

ALLEGATO A

UNIVERSITÀ DEGLI STUDI DI MILANO

Procedura di valutazione per la chiamata a professore di I fascia da ricoprire ai sensi dell'art. 24, comma 6, della Legge n. 240/2010 per il settore concorsuale _02/B2 - FISICA TEORICA DELLA MATERIA___ ,
(settore scientifico-disciplinare FIS/03 - FISICA DELLA MATERIA___)
presso il Dipartimento di _____FISICA_____, Codice concorso __5353_

Francesca BALETTO CURRICULUM VITAE

INFORMAZIONI PERSONALI (NON INSERIRE INDIRIZZO PRIVATO E TELEFONO FISSO O CELLULARE)

COGNOME	BALETTO
NOME	FRANCESCA
DATA DI NASCITA	3 MAGGIO 1975

TITOLI

TITOLO DI STUDIO

(indicare la Laurea conseguita inserendo titolo, Ateneo, data di conseguimento, ecc.)

10 Feb. 1999 Master in Physics, Physics Department, University of Genova, Italy,
110/110 cum Laude
Thesis: "Molecular Dynamics Simulations of surface diffusion and growth of metallic clusters" (in Italian, "Simulazioni di Dinamica Molecolare di Diffusione Superficiale e Crescita su Cluster Metallici"), supervisor prof. R. Ferrando

TITOLO DI DOTTORE DI RICERCA O EQUIVALENTI, OVVERO, PER I SETTORI INTERESSATI, DEL DIPLOMA DI SPECIALIZZAZIONE MEDICA O EQUIVALENTE, CONSEGUITO IN ITALIA O ALL'ESTERO

(inserire titolo, ente, data di conseguimento, ecc.)

5 Jun. 2003 PhD in Physics, Physics Department, University of Genova, Italy,
Thesis: "Energetics, Thermodynamics and Growth Kinetics of Nanoclusters", supervisor R. Ferrando

ALTRI TITOLI CONSEGUITI

(inserire titolo, ente, data di conseguimento, ecc.)

May 2023 - today Elected group spokesperson/leader of the WG- B1, Multiscale and Reduced-Scaling Methods, of the Psi-K (www.psi-k.net)

30/01/2023 ASN a prima fascia BANDO D.D. 553/2021 SETTORE CONCORSUALE 02/B2 FISICA TEORICA DELLA MATERIA

Giudizio complessivo (estratto): La candidata è valutata positivamente con riferimento al titolo 1 dell'Allegato A al D.M. 120/2016 poiché raggiunge 2 su 3 valori soglia dal D.M. 589/2018. Complessivamente le pubblicazioni presentate possono essere ritenute di qualità elevata in relazione al settore concorsuale e alla fascia per la quale è stata richiesta l'abilitazione. Per le motivazioni di cui sopra, dopo analitico esame dei titoli e delle pubblicazioni ex art. 7 D.M. 120/2016, la commissione all'unanimità ritiene che la candidata possieda la maturità scientifica richiesta per le funzioni di professore di I fascia.

Sept. 2021 - today Visiting Professor at Physics Department, King's College London
Honour agreed to accomplish research related to the CPLAS network of which I am part of.

Jan. 2021 - Dec. 2021 Elected Treasurer for the Theoretical Chemistry Group of the Royal Society of Chemistry (RSC)

Oct. 2020-July 2021 Visiting Professor at Donosti International Physics Center (DIPC), San Sebastian, Spain [such activity took place during my sabbatical year. Part of it was at the University of Pais Vasco UPV/EHU]

Oct. 2018 - Member of the London Centre of Nanotechnology (London, UK)

Sept. 2018 - Aug. 2021 Promoted Reader in Physics, Physics Department, King's College London, UK

Jan. 2017 - Dec. 2021 Elected Member of the Theoretical Chemistry Group of the Royal Society of Chemistry (RSC)

Oct. 2016 - today Member of the Institute of Physics (UK) [the IoP membership undergoes to an evaluation of a dedicated panel. It comes with a certificate]

Oct. 2016 - Member of the MMM-Hub (funded by a EPSRC grant, EP/P020194/1)

11/12/2013: ASN a seconda fascia Bando 2012 (DD n. 222/2012) SETTORE CONCORSUALE 02/B2 FISICA TEORICA DELLA MATERIA

Apr. 2013 - Aug. 2018 Promoted at Senior Lecturer in Physics, Physics Department, King's College London, UK

Dec. 2009 - Apr. 2013 "confirmed" Lecturship in Physics, Physics Department, King's College London, UK

Sept. 2007 - today Member of the Thomas Young Center (London)

Aug. 2007 - Dec. 2009 Lecturer in Physics, Physics Department, King's College London, UK

May 2006 - July 2007 Research Assistant at Dept. Of Materials Science, MIT, USA

Sept. 2000: National Qualification as High School Teacher (classe di concorso Fisica)

Apr. 1999 - Feb. 2000 INFN research student at the Physics Department, Univ. of Genova, Italy

ATTIVITÀ DIDATTICA

INSEGNAMENTI E MODULI

(inserire anno accademico, corso laurea, numero di ore frontali, eventuale CFU)

As my academic activity was for 14 years at the Physics Department, King's College London (London, UK) and only two years at the Physics Department, Aldo Pontremoli, Università di Milano, I present in all the section my activity separated in two sections related to my activities in each institution. As the UK and the Italian systems present major differences I will illustrate briefly how to interpret them. A 1-to-1 correspondence does not exist.

Any promotion and yearly-appraisal at King's College London (KCL) is done over teaching, admin, and research activities.

UNIVERSITA' di MILANO

2021/22 and 2022/23 "Physics of nanoparticles", MSc in Physics (LM-17), 42 hours, 6 CFU

2022/23 "Meccanica", BSc in Physics (LT-30), 36 hours, 8 CFU

2022/23 "BioNanoTechnology", MSc in Chemical Science (LM-54), 48 hours, 6 CFU

KING'S COLLEGE LONDON

The number of frontal hours are set to 30 per each module. Usually each academic should teach a maximum of one or two modules, expect specific figures that are hired only for teaching purposes.

Teaching at UG level: Since I began at King's College, I have taught three modules:

AY 2007/08 - 2010/11 "Introduction to Solid State (6CCP3402)", 30 frontal hours, 3rd Year module [15 CFU] mandatory for all Physics programmes

[changed because of my first maternity leave between Oct. 2011 and Jan. 2012]

AY 2008/09 - 2010/11 3rd Year Literature Review (6CCP3132) on "Hydrogen economy: hype or hope?", 30 frontal hours and deserving 15 CFU

AY 2019/20 7CCP4100/7CCP4000 "Research Project in Physics", Organiser and Manager, 4 frontal hours.

AY 2012/13 - 2019/20 "Computational Laboratory (5CCP211C)", a 30 frontal hours, 2nd Year module [15 CFU] for BSc/MSci programmes in "Physics", "Physics with Theoretical Physics" and "Physics with Medical Applications" programme.

[I did not teach during the academic year 2013/14 because of my second maternity leave followed by a period of 4 months as part-time]

AY 2012/13 - 2019/20 "Computational Laboratory" 30 frontal hours, 1st Year module as part of the Math and Computational module [30 CFU], mandatory for all BSc/MSci programmes.

Teaching activities in other insitution

Tutor of Physics to undergraduate students at Dip. di Fisica, Univ. di Genova, Spring 2001 (contract E40);

- Tutor of Calculus to undergraduate students at Dip. di Fisica, Univ. di Genova, Fall 2001 (contract E40);

- Teaching Assistant of "Introduction to Numerical Method" for Condensed Matter Diploma Course, at ICTP-Trieste (Italy), on Fall 2005;

- Lesson on 'Environmental Physics: the ozone depletion', to the students' 'Master in Science Communication' at SISSA/ILAS-Trieste (Italy), on March 2006

ATTIVITÀ DI DIDATTICA INTEGRATIVA E DI SERVIZIO AGLI STUDENTI

ATTIVITÀ DI RELATORE DI ELABORATI DI LAUREA, DI TESI DI LAUREA MAGISTRALE, DI TESI DI DOTTORATO E DI TESI DI SPECIALIZZAZIONE

(inserire anno accademico, ateneo, corso laurea, ecc.)

