


## Programme

Faraday Discussion 138: Nanoalloys - From Theory to Applications

03 - 05 September 2007

University of Birmingham, United Kingdom

**Monday 3<sup>rd</sup> September 2007**

11:00	<b>Registration – 1<sup>st</sup> Floor, Haworth Building, School of Chemistry, Edgbaston Campus</b>
12:15	<b>Lunch</b> (tickets only)
13:00	<b>Welcome and Introductions</b>
13:15 <b>Paper 1</b>	<b>Introductory Lecture: Nanoalloys: tuning structural, electronic, and thermal properties through size and composition</b> Julius Jellinek, <i>Argonne National Laboratory, USA</i>
<b>Session 1</b>	<b>Theory and simulation of nanoalloy structures and dynamics</b>
	Session Chair: Roy Johnston <i>University of Birmingham, UK</i>
14:15 <b>Paper 2</b>	<b>A study of bimetallic Cu-Ag, Au-Ag and Pd-Ag clusters absorbed on a double-vacancy-defected MgO(100) terrace</b> Giovanni Barcaro and Alessandro Fortunelli*, <i>CNR Institute for Chemical and Physical Processes, Pisa, Italy</i>
<b>Paper 3</b>	<b>Global optimization and growth simulation of AuCu clusters</b> Tefo J Toai, Giulia Rossi and Riccardo Ferrando*, <i>University of Genoa, Italy</i>
15:15	<b>Afternoon Tea</b>
15:45 <b>Paper 4</b>	<b>Mechanical properties of bimetallic crystalline and nanostructured nanowires</b> Marc Hou*, Oksana Melikhova and Stoyan Pisov, <i>Université Libre de Bruxelles, Belgium</i>
<b>Paper 5</b>	<b>Solid-solution precursor to melting in onion-ring Pd-Pt nanoclusters: a case of second-order-like phase change</b> Florent Calvo, <i>LASIM, Université Claude Bernard, Lyon 1, France</i>
<b>Paper 6</b>	<b>Atomistic computer simulations on the generation of bimetallic nanoparticles</b> M M Mariscal*, N A Oldani, S A Dassie and E P M Leiva**, <i>INFIQC, Universidad Nacional de Cordoba, Argentina</i> **work being presented by E P M Leiva
<b>Paper 7</b>	<b>Dynamical equilibrium in nanoalloys</b> F Lequien**, J Creuze*, F Berthier and B Legrand, <i>LEMHE/ICMMO, Université Paris Sud – Orsay, France</i> **work being presented by F Lequien
17:45	<b>Poster Session and Wine Reception sponsored by Johnson Matthey</b> (all delegates cordially invited)   <b>Johnson Matthey</b>

19:00 (approx)	<b>Transfer by coach from Edgbaston Campus to Selly Oak Campus</b>
20.00	<b>Dinner – Manor House (tickets only)</b>

**Tuesday 4th September 2007**

<b>0845 (approx)</b>	<b>Transfer by coach from Selly Oak Campus to Edgbaston Campus</b>
<b>Session 2</b>	<b>Electronic, optical and magnetic properties of nanoalloys</b>
	Session Chair: Riccardo Ferrando, <i>University of Genoa, Italy</i>
<b>09.30 Paper 8</b>	<b>Optical properties and relaxation processes at femtosecond scale of bimetallic clusters</b> Michel Broyer*, E Cottancin, J Lermé, M Pellarin, N Del Fatti, F Valleé, J Burgin, C Guillon and P Langot, <i>Université Claude Bernard, Lyon 1, France</i>
<b>Paper 9</b>	<b>Stability and dissociation pathways of doped Au<sub>n</sub>X clusters (X = Nb, Er, Y)</b> Nele Veldeman**, Ewald Janssens*, Klavs Hanssen, Jorg De Haeck, Roger E Silverans and Peter Lievens, <i>KU Leuven, Belgium</i> **work being presented by Nele Veldeman
<b>Paper 10</b>	<b>Laser synthesis of bimetallic nanolloys in the vapor and liquid phases and the magnetic properties of PdM and PtM nanoparticles (M = Fe, Co and Ni)</b> Victor Abdelsayed, Gary Glaspell, Minh Nguyen, James M Howe and M Samy El-Shall*, <i>Virginia Commonwealth University, USA</i>
<b>11:00</b>	<b>Morning Coffee</b>
<b>11.30 Paper 11</b>	<b>Magnetic properties of Co<sub>N</sub>Rh<sub>M</sub> nanoparticles: experiment and theory</b> M Munoz-Navia*, J Dorantes-Dávila, D Zitoun, C Amiens, B Chaudret, M-J Casanove, P Lecante, N Jaouen, A Rogalev, M Respaud and G M Pastor**, <i>Universidad Autonoma de San Luis Potosí, Mexico</i> **work being presented by G M Pastor
<b>Paper 12</b>	<b>Structure and chemical ordering in CoPt nanoalloys</b> G Rossi, R Ferrando and C Mottet*, <i>CRM-CNRS, Marseille, France</i>
<b>12.30</b>	<b>Close of Session and Lunch/Poster Session</b> (All delegates invited)
<b>Session 3</b>	<b>Nanoalloys in catalysis</b>
	Session Chair: Claude Henry, <i>CRM-CNRS, Marseille, France</i>
<b>14:00 Paper 13</b>	<b>Direct synthesis of hydrogen peroxide from H<sub>2</sub> and O<sub>2</sub> using supported Au-Pd catalysts</b> Jennifer K Edwards, Albert F Carley, Andrew A Herzing, Christopher J Kiely and Graham J Hutchings*, <i>Cardiff University, UK</i>
<b>Paper 14</b>	<b>Structures and associated catalytic properties of well-defined nanoparticles produced by laser vaporisation of alloy rods</b> Valérie Caps**, Sandrine Arrii, Franck Morfin, Gérard Bergeret and Jean-Luc Rousset*, <i>Institut de Recherches sur la Catalyse et l'Environnement de Lyon, IRCELYON, Villeurbanne, France</i> **work being presented by Valérie Caps
<b>Paper 15</b>	<b>In situ investigation of Pt<sub>100-x</sub>-Au<sub>x</sub> and Pt<sub>100-y</sub>-Sn<sub>y</sub> nanoalloys</b> Ken A Grant, Kelei M Keryou and Paul A Sermon*, <i>University of Surrey, UK</i>

