all this being a solid basis of characterization which is the support of any detailed analysis, according to the interest. Further, the objective aims at describing several exotic structures like sheets of atoms, nano-wires or interacting clusters.

The later are metastable, dynamical, states, of a special applicative interest, because they are relevant in synthesis and assembling of the clusters. Then, the objective extends the work to deposition of clusters on solid surfaces and supports, or to supramolecular assembling under geometric, or kinetic, constraints, such that the results are relevant for interfaces, contacts, junctions, deposition of thin films, layer assembling, hybrid structures, etc. All this whole multiplicity of consistent results originates in the SANTRAN superiority in comparison with traditional methods.

Liquid clusters. The atomic clusters obtained by SANTRAN method are solid clusters. They maybe viewed as the smallest, possible solids, or nuclei of condensed matter. They exhibit an impressive number of isomers, often inseparable from the ground-state, displaying together a quasi-continuum of energy. Consequently, their natural state, at finite temperatures, is a statistical ensemble of weakly undefined form, i.e. a liquid. This liquid state affects especially the surface atoms, but, under circumstances of multiple magicity, i.e for large clusters with a configuration that exhibits a multiple superposition of atomic layers, this liquid state can also be seen in the interior of the cluster. The partial liquid character of these nanostructures is a completely new property, unknown in nature as yet, entirely specific to the nanoscopic world, which may lead to applications which are difficult to foresee. It may be the key to a special, exotic, behaviour of the living cell, especially to the aging process, or to some peculiar behaviour of composite materials. The present objective aims at a preliminary investigation toward modeling the liquid, or quasi-liquid, state of nanostructures, by employing for the beginning pseudo-potentials taylored to simulate such a behaviour. The great problem raised by such results belongs to classical thermodynamics and statistical physics in fact, to the classical equation of state, where pressure is, in general, a monotonous function of volume (density), or temperature. Exotic behaviour, like the one reported recently regarding the negative heat capacities for heterogeneous mixtures of quasi-liquids, or super-dense liquids, exhibits the enormous scientific potential of bringing new contributions to classical fields, like the equation of state of condensed matter. It is also worth noting that such a quasi-fluid state of supramolecular ensembles occurs also at free surfaces, which made the physics of friction phenomena to gain new dimensions in such a context. Similarly, such curios quasi-liquid properties are partly modified on the occurrence of a contact, so that, it might be possible that fundamental notions of friction to suffer substantial changes, at least in the nanoscopic scale, as regarding their nature, their dynamic, interactive and self-consistent character. The nanoscopic tribology, with so many important applications in micro- and nano-machining, in nano-robotics, etc, receives this way a new field of unexpected research. In this respect, the importance and opportunity of the present objective of SANTRAN research is obvious. It is worth noting here the distinct relevance the fundamental research may bear upon applications of great technological interest.

Hetero-atomic clusters. At the present stage SANTRAN is limited to homo-atomic clusters, of metallic type, characterized by atomic species with upper shells orbitals of type s, or approximable by s orbitals. The electronic density of ions is thereby a function with radial symmetry, reducible in fact to a delta-function. Forthcoming developments aim at extending the computations to spatially-oriented, directional, upper shells orbitals, or to orbitals with radial dependence for ionic cores. But, in a systematic approach, aiming at long-term research, like the one proposed here by SANTRAN, there exist still many questions to be clarified at the first stages of approximation, like the hetero-atomic clusters. SANTRAN wants to

tackle such clusters formed by two chemical species, looking for structure, forms, atomic positions, spatial configurations, magic numbers, and, of course, the ground-state, isomers, vibration spectra, as functions of relative concentration of species and their nature. It is expected that for balanced relative concentrations, and for close chemical species, clusters exhibit a relatively homogeneous structure. In contrast, for unbalanced concentrations, and for largely different species, a structural segregation is expected to occur, with both surface and inner zones, or, very interesting, with spatial ruptures of domains type, and with domain walls. In this context, it occurs the possibility of a very interesting research on the dynamics of the domain walls in nanostructures, with their own vibrations, visible in spectroscopies, with a very rich phase diagram, suggesting a very interesting field of research, that of phase transitions in finite ensembles. Similarly, the electron dynamics in such segregated, or supra-structured, clusters, may exhibit new features, beside those of order-disorder type, localization, restricted mobility, like, for instance, chaotical behaviour. It is also worth remarking an inverse problem, by which it is not envisaged the nanostructures cohesion on increasing the number of atomic constituents, or chemical species, but, on the contrary, it is envisaged the clusters instability on creating successive vacancies, with definite positions, in various sequential modes. The metastable states generated this way may represent the substrate of a multitude of functionalities and functional processes, unknown yet. The investigation of the hetero-atomic clusters, as proposed by SANTRAN, represents therefore a major objective for consolidating and advancing the fundamental knowledge in nanosciences.