UNIVERSITA' di MILANO

Supervision of Research Assistant (RA)

Post Doctoral Research Assistant (Assegno A), Dr. Mirko Vanzan, Univ. of Milan, 01 Jan. 2023

Supervision of tesi di laurea

Laurea Triennale AA 2020/21 student Igor Vasiljevic, "Automated characterisation of the surface of metallic nanoparticles", LT-30

Laurea Magistrale AA 2021/22 student Sofia Zinzani, "Simulations of coalescence of Au-Pd nanoalloys in either vacuum or implicit environments", LM-17

Altri due studenti magistrali stanno attualmente svolgendo la tesi di laurea presso il mio gruppo

Mr. Giacomo Beccatti - to be defended Nov-Dec 2023

Mr. Davide Alimonti - to be defended Nov-Dec 2023

KING'S COLLEGE LONDON

In the UK system, the "tesi di laurea" e "laurea magistrale" do not exist. However, each academic might apply for specific scheme to set up research projects dedicated to undergrad students. Such project at the King's Colelge London, are named KURF. Each academic can apply to get one project per year. KURF give undergraduate students the unique opportunity to learn alongside our leading

academics during the summer. I believe they are the best match as a “Laurea” work. Please keep in mind they are limited in numbers but they come with their own research funding. Similarly to the tesi of laurea magistrale, I taught the Research Project 7CCP4100/7CCP4000

Supervision of Research Assistant (RA)

Post Doctoral Research Assistant, Dr. Vagner Rigo, KCL, 24 June 2016 - June 2017

Post Doctoral Research Assistant, Dr. GianGiacomo Asara, 7 Jan. 2015 - 4 Sept. 2016, and Nov. 2017 - 2018

Post Doctoral Research Assistant, Dr. Oliver Paz-Borbon, 1 July 2013 - 30 Oct. 2014

Post Doctoral Research Assistant, Dr. Cono Di Paola, 1 Sept. 2009 - 31 Aug 2012

Supervision of PhD student

PhD Dr. Robert M. Jones since Apr. 2019, defence on Feb. 2023

PhD Wei Zhao started in Oct. 2019 position on hold after my change of institution

PhD Laio Delgado started in Oct. 2017, defended in Jan 2022 under the supervision of Dr. K. Evgeny due to my change of institution

PhD Dr Kevin Rossi, since Sept. 2015, defence Nov. 2017

PhD Dr. Luca Pavan since April 2011, defence on 8 June 2015,

PhD Dr James Finn, since Oct. 2007, defence on 27 Sept. 2011,

I hosted the long visit of a UNAM student, Dr. Lopez-Estrada (currently RA at UNAM), in Feb-Mar. 2016, supported by a CONACyT "Movilidad en el Extranjero" and a Thomas Young Centre Junior Fellowship PhD Student

MSci/MSc project winning a prize as best project

AY 2008/09 Irina Parsina on “Growth of cobalt nanoalloys”, Wheatstone prize, given for the best M.Sci. project in the department. Led to two publications in international referred journals [Parsina and FB, JPCC (2010), Parsina, di Paola and FB, Nanoscale (2012)];

AY 2011/12 Laura Bazeley on “Growth of platinum nickel nanoparticles”. Laura won the Wheatstone prize, given for the best M.Sci. project, and was nominated for a Layton prize to complete her research project in my group before starting her M.Sc. in Environmental Science at Birbeck College

AY 2019/20 Elena Gazzarrini on “Born to be different: Cu-formation affects the conversion of CO₂ into CH₄”. Elena won the Wheatstone prize, given for the best M.Sci. project

Supervision of MSc/MSci projects

AY 2009/10 Vishal Purohit, on “Exploring the free-energy surface of nanoparticles: Metadynamics for the study of binary LJ clusters”

AY 2010/11 Alvin Got on “Metadynamics for the study of metallic nanoparticles”

AY 2011/12 Shakeel Khan on “Molecular Dynamics simulations of PtNi cluster on MgO substrate”

AY 2012/13 Myo Zaw Hein on “Jellium model study of surface plasmon resonance in Ag nanoparticles”

AY 2014/15 Tom Ellaby on “Thermal Properties of Supported Platinum Nanoclusters”

AY 2016/17 Norbert Zicher “Elucidating the Cluster-Surface Interactions”

AY 2017/18 David Schmidt on “A kinetic Monte Carlo scheme for modelling ORR on Pt-nanoparticles”

AY 2017/18 Raphael Pinto-Miles on “Post-processing on the real-space to detect thermal properties of nanoclusters”

AY 2018/19 (MSc thesis 7CCPIX10) Moerkved, Henrik “Green reduction on supported metallic nanoclusters - Exploring CO₂ reduction on Cu clusters”

AY 2019/20 Matteo Tiberi on “Modelling Gold-assembled nanowires”

AY 2019/20 Armand Aquier on “Unsupervised Machine Learning to categorize nanoparticles”

AY 2019/20 Lorenzo Espinosa-Brown Adv Literature project on “Characterising Nano-assembled Au Films”

Equivalent to a Laurea Triennale - KURF/Departmental fellowships Since Spring/Summer 2015

AY 2014/15 Norbert Zicher on “Modelling supported nanoparticles”

AY 2015/16 David Schimdt on “Kinetic Montecarlo code for nanocatalysts”

AY 2015/2016 Zac Shabka on “Implementation of vibrational properties in the LoDiS package”

AY 2015/16 Man Hou on “A new post-processing implementation for the LoDiS software” (departmental fellowship)

AY 2015/16 Mohammad Abedi on “Implementing a coalescence method in LoDiS” (not paid)

AY 2017/18 Jacopo Mascitelli (departmental fellowship) on “Nanoparticle site characterisation”

AY 2017/18 Kumar Pankaj on "Classification of nanostructures using supervised learning"
 AY 2017/18 Pascal Salzbrenner on "Melting properties of nanoparticles"
 AY 2018/19 Paul Guhenec on "Calculating pressure maps in nanoparticles"
 AY 2018/19 Russell Brooks on "Catalytic nanoparticles properties"
 AY 2019/20 Ben Jakobs on "Nanoassembly into nanowires and nanofilms"

KCL Summer internships

AY 2020/21 Antonio De Marti on "Aggregation of nanoparticles into a 3D nanofoam"

AY 2014/15, I sponsored the visit of a Malaysian MSc student, YeeYeen Soon, supported by a prestigious "MyBrain scholarship" by the Malaysian Government on the project "Modelling metallic nanoparticles".

Co-supervisions at other academic institutions

Co-supervisor (with prof. N. Marzari) of RSI thesis of K. Niemkiewicz, at Dept. of Materials Science and Engineering, MIT, USA, defence on 01/08/2006

May-July 2004 and April-July 2005 Supervisor of STEP-PhD student U.T. Ndongmouo, at ICTP

2003/04 - Co-supervisor (with prof. S. Scandolo) of Diploma Thesis of Mr M. Bakr, at ICTP, Trieste, defense on 26/08/2004.

Co-supervisor (with Prof. R. Ferrando) of Master Degree of G. Rossi at Physics Dept., Univ. di Genova, on "Global Optimization of bimetallic nanoclusters", defense on 04/06/2003.

ATTIVITÀ DI TUTORATO DEGLI STUDENTI DI CORSI DI LAUREA E DI LAUREA MAGISTRALE E DI TUTORATO DI DOTTORANDI DI RICERCA

(inserire anno accademico, corso laurea, ecc.)

Tutoring activities at the Physics Department, King's College London (KCL)

2016 - 2020 Career Tutor at KCL

As Careers tutor, I organise a few events for both UG (undergrad refers to both BSc and MSci students) and PG (postgrad refers to MSc and PhD) students, including a new career fair for Physics with the help of KCC; a teaching career day in collaboration with the Institute of Physics (Jan 2017 and 2018); promotion of internships among UG students.

2016 - 2020 Female Student Tutor for all the female cohort at UG, MSc, PhD

2014 - 2020 member of the Dept. Equality & Diversity committee (DEDC)

As Female tutor and DEDC member, on top of standard pastoral service, I played a substantial role in the recent departmental Juno Champion application.

2011 - 2016 Chair of the Physics Assessment Board; Member of the Faculty Assessment Board

Requiring the highest responsibility of all departmental, administrative jobs (as the function affects directly every student in the short as well as long term) I put in a lot of effort as Chair of the Physics Assessment board, above the standard requirements of knowing academic regulations and liaising with various College offices. I personally (a) checked that every student was treated fairly at each stage; (b) coordinated the approval of mitigating circumstances; (c) created a platform to monitor students' performance, e.g. year-by-year progression list, making it available to all staff; (d) coordinated exam preparation and marking procedures; (e) defined rescaling criteria for outlying module marks; (f) worked to get a robust mark translation for year abroad programmes; (g) liaised with internal and external examiners, who always appreciated the quality and the organization of each Programme Board meeting. I did the academic and most of the bureaucratic work alone, especially when the Physics UG office was severely understaffed (June 2015). My efforts were recognised by an excellence award.

2012 - 16 Member of the Dept. Education Committee (DEC)

For the DEC, I worked in the sub-committee for establishing a new programme in bio-physics.

