

Franco Bonafé

Personal Information

Name Franco Paul Bonafé
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Education

- 2014–2018 **PhD in Chemical Sciences**, *Dpmt. of Theoretical and Computational Chemistry, School of Chemical Sciences, UNC*, Supervisor: Prof. Cristián G. Sánchez, thesis title: “UV/visible photoinduced nuclear motion in molecular and nanoscopic systems”. Defense held on 13.12.2018
- 2009–2014 **Licenciate in Chemistry, Orientation: Physical Chemistry**, *School of Chemical Sciences, UNC, Argentina*, GPA: 9.82/10.
- 2003–2008 **Chemical Technician, Orientation: Food Industry**, *Dr. Manuel Lucero Secondary School (Córdoba)*, GPA: 9.64/10.

Teaching and Research

Publications

- 2019 **“Simulation of Impulsive Vibrational Spectroscopy”**, F. J. Hernandez, F. P. Bonafé, B. Aradi, Th. Frauenheim, and C. G. Sanchez, *J. Phys. Chem. A*, Article ASAP, DOI: 10.1021/acs.jpca.9b00307.
- 2018 **“Uniform Selenization of Crack-Free Films of Cu(In,Ga)Se₂ Nanocrystals”**, T. B. Harvey, F. P. Bonafé, T. Updegrave, V. Reddy Voggu, C. Thomas, S. C. Kamarajugadda, C. J. Stolle, D. Pernik, J. Du, and B. A. Korgel, *ACS App. Energy Mater.*, Article ASAP, DOI: 10.1021/acsaem.8b01800.
- 2018 **“Fully Atomistic Real-Time Simulations of Transient Absorption Spectroscopy”**, F. P. Bonafé, F. J. Hernández, B. Aradi, Th. Frauenheim, and C. G. Sánchez, *J. Phys. Chem. Lett.* 9 (15) 4355.

- 2017 **“Plasmon-driven sub-picosecond breathing of metal nanoparticles”**, *F. P. Bonafé, B. Aradi, M. Guan, O. A. Douglas-Gallardo, C. Lian, S. Meng, Th. Frauenheim, and C. G. Sánchez*, *Nanoscale* 9 12391.
- 2016 **“Optical Properties of Graphene Nanoflakes: Shape Matters”**, *C. Mansilla Wettstein, F. P. Bonafé, M. B. Oviedo, and C. G. Sánchez*, *J. Chem. Phys* 144 224305.
- 2015 **“Ultra-small rhenium clusters supported on graphene”**, *O. Miramontes, F.P. Bonafé, U. Santiago, E. Larios Rodríguez, J.J. Velázquez-Salazar, M. Mariscal, and M. Jose-Yacamán*, *Phys. Chem. Chem. Phys.* 17 7898.
- 2013 **“A theoretical study of the optical properties of nanostructured TiO₂”**, *V.C. Fuertes, C.F.A. Negre, M.B. Oviedo, F.P. Bonafé, F.Y. Oliva, and C.G. Sánchez*, *J. Phys.: Cond. Matter* 25 115304.

Presentations in international scientific meetings

- 2017 **“Subpicosecond breathing mode excitation in metal nanoparticles”**, *F. P. Bonafé, B. Aradi, O. A. Douglas Gallardo, Th. Frauenheim and C. G. Sánchez*, CECAM Workshop: Charge carrier dynamics in nanostructures: optoelectronics and photostimulated processes. Bremen, Germany, Poster.
- 2016 **“Absorption spectra and excitations from real time TD-DFTB”**, *F. P. Bonafé and C. G. Sánchez*, International CECAM-Workshop & Tutorial on Approximate Quantum Methods in the ab initio World. Beijing, China, Tutorial.
- 2014 **“Selenization of Automated, Ultra-Sonic Spray-Deposited Cu(In,Ga)Se₂ Nanocrystal Films for Photovoltaics”**, *T. B. Harvey, F. P. Bonafé, T. Updegrave, C. Thomas, S. Kamarajugadda, C. J. Stolle, D. Pernik, J. Du and B. A. Korgel*, AIChE Annual Meeting. Atlanta, Georgia, USA, Poster.
- 2013 **“Study of the nucleation of Pd nanoparticles on graphene”**, *F. P. Bonafé, G. J. Soldano, M. M. Mariscal*, XXII International Materials Research Congress (IMRC). Cancún, Mexico, Poster.