Nano-magnetism. Beside the electronic excitations, the magnetic excitations represent a special interest innanostructures, as they are the substrate of possible control devices on a nanoscopic scale, or for nanoscopic magnetic memories based on giant magneto-resistance, spin valves, or other phenomena and processes of magnetic nature. Magnetic excitations in nanostructures are a very special topic, for the following reasons. First, the distinction between ionic and electronic magnetic states is not sharp, then the competition between localized and delocalized magnetization is operational, then the finite size of the ensemble imposes restrictive conditions and, finally, their low energy make the magnetic excitations discernable only with difficulty from other, competitive excitations. The present objective of SANTRAN aims at investigating the dynamics of the magnetic elementary excitations in nanostructures by Bethe ansatz method. The objective requires the adaptation of this method to the finite size of the nanostructures, and envisages the conditions under which possible two-magnons bound states may appear, or resonant states, or scattering states. Preliminary research suggests possible magnetic states with a complex structure, different from those occurring in the bulk. The computations are limited at this stage to the one-dimensional case, but some partial results are envisaged for a two-dimensional case, or even for a three-dimensional case.

Spin Andreev reflexion. Pursuing further to add value to SANTRAN results regarding the cohesion and the aggregation of the nanostructures, the associated elementary excitations and their role in transport phenomena, this objective aims at investigating the behaviour of the spin polarized current on its passing through a ferromagnet-superconductor junction. It is well-known that the normal metal-superconductor junction is characterized by a reflexion and tunneling phenomenon of the one-electron elementary excitations, known as the Andreev reflexion. It occurs in all the transport phenomena where a superconducting junction is implied, as for instance in thermal conductivity, electric conductivity, etc.

Recently, a very sensitive device of thermometer type has been produced on the basis of Andreev reflexion, which may become a serious advance in the metrology of the very low heat transfer. As regard the electric conduction the Andreev reflexion is seriously affected by the nature of the metal-superconductor junction, in the sense that this junction may look like a a sharp contact, or as an extended contact, where the mutual diffusion in the two materials is important. In addition, for a sharp ideal junction the proximity effects play an important role, as the superconductivity may weakens at the junction, the superconducting coherence diminished, and a corresponding enhancement of induced superconductivity may appear at the surface of the normal metal. The objective makes use of the results established by SANTRAN regarding the deposition of the nano-clusters and nanostructure on surfaces, the formation of interfaces, contacts, junctions, description of the metastable states implied in these processes, for highlighting, as reliable as possible, the nature and the form of the normal-metal superconductor contact. In addition, the present objective has an even higher degree of complexity due to the fact that the normal metal is replaced by a ferromagnet. In a ferromagnet the electronic excitations are described by two fluids with distinct magnetizations, and distinct velocities, both contributing to transport. It is envisaged the control of the net magnetization, either by applying a magnetic field, which is more difficult experimentally in view of the superconducting junction, or by variation of the temperature. Practical realization of the device requires also the analysis of corresponding materials and working conditions, theoretical results being able to guide such a search. The objective has also a by-target regarding the control of the magnetization under the action of a spin polarized current. Recent results indicate an instability of spin-density wave type, for a magnetization interacting with a spin polarized current, where, depending on coupling strength or temperature, the spin-density wave suffers a transition toward a solitonic lattice of magnetic domains, which, in turn, has its own dynamics of domain walls, that contributes to transport. Preliminary SANTRAN analysis shows that the non-linearities are essential for describing such a complex phase diagram.

Nano-tunneling. The nanostructures offer the possibility of having control at the macroscopic level on quantum phenomena. One of such phenomena is the quantum tunneling, which may occur either in a hetero-junction which simulates a nanoscopic potential well, or in quantum dots. The phenomenon has the same origin as the molecular tunneling, reflected in the rate of chemical reactions, and, certainly, through the delocalization of the wavefunction, it bears relevance upon the modern investigations regarding the teleportation, or on classical phenomena like the waves propagation in microwaves guides, and, more recently, in photonic guides. From a fundamental standpoint the phenomenon has two distinct sides. It may be viewed either as a successive tunneling of a plane wave, or as a multiple tunneling of a wavepacket, simulating a localized particle. In other respect, the phenomenon is specific both to molecular components, which react through electronic tunneling, and to electronic transport, or of other nature (for instance thermal), in a coherent quantum regime in nanostructured hetero-junctions which simulate potential wells with corresponding potential barriers. In this context, the general theory of transport, both diffusive and, especially, coherent (balistic) or incoherent quantum transport, is of relevance, SANTRAN adding thereby value to a remarkable tradition of original research. Indeed, the scientific activities SANTRAN aims at continuing are characterized by numerous, well-known results, well-documented by numerous publications, communications, including two postgraduate monographs.