2018 - 2020 Member of the Dept. Strategy Educational Committee

We were in charge of setting the teaching strategy over a longer timescale. Managing and setting the starting of the Covid-period (March - July 2020). Weekly meeting.

Feb 2021 Msc Invited Lecture on "Introduction to atomistic simulations", Univ. of Navarra

May 2004- Jan. 2005 Tutor in “Car-Parrinello Molecular Dynamics”, in Quantum-Espresso Schools, at ICTP, Trieste (Italy)

Autumun 2005 Teaching Assistant of “Introduction to Numerical Method” for Condensed Matter Diploma Course, at ICTP-Trieste (Italy)

March 2006 Lesson on “Environmental Physics: the ozone depletion”, to the students’ ‘Master in Science Communication’ at SISSA/ILAS-Trieste (Italy)

Jan 2007 IAP lecturer on “Hydrogen economy: hype or hope?”, to IAP program at MIT (USA)

SEMINARI

(inserire titolo del seminario, luogo, data, ecc.)

Seminar at academic insitutions

Seminar at Univ. of Lancaster (Lancaster, UK) “Nanoparticles in motion: structural changes and properties”, 1 Dec. 2021 (virtual)

Seminar (virtual) at TUM (Munich, Germany) “Born to be different: how structural changes of metallic nanoparticles affect their catalytic activity”, 3 May 2021

Seminar at DIPC (San Sebastian, Spain) (virtual) “Born to be different”, 26 March 2021

Seminar at “soire Semianr” at the TYC (London, UK) “How morphology influences electrocatalysis?”, 28 Jun 2019

Seminar at York univ. (York, UK) “A geometrical apporach to nanocatalysis” 18 Oct 2019

Seminar at Univ. of Swansea (Swansea, UK) “Geometry and chemo-physical properties at the nanoscale”, 13 July 2019

Seminar at CSC/WCPM (Warwick, UK), “Size & shape dependence of the activity of metallic nanoparticles”, 24 June 2019

Seminar at Univ. of Cardiff, “How shape changes alter chemo-physical properties od nanoparticles?”, 22 Oct. 2018

Seminar at CNRS-Univ. of Marseille (Marseille, France), “The importance of geometry to predicting properties of metallic nanoparticles”, 26 March 2018

Seminar at Univ. of Milano-Bicocca (Milan, Italy), “Design of nanocatalysts: hype or hope?”, 4 Apr. 2018

Seminar at TSCM, (KCL, London UK), “Nano is different”, 7 March 2017

Seminar at EPFL (Lausanne, Switzerlandd), “Being a nano-Valentino”, 7 Jun 2017

Seminar at Soton (Southampton, UK), “Spported Pt-nanoclusters: the importance of the interface”, April 2016

Seminar at NPRL (Birmingham, UK) “Towards a rational design of supported nanocatalysts”, 23 May 2016

Seminar at Univ. of Sao Paulo (Sao Paulo, Brazil) “Nanocatalysts: when morphologies and chemical ordering matter”, May 2015

Seminar at QMUL (London, UK), “Free and supported nanoalloys; form structures to applications”, 4 March 2015

Seminar at DIPC, “Unravelling morphologies and chemical ordering at the nanoscale”, 2 Jul 2014

Seminar at Oxford Univ. (Oxford, UK), “Magnetic and chemical ordering in transition metal nanoalloys”, 11 Feb 2011

Seminata t UPV/EHU (San Sebastian, Spian), “Water clusters in atmosphere” 22 May 2009

Seminar at Oxford Univ. (Oxford, UK), “Towards a nanosolution for environmental puzzles”, 5 June 2009

Seminar at Birmingham Univ. (Birmingham, UK), “Growth simulations of Co-nanoalloys”, 11 May 2009

Seminar at UCL (London, UK), “Water clusters in atmosphere”, 20 Oct. 2008

Seminar at Univ. of Leicester (Leicester, UK), “Modelling the kinetics of Nano-particles”, on 3 Dec. 2008

Seminar at Thomas Young Center TYC (London, UK) “Modelling nanomaterials for environmetal purposes”, 2008

Seminar at King’s College London (Londin, UK), “Modelling nanomaterials for energy and the environment”, 16 Apr. 2007

Seminar at Univ. of NewHampshire (Durham, USA) “Addressing Environmental Challenges with Numerical Simulation ” 15 Feb 2007

Seminar at ICTP (Trieste, Italy), ICTP-Democritos Physics-Chemistry Seminars, “Where are the electrons in the sky?”, on 1 December 2004.

Seminar at ICTP (Trieste, Italy), ICTP-Democritos Physics-Chemistry Seminars, “Energetics, Ther-modynamics and Growth Kinetics of nanonclusters”, on 5 September 2003.

Seminar at Princeton University (Princeton, USA) invited by prof. G. Scoles, "Morphology transitions in the growth of free silver nanoclusters" on 18 October 2000.
Seminar at Helsinki University of Technology (Helsinki, Finland) invited by prof. T. Ala-Nissila, "Morphological Transitions during Growth of Silver and Gold Nanoclusters", 19 October 1999.
Seminar at CRMC2/CNRS Marseille (Marseille, France) invited by prof. G. Treglia, "Surface Diffusion and Growth on Silver and Gold Clusters", 20 April 1999

ATTIVITÀ DI RICERCA SCIENTIFICA

PUBBLICAZIONI SCIENTIFICHE

(per ciascuna pubblicazione indicare: nomi degli autori, titolo completo, casa editrice, data e luogo di pubblicazione, codice ISBN, ISSN, DOI o altro equivalente)

In short, I publish over 70 peer-reviewed publications, h-index 30 from Google Scholar (i10-index 51). Number of citations taken from Google scholar on 25 July 2023 are reported.

My reference ID numbers are:

ResearcherID: Q-2136-2017

ORCID: 0000-0003-1650-0010

<https://scholar.google.com/citations?user=zx1ZR2wAAAAJ&hl=it>

F. Martinez-Espinar, A. Salom-Català, E. Bresó-Femenia, C. Claver, **F. Baletto**, J M Ricart, B Chaudret, J. J Carbó, V Godard, S. Castillon

Bringing Selectivity in H/D Exchange Reactions Catalyzed by Metal Nanoparticles through Modulation of the Metal and the Ligand Shell

Source: Inorganic Chemistry Volume: 62 Issue: 11 Pages: 4570-4580 Published: MARCH 2023

DOI: <https://pubs.acs.org/doi/full/10.1021/acs.inorgchem.2c04442>

V. Rigo and **F. Baletto**

Pt 38 as a promising ethanol catalyst: a first principles study

Source: Phys Chem Chem Phys Volume: 26 Issue: 6 Pages: 4649-4655 Published: JAN 2023

DOI: <https://doi.org/10.1039/D2CP04323H>

R.M. Jones, K Rossi, C Zeni, M Vanzan, I Vasiljevic, A Santana-Bonilla, **F. Baletto**

Structural characterisation of nanoalloys for (photo)catalytic applications with the Sapphire library

Source: Faraday Discuss., Volume: 242, Pages: 326-352 Published JUNE 2022

DOI: [10.1039/D2FD00097K](https://doi.org/10.1039/D2FD00097K)

P Ferrari, L Delgado-Callico, OV Lushchikova, M Bejide, FJ Wensink, JM Bakker, **F Baletto**, E Janssens

Bonding Nature between Noble Gases and Small Gold Clusters

Source: J. Physical Chemistry Letters Volume: 13 Issue: 19 Pages: 4309-4314 Published: MAY 2022

Citation: 3

DOI: <https://doi.org/10.1021/acs.jpclett.2c00738>

M Vanzan, RM Jones, S. Corni, R D'Agosta, **F. Baletto**

Exploring aurh nanoalloys: a computational perspective on the formation and physical properties

Source: ChemPhysChem Volume: 23 Issue: 8 Pages: e202200035 Published APRIL 2022

DOI: <https://doi.org/10.1002/cphc.202200035>

W. Zhao, R.M. Jones, R. D'Agosta, **F. Baletto**

Making copper, silver and gold fullerene cages breathe

Source: J of Physics: Condensed Matter Volume: 34 Issue: 22 Pages: 224005 Published: 2022

Citation: 4

DOI: [10.1088/1361-648X/ac5b00](https://doi.org/10.1088/1361-648X/ac5b00)

RM Jones, R D'Agosta, **F Baletto**

The effects of Pt doping on the optical properties of Au20

Source: Eurpo. Physical Journal Applied Physics Volume: 97, Pages: 46 Published: August 2022

DOI: <https://doi.org/10.1051/epjap/2022220011>

JM Finn, **F Baletto**

A fluxional anionic water trimer

Source: Frontiers of Nanoscience Volume: 21, Pages: 43-70 Published: Jan 2022

Chap 3- volume Energy Landscapes of Nanoscale Systems Edited by David J. Wales, Elsevier