15:30	<b>Afternoon Tea</b>
16:00 <b>Paper 16</b>	<b>To alloy or not to alloy? Cr modified Pt/C cathode catalysts for PEM fuel cells.</b> Peter Wells, Yangdong Quian, Colin R King, Richard J K Wiltshire, Eleanor M Crabb, Lesley E. Smart, David Thompsett and Andrea E Russell*, <i>University of Southampton, UK</i>
<b>Paper 17</b>	<b>Structure-performance relationships of Rh and RhPd alloy supported catalysts using combined EDE/DRIFTS/MS</b> Moniek Tromp*, Andy J Dent, John Evans, Steven G Fiddy, Bhadrat Jyoti and Mark A Newton, <i>University of Southampton, UK</i>
<b>Paper 18</b>	<b>Synthesis, characterization, electronic structure and catalytic performance of bimetallic and trimetallic nanoparticles containing tin</b> John Meurig Thomas*, Richard D Adams, Erin M Boswell, Burjor Captain, Henrik Gronbeck and Robert Raja, <i>University of Cambridge, UK</i>
17:30	<b>Close of sessions</b>
17:40 (approx)	<b>Transfer between Edgbaston Campus and Selly Oak Campus</b>
19:00	<b>Pre-Dinner Drinks – Manor House (tickets only)</b>
20:00	<b>Conference Dinner – Manor House (tickets only)</b>

### Wednesday 5<sup>th</sup> September 2007

08:30 (approx) **Transfer between Selly Oak Campus and Edgbaston Campus**

<b>Session 4</b>	<b>Structural studies of nanoalloys</b>
	Session Chair: Peter Lievens, <i>KU Leuven, Belgium</i>
09:00 <b>Paper 19</b>	<b>Energy dispersive X-ray spectroscopy of bimetallic nanoparticles in an aberration corrected scanning transmission electron microscope</b> Andrew A Herzing, Masashi Watanabe, Jennifer K Edwards, Marco Conte, Zi-Rong Tang, Graham J Hutchings and Christopher J Kiely*, <i>Lehigh University, USA</i>
<b>Paper 20</b>	<b>Highly size-controlled synthesis of Au/Pd nanoparticles by inert-gas condensation</b> E Pérez-Tijerina*, M Gracia Pinilla, S Mejía-Rosales, U Ortiz-Méndez, A Torres and M José-Yacamán, <i>University of Texas at Austin, USA</i>
<b>Paper 21</b>	<b>Structures and optical properties of 4-5nm bimetallic Ag-Au nanoparticles</b> Ziyu Li*, Jess P Wilcoxon, Feng Yin, Yu Chen, Richard E Palmer and Roy L Johnston, <i>University of Birmingham, UK</i>
<b>Paper 22</b>	<b>Growth and structural properties of CuAg and CoPt bimetallic nanoparticles</b> Cyril Langlois*, Damien Alloyeau, Yann Le Bouar, Annick Loiseau, Tetsuo Oikawa, Christine Mottet and Christian Ricolleau, <i>University Paris 7, France</i>
11:00	<b>Morning Coffee</b>

11:30 <b>Paper 23</b>	<b>Controlling the density and size distribution of Pd-Au nanoparticles on TiO<sub>2</sub>(110)</b> Patrick Han and D Wayne Goodman*, <i>Texas A&amp;M University, College Station, USA</i> <b>WITHDRAWN</b>
<b>Paper 24</b>	<b>Binding energy and preferred adsorption sites of CO on gold and silver-gold cluster cations: adsorption kinetics and quantum chemical calculations</b> Marco Neumaier, Florian Weigend, Oliver Hampe* and Manfred M Kappes, <i>Karlsruhe Institute of Technology, Germany</i>
<b>Paper 25</b>	<b>Preparation of regular arrays of bimetallic clusters with independent control of size and chemical composition</b> M Marsault, G Hamm, A Wörz, G Sitja, C Barth and C R Henry*, <i>CMCN-CNRS, Marseille, France</i>
12:45 <b>Paper 26</b>	<b>Concluding Remarks</b> Brian Johnson, <i>University of Cambridge, UK</i>
13:15	<b>Acknowledgements</b>
13:30	<b>Close of Meeting and lunch</b> (tickets only)