Kevin Rossi

Education and Qualifications

Marie Curie Research Fellow, **15/09/2020 – 14/09/2022**
Chemical Engineering Department, Ecole Polytechnique Federale Lausanne
Project: "NANOCO2RE – Nanocrystals for CO2 Reduction Reaction"
Host supervisor: Prof. Raffaella Buonsanti

PostDoc, **15/09/2018 - 14/09/2020**
Materials Engineering Department, Ecole Polytechnique Federale Lausanne
Project: "Data-driven modelling and design of mineral acid catalyst for phenol hydroxylation"
Main supervisor: Prof. Michele Ceriotti – Industry Partner: Solvay S.A.

PhD student, **15/09/2014 - 14/09/2018**
Physics Department, King's College London
Thesis: "Multiscale modelling of metallic nanoparticles structural and catalytic properties"
Main supervisor: Prof. Francesca Baletto

BSc Physics – Honors, **27/09/2011 - 31/08/2014**
Physics Department, King's College London, United Kingdom
Thesis: "Modelling the self-assembly of Borazine on metal surfaces"
Main supervisor: Prof. Alessandro De Vita

Areas of Expertise

- *Design of advanced materials with applications in green energy and green chemistry*.
Through my research I've nurtured an expertise in the investigation and design of materials for the automotive sector (fuel cells), net-zero-carbon technologies (catalysts for electrochemical conversion of CO2), energy storage devices (Li-polysulfides batteries), and polymer, flavour, and fragrances industries (sustainable synthesis of value-added chemicals).

- *Data-driven prediction and numerical analysis of materials' property*.
During my career I've grown an in-depth knowledge of several computational simulation techniques (Electronic structure modelling via quantum mechanics calculations, atomistic structure modelling via molecular mechanics) and data-driven methods (linear regression, kernel methods, neural-network based approaches, physics-based methods, dimensionality reduction), which are among the state-of-the-art ones in materials design.

- *Planning and managing autonomous and collaborative research and outreach projects.*
During my past 8 years of research, I proactively and independently gathered more than 300K CHF from European, National (CH and UK), and local sources, to fund my own research (~250K CHF) and organize workshops for young researchers (~50K CHF). Also, I acted as a co-founder of a start-up for *in-silico* drug design, and have contributed to the success of R&D collaboration with industry (Solvay S.A). Currently, I am affiliated with European consortia (CECAM, PSI-K) and have close ties with two National Centre of Competence in Research (NCCR), namely, NCCR Catalysis (current member), and the NCCR Marvel (2018-2020). The former is dedicated to the computational design and discovery of novel materials. The latter aims at the design of next-gen catalysts and processes for sustainable chemistry.

Languages

English (proficient), Italian (mother tongue), Spanish, French (beginner)

Awards

Curling Prize **Jan 2019**
– Best teaching assistant award, as voted by the 2018/2019 King's College London undergraduate cohorts in the Natural and Mathematical Sciences Division.

EPSCR grant no. ER/M506357/1 **Sep 2014 – Sep 2018**
- A PhD bursary has been exceptionally awarded to me just after my Bachelor degree**.**

INA assitalia Bursary, Generali s.p.a, Trieste – £1200 **Sep 2011 – Jun 2014**
- The Bursary is awarded to bachelor students demonstrating first class performances.

Teaching activity

Student co-supervisor, **Since 2014**
A total of six undergraduate students during their Master thesis projects or "King's undergraduate research fellowships".

Examiner Assistant (Ecole Polytechnique Federale de Lausanne) **Since 2018**
Physical and Computational Organic Chemistry, Nanomaterials for Chemical Engineering, Fundamentals of Solid State.

Teaching assistant (King's College London) **2014-2018**
180h in Second Year Physics Computational Lab.
20h in Second Year Quantum Mechanics.

Teaching assistant (summer school ICTP Trieste) **July 2016**
"College on Multiscale Material Modelling for Energy Materials", Trieste.

Organization of scientific events

Workshop Organizer, **May 2022**
"Young Researcher's Workshop on Machine Learning for Materials", Trieste (IT)

Workshop Organizer, **May 2019**
"Young Researcher's Workshop on Machine Learning for Material Science", Espoo (FI)

Internal seminar co-organizer, **2016-2017**
King's College, Physics Department, Condensed Matter Theory and Simulation division

Editorial activity

Referee for international peer-reviewed journals: ACS Catalysis, npj Computational Materials, Chemical Science, Journal of Applied Physics, Engineering Reports, Fuel, Journal of Chemical Physics, International Journal of Quantum Chemistry, European Journal of Physics B, Journal of Nanoparticle Research, Chaos, Molecular Simulations.