DOI: <https://doi.org/10.1016/B978-0-12-824406-7.00010-5>

C. Zeni, K Rossi, T Pavludis, J Kioseoglou, S de Gironcoli, RE Palmer, **F Baletto**

Data-driven simulation and characterisation of gold nanoparticle melting

Source: Nat. Comm. Volume: 12 Issue: 1 Pages: 6056 Published: OCT 2021

Citation: 22

DOI: <https://doi.org/10.1038/s41467-021-26199-7>

L Delgado-Callico, P Ferrari, JM Bakker, **F Baletto**, E Janssens

Benchmarking density functional theory methods for modelling cationic metal-argon complexes

Source: Theoretical Chemistry Accounts Volume: 140 Issue: 4 Pages: 38 Published APR 2021

Citation: 8

DOI: <https://doi.org/10.1007/s00214-021-02734-z>

P Ferrari, L Delgado-Callico, OV Lushchikova, GL Hou, F Baletto, J M Bakker, E Janssens

The size-dependent influence of palladium doping on the structures of cationic gold clusters

Source: Nanoscale advances Volume: 3 Issue: 21 Pages: 6197-6205 Published: SEPT 2021

Citation: 4

DOI: <https://doi.org/10.1039/D1NA00587A>

E Gazzarrini, K Rossi, **F Baletto**

Born to be different: The formation process of Cu nanoparticles tunes the size trend of the activity for CO 2 to CH 4 conversion

Source: Nanoscale Volume: 13 Issue: 11 Pages: 5857-5867 Published: FEB 2021

Citation: 11

DOI <https://doi.org/10.1039/D0NR07889A>

L Delgado-Callico, K Rossi, R Pinto-Miles, P Salzbrenner, **F Baletto**

A universal signature in the melting of metallic nanoparticles

Source: Nanoscale Volume: 13 Issue: 2 Pages: 1172-1180 Published: DEC 2020

Citation: 16

DOI: <https://doi.org/10.1039/D0NR06850K>

P Ferrari, L Delgado-Callico, P Lievens, **F Baletto**, E Janssens

Stability of cationic silver doped gold clusters and the subshell-closed electronic configuration of AgAu14+

Source: J Chemical Physics Volume: 153 Issue: 24 Pages: 24 Published: DEC 2020

Citation: 4

DOI: <https://doi.org/10.1063/5.0033487>

K Rossi, GG Asara, **F Baletto**

Structural screening and design of platinum nanosamples for oxygen reduction

Source: ACS Cat. Volume: 10 Issue: 6 Pages: 3911-3920 Published FEB 2020

Citation: 24

DOI: <https://pubs.acs.org/doi/abs/10.1021/acscatal.9b05202>

D Schmidt, GG Asara, **F Baletto**

A kinetic Monte Carlo-blueprint for oxygen reduction on oxide-supported PtNi nanoalloys

Source: J. Chemical Phys Volume: 152 Issue: 3 Pages 034107 Published: JAN 2020

Citation: 3

DOI <https://pubs.aip.org/aip/jcp/article-abstract/152/3/034107/198913>

F Baletto, C R Miranda, V A Rigo, K Rossi

Nanoalloys for energy applications

Book Chapter on invite

Chapter 9 - Nanoalloys for Energy Applications,

Editor(s): Florent Calvo, Nanoalloys (Second Edition),
Elsevier
ISBN 9780128198476,
Pages 347-380 **Published:** SEPT 2020
DOI: <https://doi.org/10.1016/B978-0-12-819847-6.00015-2>

O Lopez-Estrada, E Orgaz, **F Baletto**
Interdependence of shape and magnetic properties in Al-nanoparticles doped with Ni and Pt
Source: J Materials Chemistry C **Volume:** 8 **Issue** 7 **Pages** 2533-2541 **Published:** JAN 20220
Citation: 2
DOI <https://pubs.rsc.org/en/content/articlehtml/2020/tc/c9tc04013g>

K Rossi, GG Asara, **F Baletto**
Correlating Oxygen Reduction Reaction Activity and Structural Rearrangements in MgO-Supported Platinum Nanoparticles
Source: ChemPhysChem **Volume:** 20 **Issue:** 22 **Pages:** 3037-3044 **Published:** NOV 2019
Citation: 5
DOI: <https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/cphc.201900564>

VA Rigo, CR Miranda, **F Baletto**
Ethanol chemisorption on core-shell Pt-nanoparticles: an ab initio study
Source: The European Physical Journal B **Volume:** 92 **Pages:** 1-7 **Published:** FEB 2019
Citation 7
DOI: <https://link.springer.com/article/10.1140/epjb/e2018-90241-3>

F Baletto
Structural properties of sub-nanometer metallic clusters
Source: Journal of Physics: Condensed Matter **Volume:**31 **Issue:**11 **Pages:**113001 **Published** JAN 2019
Citation: 44
DOI: <https://iopscience.iop.org/article/10.1088/1361-648X/aaf989/meta>

F Baletto, RL Johnston
Editorial on “Shaping nano-catalysts”
Source: The European Physical Journal B **Volume:** 92 **Pages:** 1-2 **Published:** 2019
Citation 2
DOI: <https://link.springer.com/content/pdf/10.1140/epjb/e2019-100024-9.pdf>

C Zeni, K Rossi, A Glielmo, **F Baletto**
On machine learning force fields for metallic nanoparticles
Source: Advances in Physics: X **Volume:** 4 **Issue** 1 **Pages** 1654919 **Published:** JAN 2019
Citation 31
DOI <https://www.tandfonline.com/doi/abs/10.1080/23746149.2019.1654919>

K Rossi, GG Asara, **F Baletto**
A genomic characterisation of monometallic nanoparticles
Source: Phys Chem Chem Phys **Volume** 21 **Issue** 9, **Volume** 4888-4898 **Published** 2019
Citation 23
DOI <https://pubs.rsc.org/en/content/articlehtml/2019/cp/c8cp05720f>

C Zeni, K Rossi, A Glielmo, Á Fekete, N Gaston, **F Baletto**, A De Vita
Building machine learning force fields for nanoclusters
Source: J Chem Physics **Volume:** 148 **Issue** 24 **Pages** 241739 **Published** JUN 2018
Citation 51
DOI <https://doi.org/10.1063/1.5024558>

K Rossi, LB Pártay, G Csanyi, **F Baletto**
Thermodynamics of CuPt nanoalloys
Source: Scientific reports **Volume** 8 **Issue** 1 **Pages:** 9150 **Published:** JUN 2018

Citation 24

DOI <https://www.nature.com/articles/s41598-018-27308-1>

K Rossi, L Pavan, YY Soon, **F. Baletto**

The effect of size and composition on structural transitions in monometallic nanoparticles

Source: European Physical Journal B Volume: 91 Pages: 1-8 Published FEB 2018

Citation 20

DOI <https://link.springer.com/article/10.1140/epjb/e2017-80281-6>

D Schebarchov, **F Baletto**, DJ Wales

Structure, thermodynamics, and rearrangement mechanisms in gold clusters—insights from the energy landscapes framework

Source: Nanoscale Volume: 10 Issue 4 Pages: 2004-2016 Published 2018

Citation 40

DOI <https://pubs.rsc.org/en/content/articlehtml/2017/nr/c7nr07123j>

LO Paz-Borbón, **F Baletto**

A DFT Study on the O₂ Adsorption Properties of Supported PtNi Clusters

Source: Inorganics Volume 5 Issue 3 Pages 43 Published JUL 2017

Citation 17

DOI <https://www.mdpi.com/2304-6740/5/3/43>

DiPaola, C.; Pavan, L.; D'Agosta, R.; **Baletto, F.**;

Structural stability and uniformity of magnetic Pt 13 nanoparticles in NaY zeolite

Source: Nanoscale Volume: 9 Pages: 15658-15665 Published SEPT 2017

Citation: 10

DOI: <https://pubs.rsc.org/en/content/articlehtml/2017/nr/c7nr03533k>

K Rossi, T Ellaby, LO Paz-Borbon, I Atanasov, L Pavan, **F. Baletto**

Melting of large Pt@ MgO (100) icosahedra

Source: Journal of Physics-Condensed Matter Volume: 29 Issue: 14 Published: APR 2017

Citation: 18

DOI <https://iopscience.iop.org/article/10.1088/1361-648X/aa5a1d/meta>

Rossi, K.; **Baletto, F.**;

The effect of chemical ordering and lattice mismatch on structural transitions in phase segregating nanoalloys

Source: Phys Chem Chem Phys Volume: 19 Issue: 18 Pages: 11057-11063 Published: MAY 2017

Citation: 18

DOI <https://pubs.rsc.org/en/content/articlehtml/2017/cp/c7cp01397c>

DiPaola, C.; D'Agosta, R.; **Baletto, F.**;

