EMERGING RESEARCH FRONTS - 2008

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Riccardo Ferrando & Francesca Baletto talk with *ScienceWatch.com* and answer a few questions about this month's Emerging Research Front Paper in the field of Chemistry. The authors have also sent along images of their work.

Article: Structural properties of nanoclusters: Energetic, thermodynamic, and kinetic effects
Authors: Baletto, F;Ferrando, R
Journal: REV MOD PHYS, 77 (1): 371-423 JAN 2005
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SW: Why do you think your paper is highly cited?

The pursuit of nanoscience and nanotechnology is in order to understand, control, and manipulate objects of only a few nanometres size (1-100 nm), thus comprising from a few atoms to several million. These objects, usually called nanoclusters or nanoparticles, present peculiar chemical and physical properties that are strongly dependent on the geometric structure they assume.

These properties can be qualitatively different from those of their elementary constituents (being either atoms or molecules) and of macroscopic pieces of matter. Therefore, understanding from an atomistic point of view, the conditions under which one structure is more probable than another, is a real challenge. It involves a strong interplay of experiment with theory and numerical simulation.

Coauthor
Francesca Baletto

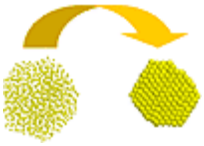
The high citation of our article is because it is a comprehensive work in that direction. It especially focuses on how external parameters, such as temperature and growth conditions, can influence the actual shape of a nanoparticle. A detailed analysis of how transformations between different structures can take place is discussed. In addition, we think that the paper is highly cited also because it can serve as a reference work for scientists entering and developing the field of research in nanoclusters.

SW: Does it describe a new discovery, methodology, or synthesis of knowledge?

It was a mix of everything. As a review paper, we summarized the state-of-the-art of this field, however, organizing the material from an original perspective. On the other hand, we also discovered, in a series of previous papers (see: F. Baletto, *et al*., "Reentrant morphology transition in the growth of free silver nanoclusters," *Phys. Rev. Lett.* 84 [5544], 2000; F. Baletto, *et al*., "Evidence of kinetic trapping in clusters of C60 molecules," *Phys. Rev. Lett.* 88 [075503], 2002), the importance of kinetic effects to determine the experimentally produced structures of nanoclusters. We singled out structural transformations of general character, occurring by the same mechanism in a variety of very different systems such as, for example, clusters of silver or copper atoms and clusters of fullerene molecules.

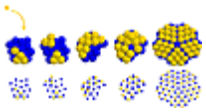
SW: Would you summarize the significance of your paper in layman's terms?

Figure 1: +enlarge



Nanoclusters are now becoming of widespread use in various applications, ranging from medicine (DNA-sequencing), to memory storage (nano-magnets), optics (quantum dots), and catalysis (fuel cells). Such a wide range of applications is possible because of the enormous variety of properties which are found in nanoparticles of different sizes and made of different materials. The properties of a nanoparticle are a consequence of its actual structure. Our paper constitutes a reference work for the structural properties of these objects.

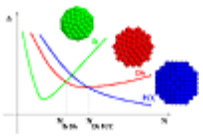
Figure 2:



SW: How did you become involved in this research and were any particular problems encountered along the way?

We entered this research field in 1998, starting with the Ph.D. work of Dr. Francesca Baletto in collaboration with Dr. Christine Mottet in Marseille, at the Centre Interdisciplinaire de Nanoscience de Marseille (CINAM/CNRS). The reason why we decided to enter the field was because we believed that it could be a rapidly developing subject, with the potential of quite exciting new physics at the borders of surface science, chemistry, and materials science.

Figure 3:



Ten years ago, the field needed a joint effort of theory and experiment, so the numerical methods would have been very useful to the interpretation of experimental results. We developed our own numerical methodologies based on molecular dynamics. Our simulations proved successful for the interpretation of experimental results. Luckily we did not encounter any particular difficulties in developing our work.

SW: Where do you see your research leading in the future?

Our computational modelling research in nanoparticles is developing in the direction of studying more and more realistic and reliable models of systems of interest for technological applications. These systems range from water clusters (M.S. Lee, *et al*., "Far-infrared absorption of water clusters by first-principles molecular dynamics," *J. Chem. Phys*. 128 [214506], 2008), to bimetallic nanoparticles (C. Mottet, *et al*., "Single impurity effect on the melting of nanoclusters," *Phys. Rev. Lett*. 95 [035501], 2005; R. Ferrando, *et al*., "Nanoalloys: from theory to applications of alloy clusters and nanoparticles," *Chem. Rev*. 108 [845], 2008), and surface-supported clusters (R. Ferrando, *et al*., "Interface stabilized phases of metal-on-oxide nanodots," *ACS Nano*, in press, DOI: 10.1021/nn800315x) for catalytic applications and memory storage, to matrix-embedded metal clusters for applications in optics and plasmonics.

SW: Do you foresee any social or political implications for your research?

Our work is basic research in physics, with multidisciplinary aspects of interest for chemistry and materials science. We would say that our work has no direct social or political implications. However, research in nanoclusters is a fundamental part of nanoscience and nanotechnology, which already have a strong impact on our society.

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Keywords: nanoclusters, nanoparticles, nanometres, nanoclusters, DNA-sequencing, nano-magnets, quantum dots,

catalysis.

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