The central point of such an activity put emphasis especially on a novel type of transport, the so-called pulse transport, with a superior efficiency in comparison with the continuous transport. The essential element of such a type of transport is the reduction, as much as possible, of dissipation, which affects the transport coefficients. The main application was directed towards the pulse thermoelectric transport, now looking for similar applications for balistic transport, or for the limit of the balistic-diffusive transport, or in the incoherent-coherent quantum transport limit. Recently, nanostructured devices configured a quasi-solitonic lattice of individual electric charges, partly trapped in a succession of nanostructured junctions, which lead to the measurement of an individual electron transport. Similarly, the nanotransport is associated not only to the nanoscopic structures (nanostructural transport), but also to nanoscopic processes (nanoscopic transport), in this direction SANTRAN initiating a forthcoming investigation regarding the thermo-acoustic and electro-acoustic transport. Such research is of utmost importance at the international level this day, because they carry an appreciable applicative potential, and requires, at the same time, a complex theoretical approach.

Through such objectives SANTRAN wants to contribute essentially to the configuration of the nanoscience and nanotechnology field, as a field with its own identity, because fundamental phenomena like cohesion, aggregation, elementary excitations, transport being essentially different in the nanoscopic zone than their counterpart in the macroscopic, or quantum, atomic and molecular zones. Nanostructures represent already a distinct field of scientific research, with an appreciable applicative potential on one hand, and with distinct methods, techniques, procedures and formulations, on the other hand. Physical phenomena that appear between 10 angstroms and 1000 angstroms in linear size are distinct, according to their nature, from both atomic and macroscopic phenomena. SANTRAN integrates itself completely in this field of activity by its superiority of the theory of matter aggregation, by original techniques of treating the interaction and the nanoscopic transport, superiority illustrated by new and original results. The SANTRAN objectives are measurable by scientific results, reports, publications and communications, electronic means of dissemination and popularization of the results (scientific movies, web sites, archives and databases), by permanent interactive seminars where the emphasis is laid upon the theory-experiment-application-social value dialog. The present Programme of Excellence aims at adding value to the technical and scientific potential of research in edge-cutting areas, among which nanoscience, nanotechnology and basic sciences like theoretical physics f condensed matter represent priorities. SANTRAN does represent indeed such an element of excellence through its structure, its objectives, scientific contents, adequate management and, especially, thorough scientific and social relevance of the envisaged results.

SCIENTIFICAl AND TECHNICAL PRESENTATION OF THE PROJECT:
SANTRAN is devoted to fundamental research in the field of supramolecular aggregation and nanostructural transport. It answers the priority requirements formulated by the Framework Programme 7 of the European research regarding the research areas of nanosciences, nanotechnologies, and, mainly, theoretical physics of nanostructured condensed matter. Through its objectives and results SANTRAN answers at the same time the necessity of adding superior value to inter-, pluri-, multi- and trans-disciplinary research in fundamental and applicative areas, regarding nano-electronics, molecular electronics, nano-transport, nanostructured interaction at the level of the living cell, nanoscopic control devices, having permanently in view both the scientific and social relevance.

