Franco Bonafé

Personal Information

Name	Franco Paul Bonafé
Date of birth	July 18th, 1990
Birth place	Córdoba, Argentina
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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 Techician, Orientation: Food Industry**, *Dr. Manuel Lucero Secondary School (Córdoba)*, *GPA: 9.64/10*.

Teaching and Research

Publications

2019 **"Simulations of Impulsive Vibrational Spectroscopy"**, *F. J. Hernandez, F. P. Bonafé, B. Aradi, Th. Frauenheim, and C. G. Sanchez*, J. Phys. Chem. A (in revision process).

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 TiO_2"**, *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)Se_2 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 breating 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 **'TiO_2 as anode material for lithium-ion batteries: a computational study"**, *F. P. Bonafé, F. Y. Oliva, G. L. Luque*, 4th. Iberoamerican Meeting "Hydrogen and susteinable energy sources", Córdoba, Argentina, Poster.

2013 **"DFT and DFT+U calculations to study lithium insertion in different polymorphs of TiO_2."**, *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 TiO_2 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 (Frauenheim 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 **Undegraduate 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 Sciencs"**, *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 conciousness from the point of view of Phylosophy 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.