Funding Record - approximately amounting to 300.000€

ERC H2020, Marie Sklodowska Curie Individual Fellowship –191.380€
- Project Title: "NanoCO2RE – Nanoparticles for CO_2 Reduction Reaction"

Aalto University, Psi-K, ICTP, and CECAM funding for ML4M 2022 workshop - 30.000€
- Conference title "Young Researcher's Workshop on Machine Learning for Materials 2022, Trieste (IT)"

Aalto University, Psi-K, and CECAM funding for ML4MS 2019 workshop - 25.000€
- Conference title "Young Researcher's Workshop on Machine Learning for Material Science 2019, Espoo (FI)"

Computational Resources - Approx 1M cpu/h
Funders: Swiss National Supercomputing Center, New Zealand National Supercomputing Center

Research projects small-grants - 15.000+€
Funders and bursary name: King's College Global research (UK), New Zealand e-Science Infrastructure (NZL), Thomas Young Center Junior Research Fellowship (UK), King's College Undergraduate Research Fellowship (UK), McDiarmid Institute (NZL)

Travel awards - 5000+€
Funding bodies: Royal Society of Chemistry (UK), Institute of Physics (UK), King's College London (UK), MacDiarmid Institute (NZL), Thomas Young Center (UK), Rideal SCI (UK)

Complete list of publications and oral presentations:

27 Publications – corresponding to 335 citations, H-index 13 (source: Google Scholar)

27) R.Jones, **K.Rossi,** I.Vasijevic, M.Vanzan, A.Bonilla-Santana, C.Zeni, F.Baletto - "Structural Characterization of Nanoalloys for (photo)Catalytic Applications with the Sapphire Library", Faraday Discussions, *accepted* (2022)

26) C.Zeni, A.Anelli, A.Glielmo, **K.Rossi** - "Exploring the Robust Extrapolation of Machine Learning Potentials", Physical Review B, *105 (16), 165145,* (2022)

25) L.Zaza, **K.Rossi,** R.Buonsanti - "Well-Defined Copper-Based Nanocatalysts for Selective Electrochemical Reduction of CO_2 to C2 products", ACS Energy Letters, *7, 1284-1291* (2022), **ACS editor choice and most read ACS article of the month**

24) **K.Rossi,** R.Buonsanti "Shaping Copper Nanocatalysts to Steer Selectivity in the Electrochemical CO_2 Reduction Reaction", Accounts of Chemical Research, *5789-5792,* (2022)

23) O.Segura, M. A.Hope, A.Venkatesh, S.Björgvinsdóttir, **K.Rossi,** A.Loiudice, L.Emsley and R. Buonsanti - "Colloidal ALD-grown hybrid shells nucleate via a ligand-precursor complex", Journal of American Chemical Society, *144 (9), 3998-4008* (2022)

22) **K.Rossi**, T.Mineva, J.Filhol, F.Tielens, H.Guesmi - "Realistic Modeling of Dynamics at Nanostructured Interfaces Relevant to Heterogeneous Catalysis", Catalysts, 12, 52 (2022)

21) C.Zeni, **K.Rossi**, T.Pavloudis, J.Kioseoglou, S.de Gironcoli, R.E.Palmer, F.Baletto - "Data-driven simulation and characterisation of gold nanoparticle melting", Nature

Communications 12 (1), 1-9 (2021), **Computation and Machine Learning for chemistry collection editor choice**

20) E.I. Andritsos, **K.Rossi** - "Accelerating the theoretical study of Li-polysulphide adsorption on single-atom catalysts via machine learning approaches", preprint arXiv:2112.115372021 (2021)

19) S.B.Varandili, D.Stoian, J.Vavra, **K.Rossi**, J.R.Pankhurst, Y.T.Guntern, R.Buonsanti - "Elucidating the structure-dependent selectivity of CuZn towards methane and ethanol in CO 2 electroreduction using tailored Cu/ZnO precatalysts", Chemical Science 12 (43), 14484-14493 (2021)

18) C.Zeni, **K.Rossi**, A.Glielmo, S.De Gironcoli – "Compact atomic descriptors enable accurate predictions via linear models", Journal of Chemical Physics, 154, 22, 223112 (2021)

17) 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 to CH conversion", Nanoscale, 13, 11, 5857-5867, (2021)

16) G.Imbalzano, Y.Zhuang, V.Kapil, **K.Rossi**, E.A.Engel, F.Grasselli, M.Ceriotti - "Uncertainty estimation by committee models for molecular dynamics and thermodynamic averages", Journal of Chemical Physics, 154, 7, 074102 (2021), **Editor Choice**

15) L.Delgado-Callico, **K.Rossi**, R.Pinto-Miles, P.Salzbrenner, F.Baletto - "A universal signature in the melting of metallic nanoparticles", Nanoscale 13, 2, 1172-1180, in press (2021)

14) **K.Rossi**, V.Juraskova, R.Wischert, L.Garel, C.Corminboeuf, M.Ceriotti – "Simulating solvation and acidity in complex mixtures with first principles accuracy: the case of CH_3SO_3H and H_2O_2 in phenol", Journal of Chemical Theory and Computation, 16 (8), 5139-5149 (2020)

13) **K.Rossi**, G.Asara, F.Baletto – "Structural screening and design of Platinum nanosamples for Oxygen Reduction", ACS Catalysis, 10 (6), 3911-3920 (2020)

12) **K.Rossi**, J.Cumby - "Representations and descriptors unifying the study of molecular and bulk systems" Invited Perspective, International Journal of Quantum Chemistry, 120 (8), e26151 (2020)