SANTRAN is motivated by the noteworthy expertise in scientific research of its team, expertise which SANTRAN aims at further developing, its adding further value, and which is accumulated in the last five years in the field of the fundamental theories of matter aggregation, chemical bonding, dynamics of elementary excitations in finite-size structures, in the field of the nanotransport and pulse transport, an expertise illustrated by numerous scientific publications, books, communications, as well as by numerous products of scientific dissemination and science popularization of the results, obtained by the specific means of the electronic information technologies, by intensive use of numerical codes of computing and simulation. In particular, the nature of the results in the field of the nanostructures is specific to advanced graphics, requiring special computational resources for simulation, archiving and storage of complex databases, including the animated presentation of the results. The scientific research activity developed by SANTRAN distinguishes itself by numerous scientific movies based on animated results of numerical calculations, on superior graphics and numerical codes of extensive computations. The development of incipient parallel computing networks adds to this research, of interconnectivities, compatibilities and securization protocols of electronic communication under the circumstances of manipulating large databases in real time. Beside the traditional methods and techniques of analysis of scientific problems SANTRAN depends essentially on a complex and superior basis of electronic computing and communication. SANTRAN is structured on 6 objectives to be developed in 3 years: metallic clusters, liquid clusters, hetero-atomic clusters, nano-magnetism, spin Andreev reflexion and nano-tunneling. These objectives add superior value to already existent major results, and envisage opening new directions of research in this area. They answer the priority research requirements in this field, especially those of the European research, and aim at scientific superiority, international visibility and extension of research activity by dissemination, popularization and creating new jobs in the Romanian scientific research by attracting graduate, post-graduate, masters, doctoral and post-doctoral students, and multiplying the international cooperation on this basis. SANTRAN starts with an ensemble of ions and electrons on the valence upper shells atomic orbitals, which are subjected to Coulomb interaction. In the Hartree-Fock energy functional SANTRAN finds out a new minimum condition, corresponding to the weak, local variation in the number of occupied one-electron energy levels. It is shown that such a variation implies quasi-plane waves, and the exchange energy is "rigid" under such variations. The solution follows then straightforwardly, leading to the screened Coulomb potential of Thomas-Fermi type for the ion-electron interaction, with an undetermined screening wavevector. This result however is strictly associated to the assumption of point-like ionic cores, whose charge density is described by a delta-type function. Forthcoming developments, envisaged by SANTRAN, take into account the radial dependence of this density, for realistic upper shells orbitals of type s, for instance, as well as the spatial dependence, especially the angular one, of valence orbitals of type p, d, f, for instance. Such developments allow for describing nanostructures with a high degree of interest, like those consisting of the life element carbon, or electronics element silicon, or the opto-electronics elements gallium, arsenic, aluminum, or the physical-chemistry elements oxygen, halogenides, etc. For the moment the computations are limited to nanostructures consisting of simple metals, or heavy elements with a high number of electrons on the upper shells which may be approximated by a charge density with radial symmetry, or even a point-like one. In the first step of the computations described above the screened potential is introduced in the energy functional, where it gives rise to effective inter-atomic potentials.

These potentials are new, original, derived from first principles, possessing very interesting properties with respect to the cohesion of the solid matter. SANTRAN continues with the minimization of the potential energy of the ensemble with respect to the atomic positions, by exploiting this way the effective potentials, leading to a generic supramolecular structure. Thereafter, the total energy is minimized with respect to the screening wavevector in the original potential, getting the final form of the cluster, atomic positions, binding energy, vibration spectrum and, especially, cluster's isomers. The clusters stability leads immediately to finding out the magic numbers. These magic numbers are structural, or geometrical, inasmuch as they refer to the ground-state. Beside them, there exist also statistical magic numbers, corresponding to the statistical ensemble which includes isomers at finite temperatures. And there are still the electronic magic numbers arising from the complete filling of the electron energy shells in clusters. For, the electron motion in clusters may be approximated by their motion in an anisotropic spatial oscillator, known also as the Clemenger-Nilson potentials in nuclear physics. In contrast to the semi-phenomenological theories SANTRAN identifies these potentials from first principles, and, in addition, it indicates higher-order corrections to them, which renders the problem anharmonic, and, in general, non-linear. In this respect SANTRAN opens the possibility to investigate the chaotic behaviour of the electrons in nanostructures, as partly documented experimentally. SANTRAN identifies the solution of matter aggregation as being that corresponding to the quasi-classical description. Consequently, SANTRAN tests the solution in various others situations, and tries its delimitation from the exact Thomas-Fermi solution, known also under the name of quasi-classical approximation, which, however, does not lead to a bound state, as it is well-known. The tests have been done on heavy atoms, where the binding energy is obtained straightforwardly by the SANTRAN method, including superior approximations to the classical computations. The second SANTRAN test was done on the bulk solid in the continuum approximation, or the generic model of the Wigner universal metal, where all the known results have been reproduced consistently, and new others have been derived (like Landau quasi-particles in solid). These tests increased the confidence in the possibilities and superiority of the SANTRAN method, and brought also improvements, at the same time. In the second step of the iterative scheme it is necessary to insert the screened potential, found out in the first step as a function of electron density, into the Hartree-Fock equations, and to solve these equations. This way the contribution of the ionic cores is taken into account, where the electron motion can not be approximated by quasi-plane waves anymore, and where the quantum corrections are important. This is the so-called step of the quantum corrections. Its contribution to relevant quantities is estimated to about 17% at most. It is shown thereafter that an additional iteration is equivalent to electronic quasi-particle lifetime, which overpasses the 3% limit of accuracy, so that such a superior iteration is immaterial under the assumption of one-particle states. These results are extended by SANTRAN to large-size metallic clusters (consisting of hundreds or thousands of atoms), to liquid clusters and to hetero-atomic clusters. Of special importance are the structural isomers in SANTRAN, since their statistical ensembles exhibit the phenomenon of quasi-liquid state, either at the surface, or in the inner shells,. The investigation of this situation which is extremely interesting is included in objective #**2 Liquid clusters**, as shown in Objectives. The segregation and structural domains brought about by the hetero-atomic clusters are of utmost importance in the physics of the nanostructures, they being completely new, being included in objective #**3 Hetero-atomic clusters**, as described in Objectives too.