Presentations in national scientific meetings

- 2018 **“Simulations of transient absorption in time dependent DFTB”**, *F. P. Bonafé, F. J. Hernández, B. Aradi, Th. Frauenheim, and C. G. Sánchez*, I Argentine Meeting of Quantum Physics, Córdoba, Argentina, Poster.
- 2017 **“An alternative explanation to laser-induced ultrafast vibrational excitations in metal nanoparticles”**, *F. P. Bonafé, B. Aradi, O. A. Douglas-Gallardo, Th. Frauenheim, and C. G. Sánchez*, XX Argentine Meeting of Physical Chemistry and Inorganic Chemistry. Villa Carlos Paz, Córdoba, Argentina, Talk.
- 2017 **“Plasmonic excitation of the breathing mode in metal nanoparticles”**, *F. P. Bonafé, B. Aradi, S. A. Paz, O. A. Douglas-Gallardo, Th. Frauenheim, and C. G. Sánchez*, IV Nanocórdoba. Villa Carlos Paz, Córdoba, Argentina, Talk.
- 2015 **“Model nanomotor driven by circularly polarized light”**, *F. P. Bonafé and C. G. Sánchez*, XIX Argentine Meeting of Physical Chemistry and Inorganic Chemistry. Buenos Aires, Argentina, Talk.

- 2013 **‘TiO₂ as anode material for lithium-ion batteries: a computational study’**, *F. P. Bonafé, F. Y. Oliva, G. L. Luque*, 4th. Iberoamerican Meeting “Hydrogen and sustainable energy sources”, Córdoba, Argentina, Poster.
- 2013 **“DFT and DFT+U calculations to study lithium insertion in different polymorphs of TiO₂.”**, *F. P. Bonafé, F. Y. Oliva, and G. L. Luque*, XVIII Argentine Meeting of Physical Chemistry and Inorganic Chemistry. Rosario, Argentina, Poster.
- 2013 **“Study of the structural parameters that influence surface reactivity of TiO₂ nanoparticles”**, *F. P. Bonafé, V. C. Fuertes, C. F. A. Negre, M. B. Oviedo, F. Y. Oliva, and C. G. Sánchez*, XVIII Argentine Meeting of Physical Chemistry and Inorganic Chemistry. Rosario, Argentina, Poster.
- 2011 **“Effect of the Hoffmeister series on the acid-base properties of human serum albumin: experimental study and theoretical model”**, *F. P. Bonafé, O. R. Cámara, and F. Y. Oliva*, XVII Argentine Meeting of Physical Chemistry and Inorganic Chemistry. Córdoba, Argentina, Poster.

Research works in foreign institutions

- jan-feb/2019 **Visiting PhD student**, “Development of tools, autotest suite and documentation for real-time Ehrenfest dynamics code within DFTB for release”, BCCMS (Fraunheim Group), Universität Bremen, Germany.
- may/2018 **Visiting PhD student**, “Development of tools, autotest suite and documentation for electronic real-time TDDFTB code”, BCCMS, Universität Bremen, Germany.
- oct-dec/2017 **Visiting PhD student**, “Applications of Ehrenfest dynamics and development of a technique to compute pump-probe spectra using real-time TDDFTB”, BCCMS, Universität Bremen, Germany.
- feb-apr/2016 **Visiting PhD student**, “Implementation of electron and Ehrenfest dynamics in DFTB+”, BCCMS, Universität Bremen, Germany.
- 2013 **Undergrad research work**, “Copper indium gallium selenide (CIGS) photovoltaic devices made using selenization of nanocrystal thin films”, Korgel Lab, Department of Chemical Engineering, The University of Texas at Austin. USA, Exchange scholarship provided by The National University of Cordoba.
4 months

Graduate teaching activities

- 2014–2018 **Teacher assistant**, *Dpmt. of Theoretical and Computational Chemistry, School of Chemical Sciences, UNC*, Courses: Calculus I, Calculus II, Calculus III.
- 2018 **Admission Course teacher**, *School of Chemical Sciences, UNC*.

Undergraduate teaching activities

- 2011–2014 **Undergraduate teacher assistant**, *Departments of Physical Chemistry and Theoretical and Computational Chemistry, School of Chemical Sciences, UNC*, Courses: Calculus I, Calculus II, Laboratory I, Laboratory III, General Analytical Chemistry, Admission Course.
- 2010–2011 **Ad-honorem teacher assistant**, *Departments of Physical Chemistry and Theoretical and Computational Chemistry, School of Chemical Sciences, UNC*.

Preparation of course handbooks

- 2017 **"Calculus II: Handbook for Practical Classes"**, *F. P. Bonafé, C. Mansilla Wettstein, C. R. Medrano, D. M. Márquez, L. Reinaudi*, School of Chemical Sciences, UNC.

