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Atomic Nano-Objects
Advanced Research in Matter Aggregation

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1 ABSTRACT

Recently, new principles of matter aggregation and chemical binding were laid,[1, 2] which allow a much faster computation of the structure and physical and chemical properties of various nano-objects, like atomic clusters, supra-molecules, atomic and molecular aggregates, nano-wires or atomic and molecular nano-structures deposited on surfaces. They were tested on homo-atomic clusters of Fe, Ba, Na of up 200 atoms, as well as on similar nano-structures deposited on surfaces, or nano-interfaces.[3] The computation takes usually from a few hours to several days, or a couple of weeks, of running a middle-class computer, yielding, beside the ground-state, the isomers too, in a statistical ensemble approach. The structure of an organo-metallic cluster Fe13(C2H2)6 has also been computed.[4]

The objectives of the project is to extend the computations to other nano-objects, to further develop and refine the methods and procedures as to increase accuracy, and, eventualy, to establish a new technology of producing nano-objects on computer from first theoretical principles. Beside simulating and modelling any known nano-structure produced experimentally, this investigation may lead to producing a database of structures, chemical and physical properties, for any nano-object of interest. It is inscribed in the general area of nano-technology and nano-science of today. Its application resides in producing scientific information on atomic nano-aggregates.

The new nano-clusters, in gaseous or liquid state, may generate a new molecular physics, as such aggregation states of matter have a much higher mass density. Consequently, they propagate sound slower, for instance, have a high heat capacity, and a low thermoconductivity. The nano-objects are spectroscopically active in far-infrared, and probably even in microwaves. Included in liquid or solid matrices the nano-objects may lead to new composite materials. Accelerated under high electric fields the nano-ions produce highly efficient particle beams. Nano-surfaces, -interfaces, -contacts and -junctions open the way toward a new electronics on a nano-scale, involving new mechanisms of electric (as well as thermal) transport. Our investigation, as based on the existence of the isomers, suggest a new state of nano-matter, characterized by a quasi-liquid surface and a solid-state core of the nano-objects, which may throw new light on various mechanical processes, like friction, e.g.

2 STATEMENT of OBJECTIVES

1 Extend the structure computation of homo-atomic clusters consisting of atoms with a quasi-classical upper atomic shell up to several hundreds of atoms, or more.

This objective involves cluster shape, atomic positions, inter-atomic distances, isomers, extension of isomer statistics as far as possible, identification of magic numbers, degree of stability, cohesion energy and vibration spectra. Mainly, it involves metallic clusters. The objective is attained by refining the computing codes (proprietary), and by using up-graded computers. The deliverables are scientific reports, electronic presentations, scientific movie, papers prepared for publication, within the first 6 months of the project. In addition, meta-stable states (clusters of clusters), nanowires and atomic clusters with constrained geometries are provided.

2 Building up atomic nano-objects deposited on solid surfaces, of the same size as above (several hundreds of atoms, or more).

The objective limits itself to the same class of atoms as above, and envisages the interplay between deposited mono- and multiple layers, the structure of the non-uniform atomic configurations, the atomic diffusion into the substrate, the inter-diffusion and the incipient interfaces, nano-contacts and -junctions. The investigation is based on deriving the effective inter-atomic potentials, including the substrate potential, and involves the up-grading of the numerical computing codes for tackling this new situation. The deliverables are as above, within the second (last) six months of the project. In addition, evidence for self-assembling will be looked for.

The project may be followed-on the next two years, with the objectives:

3 Radial dependence of the electronic charge distribution in the upper atomic shell, in order to extend the computations to other species of atoms, hetero-atomic clusters included.

This would involve new numerical codes.

4 Angular distribution of the upper atomic shell, for being able to compute clusters of carbon, silicon, aluminium, gallium, arsenic, etc, of high interest in applications.

This would require a new strategy in devising the computing algorithms.

5 Electronic properties of nano-objects, aiming at describing the spectroscopical properties.

This would require the development of the investigation of the second-order iteration procedure in the quasi-classical approach of the Hartree-Fock equations (already delineated).

6 Nano-objects under external factors (strain, stress, etc) and geometrical constraints (like a squeezed or stretched nano-wire), electric or thermal effects included.

It involves the response of the nano-objects under external factors.

3 RELEVANCE and APPROACH

The project computes for the first time the structure of large nano-objects (hundreds of atoms, or more) as based on first principles of the theory of matter aggregation and chemical binding. The state of the art attains homo-atomic clusters as large as 20 atoms by ab-initio methods. The project provides specific, quantitative information on atomic positions, inter-atomic distances, ground-state and isomer states, magic numbers and magic geometries, stability and statistical occurrence frequency, vibrations spectra for large nano-objects, including atomic clusters, clusters deposited on surfaces, nano-wires, nano-interfaces, -contacts and -junctions, free or under the

action of various external factors, geometrical constraints included. The projects aims at seting up a new technology of producing nano-objects on computer from first principles, initiating a database of relevant structural, physical and chemical information. It investigates new properties of the atomic and electronic matter constituents, like electronic spectroscopies, collective modes, finite-size effects, response to external perturbations, in the context of the nano-structured matter. Of particular importance is the characterization of the new liquid-solid inter-mixed phase, which seems to be specific to these new atomic objects. The project advances the basic scientific knowledge in the field of the nanotechnologies.

The approach is based on the quasi-classical description of the interacting ions and electrons and the associated solution to the non-linear Hartree-Fock equations. It proceeds iteratively in two steps, the former determining the atomic structure and the related properties for a quasi-classical behaviour of the binding electrons, and the latter solving for particular properties of the individual electronic states (quasi-particle excitations). The approach leads to new effective inter-atomic potentials as derived from first principles, which may have a remarkable simple form under suitable simplifying approximations. This explains partly the great saving in computing resources, like memory and time, though appropriate algorithms play also an important role. In the first year the project extends considerably the first step of the approach to large nano-objects consisting of atoms with a quasi-classical structure of the upper atomic shell, in order to get primary knowledge of these new objects, with a special attention to nano-objects built on substrates. The second step of the approach, as well as the extension to atoms with a genuine quantum character of the upper atomic shell, is planned fior the next two years of the project, in view of the more complex character of these aggregates. In particular, spatial dependence, both radial and angular, of the ionic sources of the sui-generis effective inter-atomic potentials involved by this second step, requires new algorithms and numerical strategies, which are investigated by the project.

References

[1] L. C. Cune, M. Apostol, Phys. Lett. **A273** 117 (2000)

[2] M. Apostol, J. Theor. Phys. **55** 82 (2000)

[3] L. C. Cune, M. Apostol, in NATO Workshop on Molecular Low Dimensional and Nanostructured Materials, Kluwer (2002), p. 221; in NATO Workshop on Low Dimensional Systems, Kluwer (2003), p.1

[4] L. C. Cune, M. Apostol, Chem. Phys. Lett **344** 287 (2001)