With this, SANTRAN covers its first three objectives, Metallic clusters, Liquid clusters and Hetero-atomic clusters. Further, SANTRAN tackles the magnetic excitations in nanostructures and, in this connection, phenomena of nanostructural transport. The SANTRAN method of supramolecular cohesion makes use of the upper shells orbitals of valence, which participate in the aggregation to a certain extent each, this extent being given by the effective valence. Actually, the effective valence is different for each orbital, so that one can only speak of an average effective valence for a given chemical element. Moreover, depending on partners, bond nature and even the number of atoms in the nanostructure, this effective valence changes. On the other hand, it is well-know that Hund's rule determines the magnetic moment of the ions as a function of occupied valence orbitals, so that, there appears in nanostructures a dynamic, variable, ionic magnetic moment, as expected from the experimental standpoint, but rarely described theoretically. This is an element of major interest for SANTRAN objective #**4 Nano-magnetism**. The second element of interest arises from the indication provided by Bethe's ansatz in structures with restricted geometries, like one-dimensional, two-dimensional structures, and finite-size structures, on the existence of special two-magnons states, like bound states, or resonant states, or scattering states. Such states could be a novelty in nano-magnetism, and they could represent a substrate for new possible applications of the giant magneto-resistance effect, or for controlling the magnetization by spin polarized currents, like in spin nano-valves. Investigating the nano-magnetism in this context opens up the problem of the nanostructural transport, in particular the spin transport. This is the issue included in objective #**5 Spin Andreev reflexion**, which, in turn, raises questions regarding surfaces, interfaces, contacts and junctions, which sets up the connection with the first set of SANTRAN objectives. Indeed, SANTRAN benefits from a rich experience in the field of depositing atomic clusters on solid surfaces. The method of quasi-classical description has been successfully applied to a semi-infinite solid in the continuum limit making use of the original inter-atomic potentials, leading this way to excellent results in characterizing the surface electric double layer (diode layer), work function, and, the most important perhaps, the derivation of the effective electron-surface and ion-surface potentials. The application of the SANTRAN method to solid surfaces represents a third major test for the method, and the new potentials opened the way for obtaining atomic clusters deposited on solid surfaces. Such clusters have been obtained, being characterized by interesting properties, like magic numbers, the competition between growing up along the surface or perpendicular to the surface, and, especially the diffusion. It has been established this way that there exists a multitude of metastable states by which the cluster penetrates beneath the solid surface, to a variable extent, simulating this way not only the solid-solid diffusion, but the origin of interfaces, contacts and junctions. Such results allow for establishing the conditions by which the surface bond between two solids is almost ideal, like a sharp interface, or has a controlled thickness, like a contact, or it is extended like a junction. In transport phenomena, and especially in spin transport, or in spin transport at the interface between a ferromagnet and a superconductor, the nature of such a surface bond between two solids is of capital importance. SANTRAN aims precisely at such a description. At the ferromagnet-superconductor interface occur a series of proximity phenomena, which must be clarified completely, quantitatively, before attempting to describe the transport and the injection of the spin polarized current. In this respect, the superconductivity is reduced to some extent at the surface, as depending on the coherence length, correlation length and the surface nature. Similarly, the spin polarization of the injected current is preserved on a finite distance, called sometime the spin diffusion length.