11) C.Zeni, **K.Rossi**, A.Glielmo, F.Baletto, – "On Machine Learning Force Fields for Metallic Nanoparticles", Advances in Physics X, 4 (1), 1654919 (2019)

10) **K.Rossi**, G.Asara, F.Baletto – "Correlating ORR activity and structural rearrangements of MgO-supported Pt nanoparticles", ChemPhysChem, 20 (22), 3037-3044 (2019)

9) **K.Rossi**, G.Asara, F.Baletto - "A genomic characterisation of monometallic nanoparticles", Physical Chemistry Chemical Physics, 21 (9), 4888-4898

8) C.Zeni, **K.Rossi**, A.Glielmo, N.Gaston, F.Baletto, A.De Vita – "Building machine learning forcefields for nanoclusters", Journal of Chemical Physics, 148, 241739 (2018)

7) **K.Rossi**, L.Partay, G.Csanyi, F.Baletto - "Thermodynamics of CuPt nanoalloys", Scientific Reports, Scientific reports 8 (1), 9150 (2018)

6) **K.Rossi**, Y. Soon, L. Pavan F. Baletto - "The effect of size and composition on structural transitions in monometallic nanoclusters", European Journal of Physics B, 91, 33 (2018), **special issue - "Shaping Nanocatalysis"**

5) **K.Rossi**, F.Baletto - "The effect of chemical ordering and lattice mismatch on structural transitions in phase segregating nanoalloys", Physical Chemistry Chemical Physics, 19, 11057 (2017), **Editor Choice**

4) F.Comitani, **K.Rossi**, M.Ceriotti, E.M.Sanz, C.Molteni - "Mapping the conformational free energy of aspartic acid in gas phase and aqueous solution", 146, 145102 (2017)

3) **K.Rossi**, T.Ellaby, O.Paz Borbon, I.Atanasov, F.Baletto - "Melting of large Pt@MgO(100) icosahedra", Journal of Physics: Condensed Matter, 29, 14 (2017)

2) A.Gould, **K.Rossi**, R.Catlow, F.Baletto. A.Logsdail -"Controlling Structural Transitions in AuAg Nanoparticles through Precise Compositional Design", Journal of Physical Chemistry letters, 7, 21, (2016)

1) L.Pavan, **K.Rossi**, F.Baletto - "Metallic Nanoparticles meet Metadynamics", Journal of Chemical Physics, 143, 184304 (2015)

Book Chapter

1) F.Baletto, C.Miranda, W.Rigo, **K.Rossi** – "Nanoalloys for energy applications" – Nanoalloy, edited by F. Calvo, published by Elsevier (2020)

Oral Presentations

15) On the robust-extrapolation of Machine learning methods – SISSA 2022, 11/08/2022 – Trieste – **Invited**

14) Predicting and classifying the selectivity of Cu-dilute alloys catalysts for CO_2 electroreduction – NCCR Catalysis online meeting 2022, 24/06/2022 – Online

13) Multiscale design of Pt-nanoparticles with enhanced catalytic activity for Oxygen Reduction Reaction – Cluster Meeting 2021, 18-23/06/2021 - Prague

12) Data-driven modelling, characterisation, and prediction of metallic nanocatalysts physico-chemical properties - Institut Charles Gerhardt CNRS Montpellier - 09/06/2021 – **Invited**

11) Careers in Physics – King's College London, Physics Departments, 10/03/2021 – **Invited**

10) Multiscale design of Pt-nanoparticles with enhanced catalytic activity for Oxygen Reduction Reaction – NanoGE Virtual Meeting, 23-25/11/2020

9) Machine Learning and enhanced sampling to probe the solvation, acidity, and reactions in complex mixtures – ACS PostDoc Symposium Virtual Meeting, 19/11/2020 – **Invited**

8) Multiscale design of Pt-nanoparticles with enhanced catalytic activity for Oxygen Reduction Reaction – ACS PostDoc Symposium Virtual Meeting, 19/11/2020 – **Invited**

7) Multiscale design of Pt-nanoparticles with enhanced catalytic activity for Oxygen Reduction Reaction – ACS FALL Virtual Meeting, 13-18/08/2020

6) Reduced dimensionality multiscale modelling of nanoparticles properties –
XXVIII International Material Research Congress, 19-24/08/2018 – Cancun – **Invited**

5) Reduced dimensionality multiscale modelling of nanoparticles properties –
Seminario Soterio Prieto, 06/08/2018 – UNAM, Mexico City – **Invited**

4) Fingerprinting the non-equivalent adsorption sites to predict catalytic properties –
4th TYC Energy Material Workshop, 14-16/12/2016 – London

3) Investigating structural transitions in metallic nanoalloys – 8th International Conference on Multiscale Materials Modeling, 9-14/10/2016 – Dijon

2) Investigating structural transitions in metallic nanoalloys – XVIII International Symposium on Small Particles and Inorganic Clusters, 14-20/08/2016 – Jvyskala

1) Investigating structural transition in metallic nanoalloys - European Congress and Exhibition on Advanced Materials and Processes 2015, 20-24/09/2015 Warsaw