Scholarships

- 2014–2018 **Doctoral fellowship**, *National Council for Science and Technology (CONICET)*, Director: Dr. Cristián Sánchez, from 01.04.2014.
- 2013 **Exchange studentship**, *Programa Cuarto Centenario, The National University of Córdoba*, fall semester 2013 at the University of Texas at Austin, USA.
- 2011–2012 **Undergraduate research scholarship del C (CIN)**, *National Interuniversity Council (CIN)*, Supervisors: Dr. Fabiana Oliva, Dr. Guillermina Luque, Topics: "Experimental and theoretical study of insertion of alkaline metal cations TiO_2 " (2012) and "Effect of the electrolyte on the charge development in proteins and its applications in protein adsorption on metallic oxides" (2011).

Technology transfer and entrepreneurship

- 2018 **"Empowering UK-ARG": culture and innovation exchange**, *Local coordinator*, 5 day event organised in Córdoba and Buenos Aires with experts in Innovation from the University of Cambridge, Local coordinator.
- 2015–2018 **"Quantum Dynamics": technology based startup**, *Co-founder*, Incubated at the Business Incubator, UNC, www.quantumdynamics.io.
- 2016 **"Vincular Córdoba": public-private links for innovation**, *Invited panelist*, Blas Pascal University.
- 2016 **Naves: national entrepreneurship competition**, *finalist and best scientific startup prize, representing Quantum Dynamics*, Austral University, Buenos Aires.

Courses

- 2017 **Scientific Programming Techniques Workshop**, *Universidad Nacional de Tucumán, Argentina*, Grade: 10/10.
- 2016 **Graduate course: "Pedagogical foundations involved in the teaching of the Chemical Sciences"**, *UNC*, Grade: 10/10.
- 2015 **Graduate course: "Quantum Dynamics"**, *Fac. Cs. Químicas, UNC.*, Calificación: 10 (diez).
- 2015 **Graduate course: "Quantum Espresso Spring School"**, *UNC*, Grade: 10/10.
- 2015 **Graduate course: "The problem of consciousness from the point of view of Philosophy of mind and Natural Sciences"**, *UNC*, Grade: Pass.
- 2014 **Graduate course: "The chemical sciences in Argentina"**, *School of Chemical Sciences, UNC*, Grade: 10/10.
- 2014 **Graduate course: "Quantum mechanical methods based on the DFT. Applications to nanostructured systems."**, *UNC*, Grade: 10/10.
- 2014 **Microsoft Azure for Research Training**, *School of Mathematics, Physics and Astronomy, UNC*.

- 2013 **Third school of GPGPU computing for scientific applications**, *San Carlos de Bariloche, Argentina*, Grade: Pass.
- 2013 **Courses taken at the Universidad of Texas at Austin**, *fall 2013, Austin, Texas, USA*.
- Quantum Mechanics I. Steven Weinberg. Graduate course. Grade: A.
 - Quantum Physics II. Daniel Heinzen. Undergraduate course. Grade: A.
 - Thermodynamics and Statistical Mechanics. Elaine Li. Undergraduate course. Grade: A.

Institutional activities and communication of Science

- 2016–2018 **Member of the Department Council**, *Dpmt. of Theoretical and Computational Chemistry, School of Chemical Sciences, UNC*.
- 2014–2018 **Member of the comission for activities with secondary schools**, *School of Chemical Sciences, UNC*.
- 2014–2015 **Director of “Pensando la Ciencia”**, *project to empower scientific vocation in secondary schools*.
- 2014–2015 **Speaker at the “Week of Science”**, *School of Chemical Sciences, UNC*.
- 2013 **Speaker and Organizer at University Fair “Cuatrociencia”**, *Science and technology exhibition organized as a celebration for the 400th. anniversary of the University*, Topic: Energetic revolution for a sustainable future.

Languages

- 2018 **German**, *Goethe Institute Bremen and Córdoba*, A2.1.
- 2007 **First Certificate in English**, *University of Cambridge ESOL Examinations*, B2.
Grade: A
- 2006 **Preliminary English Test**, *University of Cambridge ESOL Examinations*.
Grade: Pass with Merit

Awards

- 2015 **“10 Outstanding Young People” Award**, *Cordoba Stock Exchange*.
- 2014 **Valedictorian medal**, *Universidad Nacional de Córdoba*, for the best student of the all the University schools and faculty, class 2013.
- 2014 **Universidad Award 2013**, *Diplomma with “Mention of Honor”*.
- 2008 **Award for the academic excelence**, *Roela Bank*, for the best student of secondary school, class 2008.
- 2008 **Academic merit medal**, *Dr. Manuel Lucero Secondary School*, for the best student of the last year of the secondary school.