This length must be correlated to the junction size, and applied to new conditions, those corresponding to a superconducting state. Then, the Andreev reflexion is well-documented for a normal metal, but the ferromagnet contains two fluids of polarized spins, having distinct velocities and transport properties, whose effects superpose to each other. Such fundamental questions, and fundamental for applications questions, are the contents of this SANTRAN objective. It aims finally at obtaining the current-voltage characteristic for the ferromagnet-superconductor junction, and possibly the transition regime from diffusive to ballistic transport. The general aim is the possibility of controlling the current through such a junction, either by magnetic field, or by temperature, as in a transistor-like effect. This SANTRAN objective raises another issue that may be included or not in the present SANTRAN, or developed in the future, depending on circumstances. The issue regards the interaction between a spin polarized current and magnetization. It is well-known that such a dynamics is generally described by the Ginsburg-Landau functional. For a current however, the dynamics of the process may acquire the aspect of a one-dimensional physics, where instabilities and non-linearities may appear. Indeed, the magnons are unstable in this context, for a certain wavevector (depending on the interaction strength and temperature), the instability being of the spin-density wave type, and its investigation requires a special study. The non-linearities in the Ginsburg-Landau functional lead now to excitations of solitonic nature, and, depending on the interaction strength or temperature, to a solitons lattice, with distinct magnetic domains, with distinct domain walls, which, in turn, have their own dynamics that may contribute substantially to transport. This is a novel phenomenon, its investigation requiring a special study, either in the framework of the present SANTRAN, or in forthcoming developments. The Andreev reflexion, or spin injection, are essentially conditioned by the tunneling through the potential barrier. **Nano-tunneling** is objective #**6** of SANTRAN. First, the quantum tunneling is always associated with the wavefunction delocalization, and this looks like a teleportation phenomenon. It is a point of hot debate this day in connection with the tunneling time, resonance time, dwelling time, etc in microwaves guides, nanophotonic guides, and, generally, in periodical succession of nanostructures, or nanostructures with certain spatial patterns. SANTRAN has in view either a hetero-junction with a nanoscopic potential well, or the tunneling at molecular level, as the features of the effect are similar. SANTRAN opens thereby, by its objectives, the access to results of scientific research of major importance at international level, in strict accordance with the priorities of the European Union, whereby nanoscience, nanotechnology and the methods of the basic sciences like theoretical physics of condensed matter are fundamental. SANTRAN adds value to scientific results and expertise gained in the field of matter aggregation, atomic clusters, atomic clusters deposited on solid substrate, characterization of surfaces, interfaces, contacts, junctions, and, especially, in the field of transport, where the scientific activity SANTRAN develops further has a confirmation for a new type of transport, of high efficiency, the pulse transport. In this context, SANTRAN identifies also a few other collateral objectives, which may form the core of forthcoming scientific investigation and development.

PROJECT JUSTIFICATION: SANTRAN integrates itself in the field of the scientific research in basic sciences, physics, theoretical physics of condensed matter. This is a priority field of research for the present Programme of Excellence and for the European research. Its main relevance originates in concentrating the available scientific potential of the condensed matter physics in the nanoscience and nanotechnology area.

The nanoscience and nanotechnology is another priority area for the European research, especially for the Framework Programmes 6 and 7. SANTRAN is devoted precisely to these issues related to the nanostructures physics. The major interest for nanostructures arises from the ultraminiaturization (nanomization) of electronics, with profound implication on the data storage and manipulation, on electronic communications, with a hard-to-evaluate relevance on the electronization of biology, on elaboration of superior materials, processes and devices. The nanostructures have several central issues. Among them, the aggregation of matter at the supramolecular level, elementary excitations with relevance in spectroscopies and transport, and nanotransport. SANTRAN aims precisely at these three major directions of research in the field of theoretical physics of condensed nanostructures. The nanostructures are very flexible and versatile for complex constructions, like nano-dots, nano-wires, self-assembled layers, serial junctions, hetero-lattices, quantum wells, etc, all exhibiting novel phenomena, or phenomena transposed from the quantum or condensed matter zones, in new contexts, with new functionalities. SANTRAN aims precisely to such fundamental aspects of the nanostructures, like supramolecular aggregation, quasi-liquid state of the nanostructures, nanostructured domain segregation in hetero-atomic clusters, as well as the nanomagnetism and the nanostructural transport. A special importance is attached to spin diffusion and magnetization control through the reflexion on the superconducting state, and fundamental characterisation of the nano-tunneling. SANTRAN benefits of a rich expertise in the field of matter aggregation, nanostructures deposited on solid substrate, transport, ballistic transport included. SANTRAN aims especially at functionalities, processes and devices that may add value to such fundamental knowledge. The SANTRAN objectives aim at continuing and further developing such knowledge, so that SANTRAN risks are minimal. There exist in SANTRAN three collateral objectives which might be conditionally tackled. They are the only elements which may represent a higher risk factor. The first is the investigation of the coupling between the spin polarized current and magnetization, for describing the new dynamics of the domain walls. The second is the individual electronic transport in serial junctions of potential-well type. The third may be represented by the assembling of nanostructured layers, in a one-dimensional series, by making use of the effective potentials derived by SANTRAN. These three objectives involve, among others, superior computational techniques and resources. Depending on the assumed hypotheses, SANTRAN may bring minor changes to the objectives during the development of the activities, or to the strategy and tactics of the research described at this moment. A fundamental hypothesis in this respect is the course of the research trends in the field at international level.

