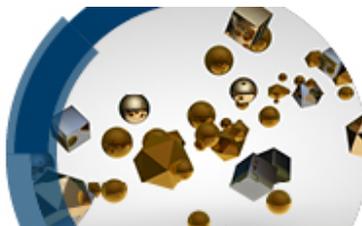




Wednesday 21 September 2022

11:00	Registration, tea and coffee
11:45	Lunch
12:45	Welcome and introductions Ewald Janssens, Chair of the Scientific Committee
12:55	Outline of Discussion format <i>Royal Society of Chemistry Publishing Editors</i>
13:00	Introductory Lecture (Session Chairs: Riccardo Ferrando and Ewald Janssens) Miguel Jose Yacaman <i>Northern Arizona University, United States</i>
14:00	Break
14:15	Session 1: Nanoalloy structures 1 (Session Chairs: Ewald Janssens and Riccardo Ferrando)
14:15	On the mechanical response in nanoalloys: the case of NiCo Marcelo M. Mariscal <i>University of Córdoba, Argentina</i>
14:20	Combined atomistic simulations to explore metastability and substrate effects in Ag–Co nanoalloy systems Georg Daniel Förster <i>ICMN UMR 7374, Université d'Orléans, France</i>
14:25	Interplay between interdiffusion and shape transformations in nanoalloys evolving from core-shell to intermixed structures Diana Nelli <i>University of Genoa, Italy</i>
14:30	Discussion
15:45	Break
16:15	Session 2: Nanoalloy catalysis 1 (Session Chairs: Francesca Baletto and Pascal Andreatza)
16:15	Oxidative dehydrogenation of cyclohexene on atomically precise subnanometer Cu_{4-n}Pd_n (0 ≤ n ≤ 4) tetramer clusters: the effect of cluster composition and support on performance Štefan Vajda <i>J. Heyrovský Institute of Physical Chemistry, The Czech Academy of Sciences, Czech Republic</i>
16:20	Doped metal clusters as bimetallic AuCo nanocatalysts: insights into structural dynamics and correlation with catalytic activity by <i>in situ</i> spectroscopy Noelia Barrabés <i>TU Wien, Austria</i>
16:25	Discussion
17:15	Invited lightning presentations
17:30	Poster session and wine reception
19:30	Close of sessions



Thursday 22 September 2022

09:00	Session 1 Contd: Nanoalloy structures 2 (Session Chairs: Catherine Amiens and Francesca Baletto)
09:00	Synthesis and structural properties of high-entropy nanoalloys made by physical and chemical routes Damien Alloyeau <i>MPQ Lab. - Univ. of Paris, France</i>
09:05	Melting properties of Ag_xPt_{1-x} nanoparticles Alexis Front <i>CINaM - AMU/CNRS, France</i>
09:10	Mixed-metal nanoparticles: phase transitions and diffusion in Au–VO clusters Wolfgang E. Ernst <i>Graz University of Technology, Austria</i>
09:15	Discussion
10:30	Break
11:00	Session 2 Contd: Nanoalloy catalysis 2 (Session Chairs: Jaysen Nelayah and Christine Mottet)
11:00	Oxidation and de-alloying of PtMn particle models: a computational investigation Alessandro Fortunelli <i>CNR-ICCOM, Istituto di Chimica dei Composti Organometallici, Italy</i>
11:05	Methanol synthesis from CO₂ and H₂ using supported Pd alloy catalysts Graham Hutchings <i>Cardiff University, UK</i>
11:10	Discussion



12:00	Lunch
13:00	Session 3: Magnetic and optical properties of nanoalloys 1 (Session Chairs: Jeffrey Shield and Riccardo Ferrando)
13:00	Joint electric and magnetic beam deflection experiments and quantum chemical studies of $M\text{Sn}_{12}$ clusters ($M = \text{Al, Ga, In}$): on the interplay of geometric structure and magnetic properties in nanoalloys Rolf Schäfer <i>TU Darmstadt, Germany</i>
13:05	Tuning the degree of CO_2 activation by carbon doping Cu_n ($n=3-10$) clusters: an IR spectroscopic study Joost M. Bakker <i>Radboud University, the Netherlands</i>
13:10	Radiative cooling in silver and palladium doped gold clusters Piero Ferrari <i>KU Leuven, Belgium</i>
13:15	Discussion
14:30	Break
14:45	Session 4: Applications of nanoalloys (Session Chairs: Christine Mottet and Riccardo Ferrando)
14:45	Structural evolution under physical and chemical stimuli of metastable Au-Fe nanoalloys obtained by laser ablation in liquid Vincenzo Amendola <i>University of Padova, Italy</i>
14:50	Disproportional surface segregation in ligand-free gold–silver alloy solid nanoparticles solution, and its implication for catalysis and biomedicine Stephan Barcikowski <i>Technische Chemie I, University of Duisburg-Essen, Germany</i>
14:55	Discussion
15:45	Break
16:00	Session 1 Contd: Nanoalloy structures 3 (Session Chairs: Pascal Andreazza and Francesca Baletto)
16:00	Structural characterisation of nanoalloys for (photo)catalytic applications with the Sapphire library Robert Jones <i>King's College London</i>
16:05	<i>In situ</i> study of the evolution of NiFe nanocatalysts in reductive and oxidative environments upon thermal treatments Catherine Amiens <i>CNRS, France</i>
16:10	Cu segregation in Au-Cu nanoparticles exposed to hydrogen atmospheric pressure: how is fcc symmetry maintained? Hazar Guesmi <i>CNRS-ICGM-Montpellier, France</i>
16:15	Discussion
17:30	Close of sessions
18:30	Pre-dinner drinks
19:00	Conference dinner



Friday 23 September 2022

09:00	Session 2 Contd: Nanoalloy catalysis 3 (Session Chairs: John McGrady and Christine Mottet)
09:00	Isoprene selective hydrogenation using AgCu-promoted Pd nanoalloys Daojian Cheng <i>Beijing University of Chemical Technology, China</i>
09:05	Density functional theory based computational investigations on the stability of highly active trimetallic PtPdCu nanoalloys for electrochemical oxygen reduction Lichang Wang <i>Southern Illinois University, USA</i>
09:10	The role of the gold-platinum interface in the AuPt/TiO₂-catalyzed plasmon-induced reduction of CO₂ with water Valérie Caps <i>CNRS (ICPEES, UMR 7515, Université de Strasbourg), France</i>
09:15	Discussion
10:30	Break
11:00	Session 3 Contd: Magnetic and optical properties of nanoalloys 2 (Session Chairs: Hans-Christian Weissker and Pascal Andreatza)
11:00	Characterization of Pt-doping effects on nanoparticle emission: a theoretical look at Au₂₄Pt(SH)₁₈ and Au₂₄Pt(C₃H₇)₁₈ Christine Aikens <i>Kansas State University, USA</i>
11:05	Structural and optical characterization of nanoalloys mixing gold or silver with aluminium or indium: evolution under various reactive environments Emmanuel Cottancin <i>University Claude Bernard Lyon 1, France</i>
11:10	Plasmon-driven methanol oxidation on PtAg nanoalloys prepared by improved pulsed laser deposition Junpeng Wang <i>Northwestern Polytechnical University, China</i>
11:15	Discussion
12:30	Break
12:45	Concluding Remarks Lecture (Session Chairs: Ewald Janssens and Riccardo Ferrando) Florent Calvo <i>University Joseph Fourier - Grenoble 1, France</i>
13:25	Presentation of poster prizes and acknowledgements Ewald Janssens, <i>Chair of the Scientific Committee</i>
13:30	Close of meeting and lunch