Geometrical effects on the magnetic properties of nanoparticles

Source: Nano Letters Volume: 16 Issue: 4 Pages: 2885-2889 Published: APR 2016

Citation 46

DOI <https://pubs.acs.org/doi/abs/10.1021/acs.nanolett.6b00916>

Asara, G.G.; Paz-Borbon, L.O.; **Baletto, F.**;

'Get in Touch and Keep in Contact': Interface Effect on the Oxygen Reduction Reaction (ORR) Activity for Supported PtNi Nanoparticle

Source: ACS Catalysis Volume: 6 Issue: 7 Pages: 4388-4393 Published: JUL 2016

Citation: 38

DOI <https://pubs.acs.org/doi/abs/10.1021/acscatal.6b00259>

Gould, A.L; Rossi, K.; Catlow, C.R.A; **Baletto, F.**; Logsdail, A.J.;

Controlling Structural Transitions in AuAg Nanoparticles through Precise Compositional Design

Source: J Physical Chemistry Letters Volume: 7 Issue: 21 Pages: 4414-4419 Published: NOV 2016

Citation: 20

DOI <https://pubs.acs.org/doi/abs/10.1021/acs.jpcllett.6b02181>

Davis, J.B.A; **Baletto, F.**; Johnston, R. L.;
The Effect of Dispersion Correction on the Adsorption of CO on Metallic Nanoparticles
Source: Journal of Physical Chemistry a Volume: 119 Issue: 37 Pages: 9703-9709 Published: SEP 2015
Citation: 63
DOI <https://pubs.acs.org/doi/abs/10.1021/acs.jpca.5b05710>

L Pavan, K Rossi, **F Baletto**,
Metallic nanoparticles meet metadynamics
Source: J. Chem. Phys. Volume 143 Pages 184304 Published: 2015
Citation: 33
DOI: <https://pubs.aip.org/aip/jcp/article/143/18/184304/562725>

F Baletto, R Ferrando,
Doped golden fullerene cages
Source: PCCP Volume: 17 Pages 28256 Published: NOV 2015
Citation: 16
DOI <https://pubs.rsc.org/en/content/articlehtml/2015/cp/c5cp01061f>

L Pavan, **F Baletto**, R Novakovic,
Multiscale approach for studying melting transitions in CuPt nanoparticles,
Source: PCCP Volume: 17 Pages: 28364 Published: 2015
Citation 25
DOI <https://pubs.rsc.org/en/content/articlehtml/2015/cp/c5cp01096a>

C DiPaola, **F Baletto**,
Chemical order and magnetic properties in small Mx-2N2 nanoalloys,
Source: Eur. Phys. J D Volume: 67 Pages: 49 Published: 2013
Citation 16
DOI <https://link.springer.com/article/10.1140/epjd/e2013-30561-4>

L Pavan, C DiPaola, **F Baletto**,
Sampling the energy landscape of Pt13 with metadynamics,
Source: Eur. Phys. J D Volume 67 Pages: 24 Published: FEB 2013
Citation 20
DOI <https://link.springer.com/article/10.1140/epjd/e2012-30560-y>

F. Baletto
Modelling Janus nanoparticles
Book Chapter In: Metal Clusters and Nanoalloys. Nanostructure Science and Technology.
Springer, New York, NY.
Published May 2012
Print ISBN 978-1-4614-3267-8
Online ISBN 978-1-4614-3643-0
DOI https://doi.org/10.1007/978-1-4614-3643-0_8
Citation 8

I Parsina, C DiPaola, **F Baletto**,
A novel structural motif for free CoPt nanoalloys,
Source: Nanoscale Volume 4 Pages 1160 Published 2012
Citation 27
DOI <https://pubs.rsc.org/en/content/articlehtml/2012/nr/c1nr11171j>

C di Paola, **F Baletto**,
Oxygen adsorption on small PtNi nanoalloys,
Source: PCCP Volume 13 Pages 7701 Published 2011
Citation 46
DOI <https://pubs.rsc.org/en/content/articlehtml/2011/cp/c0cp01662d>

I Parsina, **F Baletto**,
Tailoring the structural motif of AgCo nanoalloys: core/shell versus Janus-like,
Source: J. Phys. Chem. C Volume 114 Pages 1504-1511 Published JAN 2010

Citation 106

DOI <https://pubs.acs.org/doi/abs/10.1021/jp909773x>

SK Bhattacharya, JM Finn, VP Diep, **F Baletto**, S Scandolo,
CCl4 dissociation on the ice Ih surface: an excess electron mediated process,
Source: PCCP Volume 12 Pages 13034 Published 2010

Citation 11

DOI <https://pubs.rsc.org/en/content/articlehtml/2010/cp/c0cp00439a>

U. Bovensiepen, C Gahl, J Stahler, M Bockstedte, M Meyer, **F Baletto**, S Scandolo, X-Y Zhu, A. Rubio, M. Wolf,

A Dynamic Landscape from Femtoseconds to Minutes for Excess Electrons at Ice-Metal Interfaces,
Source: J. Phys. Chem. C Volume 113 Pages 979-988 Published 2009

Citation 81

DOI <https://pubs.acs.org/doi/abs/10.1021/jp806997d>

MS Lee, **F Baletto**, DG Kanhere, S Scandolo,
Far-infrared absorption of water clusters by first-principles molecular dynamics,
Source: J. Chem. Phys. Volume 128 Pages 214506 Published JUN 2008

Citation 50

DOI <https://pubs.aip.org/aip/jcp/article/128/21/214506/959095>

UFT Ndongmouo, MS Lee, R Rousseau, **F Baletto**, S Scandolo,
Finite-temperature effects on the stability and infrared spectra of HCl-(H2O)₆ clusters,
Source: J. Phys. Chem. A Volume 111 Pages:12810-12815 Published DEC 2007

Citation 34

DOI <https://pubs.acs.org/doi/abs/10.1021/jp0765603>

F Baletto, C Cavazzoni, S Scandolo,
Surface trapped excess electrons on ice,
Source: Phys. Rev. Lett. Volume 95 Pages:176801 Published OCT 2005

Citation 65

DOI <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.95.176801>

C Mottet, G Rossi, **F Baletto**, R Ferrando,
Single impurity effect on the melting of nanoclusters,
Source: Phys. Rev. Lett. Volume 95 Pages: 035501 Published JULY 2005

Citation 219

DOI <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.95.035501>

F Baletto, R Ferrando,
Structural properties of nanoclusters: Energetic, thermodynamic, and kinetic effects,
Source: Rev. Mod. Phys. Volume 77 Pages: 371 Published MAY 2005

Citation 2052

DOI <https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.77.371>

-Selected as Emerging paper by **Reuters** in **2008** This review contains the first prediction of how kinetic processes influences the formation of nanoclusters. The reference paper to address kinetics effect in monometallic systems. Selected to appear in the Emerging Research Fronts Paper in the field of Chemistry, over 6-year period, 2002-2008, interview published on the ScienceWatch.com website on October 2008: <http://sciencewatch.com/sciencewatch/dr/erf/2008/08octerf/08octerfFerrET/>.

C Mottet, J Goniakowski, G Rossi, R Ferrando, **F Baletto**,
Melting of metallic nanoclusters: alloying and support effects
Source: Annales de Chimie-Science des Matériaux Volume 30 Pages:303 Published 2005

Citation 5

DOI <https://air.unimi.it/handle/2434/932160>

E Apra, **F Baletto**, R Ferrando, A Fortunelli,
Amorphization mechanism of icosahedral metal nanoclusters,
Source: Phys. Rev. Lett. Volume 93 Pages:065502 Published AUG 2004

Citation 127

DOI <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.93.065502>

F Baletto, A Rapallo, G Rossi, R Ferrando,
Dynamical effects in the formation of magic cluster structures,
Source: Phys.Rev. B Volume 69 Pages:235421 Published JUN 2004
Citation 78

DOI <https://journals.aps.org/prb/abstract/10.1103/PhysRevB.69.235421>

F Baletto, R Ferrando, AC Levi
Growth simulations of nanoclusters - Chapter Book
Source: Encyclopedia of Nanoscience and Nanotechnology Volume 3 (890), Pages 865-890
Published MARCH 2004
American Scientific Publishers
DOI <https://scholar.google.com/scholar?cluster=1176551507001691251&hl=en&oi=scholar>

GE Tommei, **F Baletto**, R Ferrando, R Spadacini, A Danani,
Energetics of fcc and decahedral nanowires of Ag, Cu, Ni, and C60: a quenched molecular dynamics study,

Source: Phys. Rev. B Volume 69 Pages:115426 -115426 Published 2004

Citation 35

DOI <https://scholar.google.com/scholar?cluster=6812273964844680718&hl=en&oi=scholar>