DIAGRAM OF PROJECT EXECUTION: SANTRAN develops its activity with the aim of fulfilling its 6 major objectives: metallic clusters, liquid clusters, hetero-atomic clusters, nanomagnetism, spin Andreev reflexion and nano-tunneling. During each stage SANTRAN has in view the development of the main activity, such that each stage has a finality in producing the interim scientific report as well as the finite form of the texts prepared for scientific publications. Beside this main activity corresponding to each stage SANTRAN initiates the preliminary activities for the next stage, with a time horizon of about 2-3 stages in advance, such that the specific targets be prepared in advance. According to the previous experience, this type of activity is best developed under circumstances of satisfactory efficiency by graduate, post-graduates, masters or doctoral students, who work independently in advance, their results being finished in each specific stage. The monitorization of SANTRAN activity is permanent, by specific working means and techniques, such that immediate action can be taken, in real and efficient time, for changing and correcting the course of activities, for changing the strategy, if situation requires so.

A special feature of SANTRAN is the originality of its proposed research. Consequently, the cooperation with external and internal partners are of utmost importance. At the national level SANTRAN is unique in its technical and scientific potential. Consequently, the partnership is ensured on a dynamic, interactive basis, through the permanent seminars and working meetings organized by SANTRAN, with participation of theoreticians, experimentalists, applicationists and private companies or enterprises of science and research At the external level, SANTRAN maintains and develops regular informative cooperations with researchers in the field, in order to permanently exchange relevant scientific information, in order to eliminate redundancies, finding out the niches of exploitation of the results, to maximize the efficiency of its own research and to integrate itself completely and definitively in the international course of cutting-edge research in the field. SANTRAN concentrates the efforts of a complex consortium consisting of cca 25 relevant experts from four national institutes of research and a university (P1,2,3,4), is fully connected to the objectives of the European Research Area and aims at a major strategic objective, both at national and European level, namely the basic knowledge in physics at nanoscopic level.

RESULTS / PROFITS AND DIAGRAM/ CAPITALISATION PLAN/ DISSEMINATION: The expected results for SANTRAN are: 1) the enhancement of detailed information on the structure, form, cohesive energy and isomers for free or surface deposited metallic clusters, as well as for various nanostructures with geometric constraints, and their interaction; 2) the nature of the supra-dense liquid state and its localization (core, surface, inner interfaces) for liquid clusters, its properties and the general aspect of the equation of state in these anomalous conditions; 3) segregation and occurrence of structural domains in hetero-atomic clusters; 4) nature of the two-magnons bound states in clusters nano-magnetism; 5) current-voltage characteristic of the injection of spin polarized currents at the ferromagnet-superconductor interface on the basis of spin Andreev reflexion; 6) nano-tunneling characteristics, in molecular or nano-structures, for derivation of the rate of the chemical reactions and possibly for the individual one-electron transport. All these scientific results regarding the advancement of new basic knowledge are quantified, numerable, finite, definite, distinct and communicable. The benefits of SANTRAN are: 1) advancing the fundamental knowledge in the field of theoretical physics of nanostructured condensed matter; 2) upgrading to a superior level the existent expertise and potential of scientific research; 3) increase the international visibility through scientific results obtained in European and international priority directions of research; 4) dissemination on a large scale of the results, through publications, books, communications, conferences, talks, scientific movies, electronic audio-visual and animated means; 5) attracting experimentalists, applicationists, science and research entrepreneurs to the technical and applicative potential of the nanoscience and nanotechnology; 6) attracting the graduates, post-graduates, masters, doctoral students and post-docs to original, edge-cutting research, creating new jobs for research. The estimated profit of SANTRAN is above the average, consisting of 6 new, original, major results in priority directions of research, very competitive, and collateral products. The high rentability comes from the 3 years range of complex activities developed by a highly-competent team, with complementary competencies, the costs being efficientized as to cover the manpower, equipment and consumables, mobilities. The SANTRAN superiority comes from exploiting the experience accumulated in the last 5 years in this area of research which is very competitive at worldwide level. Adding value to the results is made by scientific publications, books, communications and participation in conferences, workshops, as to promote the scientific consensus at the community level on the novelty and originality of the research.

