cecam Centre Européen de Calcul Atomique et Moléculaire	**Workshop Scientific Report** Please do not repeat the program (unless there were last-minute changes) or the initial description - we already have this material.
Title	Nanoscale Alloys: from experiment and theory to quantitative modelling
Organizers	F. Calvo (CNRS and University of Lyon, France) G.M. Pastor (University of Kassel, Germany) A. Fortunelly (CNR, Pisa, Italy)

Scope of the workshop (one-two paragraphs)

This workshop aimed at bringing together physicists and chemists working in the increasingly broad field of metallic alloys at the nanoscale. Nanoalloys are currently at the frontline of many avenues of research ranging from catalysis, magnetic storage, to optical sensors for medical applications. This has triggered a formidable wealth of theoretical and computational studies, however poorly coordinated until the first conference on the subject was organized in 2007.

By focusing on the objects rather than the methods, we were able to bring several experimentalists, whose lectures have

considerably fed the meeting. The majority of participants, though, were from theoretical sides. This mixing contributed to better understanding each other and developing a common language, one of our primary objectives when this proposal was submitted.

The other important goal was to provide an overview of the current state of the art in theoretical and computational methods to address nanoalloys. This goal was achieved by devoting 80% of the talks to simulation experts, and inserting a 90 minute long round table on various subjects.

Main **outcomes** of key presentations (one page)

The workshop included both experimental and theoretical contributions.

On the experimental side, the impressive resolution recently achieved by electron microscopy (Yacaman, delivered in a slightly shortened version by Mariscal) together with more traditional methods (Kaszkur) were highlighted, by which nanoalloys particles' size, shape, morphology and chemical ordering can in principle be elucidated. Advances on single particle characterization were presented in terms of optical (Pellarin) and magnetic (Brune) properties. Latest magnetic experiments on gas-phase small clusters were also included (Janssen). Relationships between structure and magnetic (Dupuis, Respaud, Farle, Brune) or catalytic (Belic) properties were convincingly proven.

On the theoretical side, state-of-the-art and most recent advances were illustrated in different fields.

In terms of total energy methods, novel effective Hamiltonian approaches (Rubinovich) or new parametrization of empirical force fields (Mariscal, Negreiros, Ferrando) were discussed. In terms of structure, novel motifs were presented among the first times: off-center core-shell or Janus particles (Baletto, Johnston) and chiral icosahedra (Ferrando) at the level of force fields; gas-phase (Aguado) or supported (Barcaro, Negreiros) non-crystalline configurations (such as poly-icosahedra) at the density-functional level. In terms of coated particles, the prediction of their chemical (Groenbeck) and structural (Mariscal) properties was achieved via either density-functional or empirical approaches, respectively. In terms of catalytic properties, general relationships between structure, segregation patterns and chemisorption (Neyman), detailed accounts on the activity of medium-sized particles (Lopez) and the fascinating possibilities provided by very small clusters together with an overview of the main issues involved (Jellinek) were presented. In terms of magnetic properties, relationships between morphology and magnetism (Entel), novel phenomena with in-principle single-spin control arising from quantum confinement (Stepanyuk), the interplay of structure and spin-orbit interactions (Ebert), support effects on magnetic spin and anisotropy (Ebert, Barcaro) and the structure of very small clusters (Mokkath) were highlighted. Latest developments in the statistical mechanics treatment of equilibrium and non-equilibrium phenomena in nanoscale alloys were presented, their relative merits discussed in detail, and applied using either force-field (Caro, Mottet, Hou, Albe), effective Hamiltonians (Rubinovich, Creuze) or first-principles (Negreiros) approaches to the study of phase transitions in nanostructured bulk alloys (Caro), segregation patterns and order-disorder transitions (Hou, Mottet, Albe, Creuze), dynamic transformations and achievement of equilibrium (Hou, Negreiros).

Report on selected discussions (one page)

eg. Were there interesting hints for new research? for new developments? for collaborations?

A significant time for discussion after each oral presentation has been allocated by the organizers of the workshop. As expected the participants contributed very actively to these exchanges, which have been particularly lively and which contributed decisively to the achievement of the goals of the meeting. In addition, the poster session allowed for additional discussions not only among young researchers, most of which were presenting their current research in this form, but also between invited speakers and young researchers.

A 2 hour round-table discussion was organized on the third day of the meeting in order to allow further opportunities for scientific exchanges on some general, critical or controversial issues. This type of discussions are per se rather informal, at times disordered but certainly very stimulating. The discussion was moderated by the organizers of the workshop. Several subjects have been discussed on the basis of previous and spontaneous propositions of the participants: i) Goals, difficulties and prospects of improving of the interaction between theoretical and experimental research on nanoalloys, ii) Theoretical challenges from the experimentalists' perspective, iii) Experimental goals from the theorists' viewpoint, iv) Scope and limitations of effective interaction potentials, v) Global optimization versus kinetic conditioned nanoalloys structure and chemical order, vi) Implications of magnetism on electronic structure, modeling, and reactivity .

The scientific level of the exchanges, the commitment of the participants and the feedback we received shows that the round table discussion was very successful.

Goals for the immediate future:

The need for a closer link and integration among first-principles, empirical potentials and effective Hamiltonians methods strongly emerged from the questions and discussions, both in structure exploration and clarification of structure-property relationships, and both at the static or thermodynamic level and in the study of the largely unexplored kinetic and non-equilibrium processes. This is thought to be crucial to achieve closer agreement between theory and experiment, especially in terms of optical and magnetic phenomena, and entails establishing or reinforcing collaborations among several of the groups participating to the workshop.

Several chances of possible collaborations between theoretical and experimental groups were actually proposed in the lively discussions after the presentations, covering all aspects of chemical, structural, magnetic and optical phenomena.

To what extent were the **objectives** of the workshop achieved (strong points, weak points)? (one paragraph at least)

Our initial objective to bring together experimentalists and theoreticians was successful, despite the late cancellation of two prominent researchers (one of them could have his talk given by another participant). We velieve everyone enjoyed this mixed audience which, although somewhat unusual for a CECAM meeting, allowed more fruitful discussions on the physics and chemistry. The obvious downside is that the most technical theoretical issues were sometimes barely discussed, probably so as not to frighten the experimentalists in the room. This was anticipated, but we constantly witnessed the strong interest of experimental researchers toward computation, as well as numerous private discussions during the coffee breaks or the two poster sessions. One very strong outcome of the workshop is to strengthen the community working on nanoalloys. After two previous meetings held in 2007 (Faraday Discussion, Birmingham) and 2008 (SimBioMa workshop, Pisa), a nucleus of 30 groups around the world has made strong bonds and the CECAM meeting should trigger new collaborations among those groups.

On more specific grounds, the general atmosphere of the workshop was very good, and we felt most participants highly satisfied and wanting more (on their own topics). The chosen duration of 3 days and a half, however, was probably adequate for about 40 active participants. The round table, moderated by the three organizers, was lively and constructive, we think of it as a highlight.

Do you have suggestions for new workshops/tutorials/conferences on the topic?

All participants seemed eager to meet again in the future, which to some extent will be achieved through a COST action starting in 2010. But more focused workshops (rather than tutorials) could be anticipated to extend our own CECAM meeting and bridge gaps between subfields, or with related fields:

-Modeling the interactions from molecular to meso scales
-Interplay between bonding, magnetism, and reactivity
-Optical spectroscopy and plasmonics at the nanoscale
-Tailoring the structure of nanoalloys: thermodynamics and kinetics
-etc.