F Baletto, C Mottet, A Rapallo, G Rossi, R Ferrando,
Growth and energetic stability of AgNi core-shell clusters,
Source: Surf. Sc. Volume 566, Pages:192-196 Published SEPT 2004
Citation 75

DOI <https://www.sciencedirect.com/science/article/pii/S0039602804005370>

G Rossi, A Rapallo, C Mottet, A Fortunelli, **F Baletto**, R Ferrando,
Magic polyicosahedral core-shell clusters,
Source: Phys. Rev. Lett. Volume 93 Pages:105503 Published SEPT 2004
Citation 431

DOI <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.93.105503>

C Mottet, J Goniakowski, **F Baletto**, R Ferrando, G Treglia,
Modeling free and supported metallic nanoclusters: structure and dynamics,
Source: Phase Transitions Volume 77 Pages:101-113 Published JAN 2004
Citation 122

DOI <https://www.tandfonline.com/doi/abs/10.1080/1411590310001622473>

F Baletto, JPK Doye, R Ferrando, C Mottet,
Adsorption and diffusion on nanoclusters of C60 molecules,
Source: Surf. Sc. Volume 532, Pages:898 Published JUN 2003
Citation 7

DOI <https://www.sciencedirect.com/science/article/pii/S0039602803001353>

F Baletto, C Mottet, R Ferrando,
Time evolution of Ag-Cu and Ag-Pd core-shell nanoclusters,
Source: Eur. Phys. J. D 2 Volume 4 Pages:233 Published JUN 2003
Citation 27

DOI <https://link.springer.com/article/10.1140/epjd/e2003-00157-x>

F Baletto, C Mottet, R Ferrando,
Growth of three-shell onionlike bimetallic nanoparticles,
Source: Phys. Rev. Lett. Volume 90 Pages:135504 Published APR 2003
Citation 303

DOI <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.90.135504>

F Baletto, C Mottet, R Ferrando,
Freezing of silver nanodroplets,

Source: Chem. Phys. Lett. Volume 354 Pages: 82 Published MARCH 2002

Citation 70

DOI <https://www.sciencedirect.com/science/article/pii/S0009261402001070>

F Baletto, R Ferrando, A Fortunelli, F Montalenti, C Mottet,

Crossover among structural motifs in transition and noble-metal clusters,

Source: J. Chem. Phys. Volume 116 Pages: 3856-3863 Published MARCH 2002

Citation 530

DOI <https://pubs.aip.org/aip/jcp/article-abstract/116/9/3856/185110>

F Baletto, JPK Doye, R Ferrando,

Evidence of kinetic trapping in clusters of C 60 molecules,

Source: Phys. Rev. Lett. Volume 88 Pages: 075503 Published JAN 2002

Citation 42

DOI <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.88.075503>

F. Baletto, C. Mottet, R. Ferrando,

Growth simulations of silver shells on copper and palladium nanoclusters,

Source: Phys. Rev. B Volume 66 Pages 155420 Published OCT 2002

Citation 211

DOI <https://journals.aps.org/prb/abstract/10.1103/PhysRevB.66.155420>

F Baletto, C Mottet, R Ferrando,

Non-crystalline structures in the growth of silver nanoclusters,

Source: Eur. Phys. J. D Volume 16 Pages 25 Published OCT 2001

Citation 16

DOI <https://link.springer.com/article/10.1007/s100530170052>

F Baletto, R Ferrando,

Island adsorption and adatom diffusion on 3D non-crystalline silver nanoclusters

Source Surf. Sc. Volume 490 Pages 361 Published 2001

Citation 23

DOI <https://www.sciencedirect.com/science/article/pii/S0039602801013553>

F Baletto, C Mottet, R Ferrando,

Microscopic mechanisms of the growth of metastable silver icosahedra

Source: Phys. Rev. B Volume 63 Pages: 155408 Published MARCH 2001

Citation 254

DOI <https://journals.aps.org/prb/abstract/10.1103/PhysRevB.63.155408>

F Baletto, C Mottet, R Ferrando,

Reentrant morphology transition in the growth of free silver nanoclusters

Source: Phys. Rev. Lett. Volume: 84 Pages: 5544 Published JUN 2000

Citation 168

DOI <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.84.5544>

F Montalenti, F Baletto, R Ferrando,

Diffusion of one-dimensional clusters on Au and Pt (110)(1× 2)

Source: Surf. Sc. Volume 454, Pages: 575 Published 2000

Citation 6

DOI <https://www.sciencedirect.com/science/article/pii/S0039602800000947>

F Baletto, C Mottet, R Ferrando,

Molecular dynamics simulations of surface diffusion and growth on silver and gold clusters

Source: Surf. Sc. Volume 446 Pages: 31-45 Published: FEB 2000

Citation 142

DOI <https://www.sciencedirect.com/science/article/pii/S0039602899010584>

I have also contributed to outreach and editorials:

Geometric control of noble-metal nanoparticles,

R. D'Agosta & F. Baletto,
<https://mappingignorance.org/2018/07/23/geometric-control-of-noble-metal-nanoparticles/>
Published July 2018

Catalysis bit by bit,
F. Baletto & R.L. Johnston,
Research Futures, <https://researchfeatures.com/designing-catalysts-bit-by-bit/>
Published Oct 2017

Modelling 'Magic': the Search for Nanocatalysts,
F. Baletto,
SES interview at <https://www.ses.ac.uk/modelling-the-magic-the-search-for-nanocatalysts/>
Published May 2017

2nd TYC workshop on energy materials,
F Baletto, J Blumberger, A Shluger,
Source: PCCP Volume 15 Pages: 4475 Published 2013
DOI <https://pubs.rsc.org/en/content/articlehtml/2013/cp/c2cp90214a>

1st TYC workshop on energy materials,
J Blumberger, F Baletto, A Shluger,
Source: PCCP Volume: 13 Pages: 7602 Published 2011
DOI <https://pubs.rsc.org/en/content/articlehtml/2011/cp/c1cp90044g>

F. Baletto, <https://www.chemistryworld.com/news/gold-melted-at-room-temperature-using-electric-fields/3009802.article>

F. Baletto acted as KCL representative at Japanese Embassy,
personal interview on "Machine learning collaborations accelerate materials discovery"
<https://physicsworld.com/a/machine-learning-collaborations-accelerate-materials-discovery/>
Published 2019

ORGANIZZAZIONE, DIREZIONE E COORDINAMENTO DI CENTRI O GRUPPI DI RICERCA NAZIONALI E INTERNAZIONALI O PARTECIPAZIONE AGLI STESSI

(per ciascuna voce inserire anno, ruolo, gruppo di ricerca, ecc.)

My personal research income is exceeding 1M€, including main research grant, equipment, travel grants.

June 2023 Linea 2 di Ricerca (Unimi) "HyG: hydrogen production on GDY and decorated GDY", co-PI together with Dr. Simona Achilli, value €9200

December 2022 HORIZON-EIC Pathfinder

The project is a 42-month research named CHIRALFORCE, see <https://chiralforce.eu/>

Role FB only PI at Univ of Milan (personal budget ~260000€)

June 2022 LINEA DI RICERCA PER BANDO ASSEGNI 2022 (Unimi)

Role: primary PI of the project "The beauty of particles: from nano to astro" ended in funding two Assegno A fellowship for two-years, value 24500€ per year.

May 2022 programme grant EPSRC CPLAS led by prof. Anatoly Zayats (KCL) £10M,

Role: I was one of the co-I at KCL under the submission of the proposal (3-stages). Now, I have a research role but without funding as the grant is only for UK-based researchers, see <https://www.cplas.org/>

Feb 2022 Linea2 di Ricerca (Unimi) "PATOIS: OpTICaL PROPERTIES oF ATMOSPHERiC AEROsOL: numerical approaches",

Role PI with profs. Bernardoni and Guerra, total budget €14000

April 2021 DIPC Visiting professorship

Role PI the funding covered three onths of my salary ~ 10000€

2021 Feb-Apr: EU-HPC3 travel grant and HPC-time

Role co-I host and supervisor of the visit of Mr Mirko Vanzan (Univ of Padua) €2800

2020 Feb-Mar: EU-HPC3 travel grant and HPC-time

Role co-I host and supervisor of the visit of Dr. Piero Ferrari (Leuven) €3000

2019 Sep-Dec: EU-HPC3 travel grant and HPC-time

Role co-I host and supervisor of the visit of Mr Antoni Salam (URV, Spain) €3500

Jan 2019: EPSRC-IAA grant on “Software factory for nanoscaled materials: the LoDiS suite”,

Role PI of the project hired for a 6-month period a research student, ~13000€

Jul 2018: Visiting professorship scheme funded by Programa "Salvador de Madariaga" 2018

The grant #PRX18/00460 supported the visit of prof. J. J. Carbo' in my reserach group at KCL.