The benefits are in the favor of the national and international scientific community, applicationists and enterpreneurs of science and research, young researchers, all these being the target groups of SANTRAN. All this activity is being made over the entire period of developing the SANTRAN research, both in interim stages and in the final stage, which summarizes all the results. Dissemination of the SANTRAN results is ensured by specific electronic audio-visual means, CDs, booklets, dedicated websites, scientific movies, popularization conferences.

TECHNICAL, ECONOMICAl AND SOCIAL IMPACT The main impact of SANTRAN is upon the scientific mental environment, which benefits from a manifold of new and original scientific results in a field that is a priority in the international and European research. The scientific community acquires through SANTRAN new horizons of scientific knowledge in the field of theoretical physics of condensed matter in nanostructured forms, processes and devices at the nanoscopic level. Thereby, the technical impact of possible applications is enhanced, for the present or in the future, toward nano-electronics, nano-biology, control nano-devices, nano-opto-electronics, nano-photonics, nano-materials and, not in the least, basic knowledge which represents the necessary condition for any advance in this high -tech and high-sci field.the databases, electronic archives and communications promoted by SANTRAN during its research activities are applications with a high economic impact. Dissemination of the results and attracting the young researchers and students to the SANTRAN activities in the priority domain of nanoscience is a high-level, noteworthy, social impact. The opportunities open by SANTRAN toward preparation of diploma, masters works, PhD theses are another major element of social impact upon the professional environment. The professional elevation, mathematical and physical rigor, are another element of intellectual impact upon the professional environment, which becomes an attraction point of superior value-adding at the socio-professional level. The activities developed by SANTRAN provide for conservation and reconditioning of the professional environment of scientific research and high education in science, reconditioning the professional resources which are greatly damaged at this moment, conservation of the expertise and human basis in the advanced scientific research. SANTRAN gives a special importance to the less-advanced regions in the scientific research, by attracting relevant human resources, in order to contribute to a harmonious regional development, both at the national level and at the European-regional level. The permanent contact with elements of technological transfer, intellectual, scientific and professional transfer are continuously in the attention of SANTRAN, with targets the scientific and technological minority groups.

PROJECT MANAGEMENT: The SANTRAN management is provided by a leading team consisting of the project director, workpackages and stages administrators, and the monitorization council. The administration of unrolling activities scrutinizes closely the fulfillment of the objectives in time and good conditions, in agreement with the working, following-up, monitorizing, valorisation, spendings, refundings and budgetary allocations plans, the plan of advancement of the tasks and the plan of changing strategy and tactics, in accordance with the assumed risks and hypotheses. The communication is maintained continuously, between all the team members, on a permanent basis, for a permanent control of the stage of the scientific operations. A basic component of the project management is the permanent briefing on the results and the evolution stage of workpackage sub-teams, on the activity of all the researchers being in cooperation contacts with SANTRAN and/or in competition with SANTRAN. The adequate study of the information originating in coworkers, associates, interested persons or competitors represents for SANTRAN a valuable working basis for maximizing the success chances.

DESCRIPTION OF REQUIRED RESOURCES FOR PROJECT EXECUTION:
SANTRAN needs 25 scientific researchers for attaining its goals, grouped in sub-teams of 4-5 according to the objectives and stages in the Scheme of Realization, with an adequate balance between principal investigators and researchers, with a complementarity of competences. In addition SANTRAN may employ 2-3 graduates, post-graduates, masters or doctoral students at least, for covering the current tasks. SANTRAN needs also a net administrator and a soft responsible. The material resources of SANTRAN are at the level of current corresponding consumables and electronic computing equipment, of the order of 10-15 evolute PCs, dedicated softs, cca 5 associated peripherals, a graphic station for producing and presenting specific materials, according to the Plan of Realization and List of Equipment. Partner 1 has special tasks in numerical modelling and simulations, Partner 2 has specific tasks in numerical computations and associated graphics, Partner 3 aims at confronting the theoretical results with its own experimental research, and Partner 4 aims at numerical computations, simulations and dissemination of the results. Financially, SANTRAN needs cca 20 GROL (old) for fulfilling its objectives, the allocation being made according to the recorded objectives and stages.