Role: co-I I wrote a letter and I provided the place and facilities for the visit ~€19000

2018 Oct-Dec: EU-HPC3 travel grant + HPC- time

Role: co-I host and supervisor of the visit of prof. R. D'Agosta (EPV/EHU Spain)~€3200

June 2016 Research Assistant fellowship - Project ID number 202256/2015- 4 funded by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Pós-doutorado no Exterior, Programa Ciência sem Fronteiras.

Role: FB was the co-I of the application as unique supervisor of the project and host at the KCL, value ~30000€

2016 Feb-Mar: CONACyT "Movilidad en el Extranjero" (Grant 291062) and Thomas Young Centre Junior Fellowship on "Theoretical study of the magnetic properties in PtNi and NiAl small-sized aggregates"

Role: co-I sponsor and host of Mr. Omar Estrada's 2-month fellowship

2015 Oct - Jan 2016: “Modelling metallic nanoparticles”funded by the "MyBrain scholarship", Malaysian Government,

Role: co-I sponsor and host of Miss Yee-Yeen Soon for her research visit ~€3000.

2010 May- 2014 May: COST-Action MP0903 on Nanoalloys

Role: UK representative and manager of the short-term mission, I was administrating about €20000 each year in mission.

2012 Dec - 2013 Nov: Royal Society Research Grant on "Physical properties of PtNi nanoalloys at oxide interfaces",

Role: Unique PI, major grant €18000

Sept. 2012 5-years EPSRC Critical Mass Research Grant

Role: I was the only PI at KCL of the EP/J010812/1 project (value £ 250231) related to the critical mass UK collaboration named TOUCAN. On top we were granted HPC-time at Hector/ARCHER worth ~€2M.

2015 Apr-Jul: Gobierno Basco, Movilidad del Personal Investigador 2014

Role: co-I host and sponsor of the visit by prof. R. D'Agosta (UPV/EHU Spain) €9485

2011– 2015 International collaboration FAPESP collaboration between KCL and San Paulo University (Brazil) on "Computational Nanoscience for Energy Materials

Role: co-I, but unique PI at KCL, USP-PI profs. Miranda & Antonelli, we worked on hydrogen storage and production and ethanol catalysis through metallic nanoalloys", €11000

2011 Jul-Aug: EU-HPC2 grant on “Optical properties of nanoparticles”,

Role: PI grant to support my visit to the group of Prof. Rubio (Nano-bio, ETSF/EHU-UPV) and to use BSC supercomputers. ~€2500, excluding computational time (project # hpce08173)

August 2009 5-years EPSRC First Grant Research Grant on "CPLACES: Clusters of platinum alloys for fuel cell applications"

Role: I was the only PI to create my own research group as promising future leader, value £398850

Computational research grants (worthy over 50000€)

2022 Oct: (PI, HPC-time) Indaco grant HPC@University of Milan for having a dedicated queue

2021 Feb-Jun: (PI, HPC-time) EPSRC-MCC-grants for using HPC-Tier1-Archer2 and Tier2-Young,

2020 Jan-Oct: (PI, HPC-time) EPSRC-MCC-grants for using HPC-Tier1-Archer and Tier2-Thomas,

2018 Jul-Oct: (PI, HPC-time) EPSRC-MCC-grants over three different projects,

2018 Jan - Jul: (PI, HPC-time) EPSRC-MCC, (25 MAu over two projects)

(The Materials and Chemistry Consortium (MCC) is funded by EPSRC-EP/R029431/1 (2018 - 2022) of the value of £489316)

2017 Jan-Dec: (PI, HPC-time) MMM grant on HPC- Tier 2 - Hub

(Materials and Molecular Modelling -MMM- is supported by EPSRC- EP/P020194/1 value £4,000,000)

June 2010: (PI, HPC-grant) Hector-phase 2b project (number e169) on "NOR: nanoalloys for oxygen reduction in fuel cell"

2006 Jan.-Dec: TWO CINECA-HPC grant projects: "Heterogeneous Catalysis on ice surfaces in stratospheric conditions" and "Water Clusters: Application of the density functional theory to the physics of water clusters"

Travel Grants to support my visits/conference travel (over 4000€)

2019 Jun: (PI, travel grant) GRC-conference

2010 Sept: (PI, travel grant) CECAM-conference

2010 Aug: (PI, travel grant) MRS/ICMR for conference

2008 Aug: (PI, travel grant) Royal Society to attend International conferences

2007 Jan: (PI, travel grant) ESF, ICMR and MCC to attend to International conferences

Funding raised to organise conferences

2016 Aug-Dec: Funding raised to organize the TYC-Toucan workshop, several funding agencies including Psi-K, IoP, RSC, CCP9 and Overleaf, ~€18000

ATTIVITÀ QUALI LA DIREZIONE O LA PARTECIPAZIONE A COMITATI EDITORIALI DI RIVISTE SCIENTIFICHE

(per ciascuna voce inserire anno, ruolo, rivista scientifica, ecc.)

Associate Editor for Modelling, Theory and Computational Catalysis

Frontiers in Catalysis

<https://www.frontiersin.org/journals/catalysis/sections/modelling-theory-and-computational-catalysis/editors>

TITOLARITÀ DI BREVETTI

(per ciascun brevetto, inserire autori, titolo, tipologia, numero brevetto, ecc.)

PREMI E RICONOSCIMENTI NAZIONALI E INTERNAZIONALI PER ATTIVITÀ DI RICERCA

(inserire premio, data, ente organizzatore, ecc.)

Dec. 2015 Recognition Pay Scheme on the basis of my "exceptional performance over the previous 12 months has been recognised. The success of the Department, the Faculty, and King's as a whole, relies on contributions like yours" awarding body King's College London

March 2009 Finalist ERC-starting grant interview stage on "MONALISE: Modelling nanoparticles for environment and sustainable energy"

Nov. 2006 Finalist for a MRS award Poster on "Unusual alloying effect on the melting temperature of metal nanoclusters", MRS2006, Boston (USA) on 27-30 November 2006

August 2003

Winning an UNESCO fellowship to perform research at the International Centre for Theoretical Physics, Trieste, Italy (competitive)

June 2002 Finalist at the NANOECOSS-PRIZE Poster competition "Kinetic Trapping Effects during nanocluster growth", at NANO7-ECOSS21, at Malmo (Sweden) on 24-28 June 2002

PARTECIPAZIONE IN QUALITÀ DI RELATORE A CONGRESSI E CONVEGNI DI INTERESSE INTERNAZIONALE

(inserire titolo congresso/convegno, data, ecc.)

1. Invited Talk at the ISSPIC XXIX, "And yet it moves: dynamical processes at the nanoscale: Berlin 3-8 Sept. 2023
2. Invited talk at the ClusterMeeting, "Nanofaceting and catalysis", Prague (CZ) 18-23 June 2023
3. Invited Talk at 108 Congress SIF, "and yet it moves": A journey at the nanoscale", Milan 16 Sept. 2022
4. Talk at Psi-K 2022, "and yet it moves: modelling formation processes at the nanoscale", Lausanne 23 Aug. 2022
5. Invited Talk at the CECAM-Flagship Workshop on "Born-to-be-different", 7-9 July 2021 (virtual)
6. Invited Talk at the SIAM Minisymposium-Nanocrystals and Epitaxial Nanoclusters, on "Born to be different: modelling formation of metallic nanoparticles and their consequences", May 2021 (virtual)
7. Invited Talk at the IMN 2021 on "Double-doping and magnetic effects", 15 April 2021 (virtual)
8. Keynote Lecture at the Int. Conf. Theo. Aspects of Catalysis (ICTAC), "Born different: modelling the formation of nanoparticles and nanoalloys -consequences on catalysis", Lyon (France) 13-17 June 2022
9. Invited Talk at the Gordon Research Conference on "Cluster and nanostructures", "Size (&shape) dependence of chemical properties of small clusters", Les Diablerets (CH) Jun. 2019
10. Invited talk at the IMN2019 meeting, "Elucidating structural transitions in nanoalloys", Genova (Italy) June 2019
11. Invited Talk at the Forum 2- WCF 2019, "Understanding structural changes for a better design of nanocatalysts", Barcellona (Spain) May 2019
12. Invited Talk at the ICTP-Workshop on "Crystal Structure Prediction", "Modelling structural changes at the nanoscale: the fluxionality of metallic nanoparticles" Trieste (Italy) 14 Jan. 2019
13. Invited Talk at 3rd Workshop Condensed Matter Highlights, Univ. of Milan, "How structural transformation of metallic nanoclusters could affect their catalytic, magnetic and optical properties", 15 Feb. 2019
14. Invited Talk at the CECAM Flagship Workshop on "Modelling metal-based nanoparticles: environment and dynamical effects", "How shape changes alter chemo-physical properties of nanoparticles?" Grenoble (France) 3-5 Dec. 2018
15. Invited Talk at the ISSPIC-XIX, "How shape changes alter the physical chemical properties of nanoparticles" Hangzhou (China) Aug. 2018
16. Invited Talk at the COST-Action CM-1405 MOLIM, "Small molecules on metallic nanoparticles", Graz (Austria) 5 Feb. 2018
17. Invited Talk at MMM-Hub for the launch of the EPSRC-Tier 2, "Modelling magic nanoparticles", London (UK) 12 Sept. 2017
18. Invited Lecture at the CATSENSE Summer School, on "Towards a rational design of nanocatalysts" Leuven (Belgium) 11 Sept. 2017
19. Invited Talk at the Faraday Joint Interest Group Conference, "Towards a rational design of nanocatalysts", Warwick (UK) Apr. 2017
20. Invited Talk at International Symposium FOR1282, on "Numerical modelling for a rational design of nano catalysts", Berlin 22-24 Feb 2017
21. Invited Talk at the Inter. Symposium Semiconductor Clusters and Nanoparticles, Berlin (Germany) Feb. 2017 13.
22. Talk at the International Workshop on Nanoalloys, Birmingham (UK) Dec. 2016

23. Invited Lecture at the ICTP-College on Multiscale Computational Modelling of Materials, Trieste (Italy) Jul. 2016
24. Lecture at the TYC/Toucan Int. Workshop on Energy materials, "Modelling structural transistions at the nanoscale" London (UK) Dec. 2016
25. Invited Talk at the PacificChem 2015, "Supported metallic and bimetallic nanocatalysts", Hawaii (USA) Dec 2015
26. Invited Talk at the EMN-2015, "Topological effects in magnetic platinum nanoparticles", San Sebastian (Spain) 3 Sept. 2015
27. Invited Talk at the ECOSS-2015, "Supported metallic and bimetallic nanonocatalysts" Barcelona (Spain) 1 Sept. 2015
28. Invited Talk at the CECAM workshop, "Dynamical Behaviour of supported Pt-clusters", Toulouse (France) Jun 2015
29. Invited Talk at the COST-Action-MP0903 Inter. workshop, "AuCu and AgAu nanocages" Santa Margherita (Italy) 6-9 Apr. 2014
30. Invited Lecture at the TOFA 2012, "Energetics, thermodynamics, and kinetics of metallic nanoalloys" Pula (Croatia) Sep. 2012
31. Hot Topics -Talk at the ISSPIC XVI, "Oxygen chemisorption upon PtNi clusters deposited over MgO(001)", Leuven (Belgium) 12 Jul. 2012
32. Invited Talk at the COST-Action MP0903 Meeting, Genoa (Italy) Oct. 2010
33. Invited Talk at the CECAM Workshop, "Fancy motifs for Co-based nanoalloys", Lausanne (CH) 13-16 Sept. 2010
34. Invited Talk at the IMRC/MRC XIX on "Magnetic and chemical order in transition metal nanoalloys", Cancun (Mexico) 16 Aug. 2010
35. Talk at ECOSS26, "First-principles simulations of water systems in atmosphere", Parma 31 Aug. 2009
36. Maxwell Lectuer on "New fuel or new cars?", King's College London, 14 Feb 2008
37. Talk at Workshop in New horizonzs in modelling surfaces, "Excess electron on ice surfaces", London 1 Apr. 2008
38. Talk at APS Meeting 2008, "Dynamical investigation of water clusres in atmospheric conditions", Denver 13 March 2008
39. Invited Talk at IMRC, "Dynamical concepts in the nanoworld", Cancun (Mexico) on 22-26 August 2004;
40. Invited Talk at International Workshop on Fundamental Aspects and Practical Applications of Surface Diffusion, "Growth of three-shell onion-like bimetallic nanoparticles", Trest Castle (Czech Republic) on 14-17 September 2003;
41. Invited Talk at Fourth International Workshop on Surface & Interface Segregation (IWSIS-4), "Growth of multishell metallic nanoparticles", Cape Town (South Africa) on 17-22 August 2003;
42. Invited Talk at Colloque Annuel Groupement Quasicristaux, "Growth of non-crystalline silver structures", Marseille (France) on 27-29 June 2001;
43. Invited Talk at XX Convegno di Fisica Teorica e Struttura della Materia, "Transizioni morfologiche durante la crescita di nanocluster di argento", Fai della Paganella (Italy) on 25-28 March 2001
44. Invited Talk at CECAM Workshop Dynamical correlations in single-particle and collective diffusion on surfaces, "Simulation of surface diffusion and growth on noble-metal clusters", Lione (France) on 26-28 May 1999

ATTIVITÀ GESTIONALI, ORGANIZZATIVE E DI SERVIZIO

INCARICHI DI GESTIONE E AD IMPEGNI ASSUNTI IN ORGANI COLLEGIALI E COMMISSIONI, PRESSO RILEVANTI ENTI PUBBLICI E PRIVATI E ORGANIZZAZIONI SCIENTIFICHE E CULTURALI, OVVERO PRESSO L'ATENEO O ALTRI ATENEI

(inserire incarico/impegno, ente, data, ecc.)

• INSTITUTIONAL RESPONSIBILITIES

2023 - now

2022 - now Assistant of the 4EU+ per il dipartimento di Fisica (European Alliance University)
 2023 - now co-I del progetto Fiorire con la Scienza Unimi Connect
 2022 - now Unico Referente per il dipartimento di fisica "Reti delle Politiche di genere", Univ. of Milan
 2020 - 2021 Member of the Research Culture Task & Finish Working Group, King's College London
 2018 - 2020 Member of the Dept. Strategy Educational Committee, King's College London, UK
 2018 - 2020 Member of the Dept. Research Committee, King's College London, UK
 2018 - 2020 Post-doctoral researcher Mentor, King's College London, UK
 2016 - 2020 Career Tutor, King's College London, UK
 2016 - 2020 Female Tutor, King's College London, UK
 2014 - 2020 Member of the Diversity and Equality Depart. committee, King's College London, UK
 2011 - 2016 Chair of the Departmental Assessment Committee, King's College London, UK
 2011 - 2016 Member of the Faculty Assessment Committee, King's College London, UK
 2011 - 2016 Member of the Departmental Educational Committee, King's College London, UK
 2007 - 2008 Organiser of the Internal Seminar, King's College London, UK

• ORGANISATION OF SCIENTIFIC MEETINGS

2022 In the organisation of the "Tempo delle Donne" day at Unimi
 2022 Organising Committee Faraday-Discussion on Nanoalloys
 2021 Organising committee for CCP2020 section on "Materials and nano-science"
 2020 Organising committee for MMM10-Symposium 14 on "Metals at the nanoscale and metals-based nanoparticles: environmental, mechanical and kinetic properties" (postponed)
 2020 Organising committee for TYC Energy Workshop 2020 (postponed)
 2018 Steering committee of the RSC-TCG Conference 2018
 2012-2014-2016 Organiser of the Energy Materials workshop series on behalf of the Thomas Young Centre, London, UK. Main organiser for the 2016 edition 2016, dedicated to "Shaping Nanocatalysts" in conjunction with the final international conference for the TOUCAN project.
 2016 USP-KCL meeting, webinar meeting between KCL and USP delegation, May 2016
 2015 Organising Committee for Condensed Matter Physics-2015, Boston, USA
 2014 TAMC VII, local organiser, Birmingham, UK

• MEMBERSHIPS OF SCIENTIFIC SOCIETIES

2023 Elected spokesperson/leader of the Psi-K Working Group "Bridging length and time scales"
 2021-2022 Member of the Psi-K Working Group B3 "Bridging length and time scales"
 2021 Treasurer for the Royal Society of Chemistry Theoretical Chemistry Group
 2018 - Member of the London Centre of Nanotechnology (UK)
 2017-2021 Elected Member of the Royal Society of Chemistry Theoretical Chemistry Group, renewed in 2019
 2017- Member of the MCC (EPSRC, EP/R029431/1 and previously EP/L000202/1)
 2016 - Member of the MMM-Hub (EPSRC, EP/P020194/1)
 2016 - Member of the Institute of Physics (UK)
 2010-2014 Elected UK representative of the MP0903-COST-Action Board and Manager of short-term scientific missions
 2009 - Member of Royal Society of Chemistry (UK)
 2007 - Member of the Thomas Young Centre (TYC, London)

ATTIVITÀ CLINICO ASSISTENZIALI

(indicare, data, durata, ruolo, ente presso il quale si è prestata attività assistenziale, ecc.)

NA

Data

25 July 2023

Luogo

Milano, Italy