

CURRICULUM VITAE

CARLOS JOSÉ FERNÁNDEZ SOLANO

First Names: Carlos José
Other Name : Solano **Sex:** Male
Address: Friedrich-Humbert-Str. 159
City: Bremen **Province:** Bremen
Telephone: +4915118901525
Personal Website: cjfsolano.com

Last Name: Fernández
Birthday: 21-02-1977
Postal code: 28759
Country: Germany
E-mail: cjfqct@gmail.com

EDUCATION

1. 2004–2009 **PhD in Physical Chemistry** (Honours). University of Oviedo, Asturias, Spain.

PROJECT

Design and implementation of classical and quantum methods for atomistic simulation in materials

Research Supervisor: Dr. Miguel Álvarez Blanco

Source of Funding: FPI doctoral fellowship. Spanish Ministry for Science and Innovation

SUBJECTS

Atomistic simulation in aggregates and nanostructures: computational implementation for *periodic* nanobelts and nanorings; theoretical simulation of AlN nanocrystals, nanobelts and nanorings.

The Quantum Theory of Atoms in Molecules: new software for improving the multipolar expansion convergence in the electrostatic interactions between topological atoms directly bonded; and a study of bipolar expansion in 1,2 Coulomb interactions between topological atoms.

The generalized perturbed ion method: development and computational implementation of local quantum methods for *ab initio* simulation using ionic materials.

2. 2004–2006 **MPhil in Physical Chemistry** (Highest grade achieved). University of Oviedo, Asturias, Spain.

RESEARCH PROJECT

Periodic cluster model and atomistic simulation in AlN nanostructures

Research Supervisor: Dr. Miguel Álvarez Blanco

Source of Funding: FPI doctoral fellowship. Spanish Ministry for Science and Innovation

SUBJECTS

Atomistic simulation in aggregates and nanostructures: computational implementation for *periodic* nanobelts and nanorings; theoretical simulation of AlN nanobelts and nanorings.

3. 1996–2001 **BSc in Inorganic and Physical Chemistry**. University of Oviedo, Asturias, Spain.

Final year dedicated to a deep insight into theoretical chemistry fundamentals and inorganic experimental techniques.

RESEARCH EXPERIENCE

1. Sept 2013–today 2017 **Department of Physics and Earth Sciences**. Jacobs University Bremen (Germany). Post-Doctoral Fellow.

Ion permeation and antibiotic translocation across outer membrane porins of Gram-negative Bacteria.

- Research belongs to the *IMI* european project in which main goal is to understand the molecular basis of the bacterial cell wall permeability. Such a detailed understanding is potentially very helpful in guiding the development of next generation antibiotics.
- I've implemented BROMOCEA code, which is an extension of the Brownian dynamics scheme including conformational dynamics. To this end, an improved GCMC/BD algorithm has been developed in which the dynamics of amino-acid residues is incorporated into the many-body potential of mean force and into the Langevin equations of motion.
- Theoretical study concerning the diffusion route of ciprofloxacin across the outer membrane porin OmpC from *E. coli*. To this end, we establish a protocol to characterize meaningful permeation pathways by combining metadynamics with the zero-temperature string method.

- I've implemented BRODEA code for studying ion permeation and substrate translocation across a nanopore, which is an extension of our previous BROMOCEA code. BRODEA enables one to achieve long simulation times at a low computational cost.
- 2. Feb 2011–Jun 2013 **Laboratory for Chemistry of Novel Materials**. The University of Mons (Belgium). Post-Doctoral Fellow.

Multiscale modeling of ionic liquids and dyes synthesized solar cells.

- Research belonged to the *ORION* european project in which main goal was for advancing the fabrication of inorganic-organic hybrid materials using ionic liquids.
 - Transferable, quantum-chemistry-based, Atomistic many-body Polarizable Potential for Liquids, Electrolytes, and Polymers force field was used for running molecular dynamics of ionic liquids.
 - I implemented a *post-analysis* package for obtaining transport properties, structural properties and atomic (molecular) trajectories.
 - I developed a new methodology for studying interfaces between a semi-conductor surface and ionic liquids as those appearing in new generations of dye sensitized solar cells.
- 3. Jan–Dec 2010 **Institute of Biocomplexity and Informatics**. The University of Calgary (Canada). Post-Doctoral Fellow.

DNA translocation across nanopores using the GCMC/BD algorithm and DNA mesoscale models.

- I was the primary developer of this new approach, which can simulate a much broader range of DNA conformations.
 - I implemented a more robust code, building upon previous implementations of GCMC/BD developed by Noskov, Im, and Roux.
- 4. 2004–2009 **Quantum Chemistry group**. University of Oviedo (Spain). PhD student.

The research work developed in the Quantum Chemistry group can be divided into three blocks: (i) the periodic cluster model, (ii) the bonded Coulomb interactions between topological atoms, and (iii) the generalized perturbed ion method. The main objective was to design new methodologies, algorithms and softwares for materials simulation in a wide range of sizes.

- Achieved ability to work independently.
 - Organised own work as part of a research project.
 - Developed project management skills including scheduling work and prioritising tasks.
- 5. Mar–May 2007 **Manchester Interdisciplinary Biocenter**. The University of Manchester (UK). Academic Visitor.

Study of alternative routes to obtain convergent series for short–range Coulomb interactions between topological atoms: the shift multipole method; L. S. Salmon, F. W. Birss and K. Ruedenberg bipolar expansion; and Padé approximation for multipolar expansion.

- Worked well as a member of a team under considerable pressure maintaining a high degree of accuracy.
 - Conducted extensive planning to fit in the time schedules of my studies with other collaborators.

OTHER EXPERIENCE

1. 2002–2004 Commercial agent in the *Europea de Pinturas Especiales* company. Asturias, Spain.
2. 2006–2007 Private tuition on the Quantum Mechanics principles to BSc Chemistry students. *Academia Urania*, Gijón, Spain.
3. 2013–2017 Lectures about *Electrostatics* in the courses *Introduction to Computer Simulation Methods* and *Computational Challenges in Biology and Biophysics* for Physics and Computational Life Science undergraduate programs. *Jacobs University*, Bremen, Germany.

SKILLS

1. **COMPUTING.** Well versed in various software packages like Microsoft Office, Gnuplot, Adobe Reader and Writer, Ghostview, LaTeX, etc. and operative systems like Windows Vista, XP (and older versions), Linux, UNIX. Elevated experience in C and Python programming languages. Expert in FORTRAN programming language.
2. **COMMUNICATION.** Developed good communication skills thanks to the many articles and reports that were written for several international journals and conferences.
3. **LANGUAGES**
 - Spanish: mother tongue.
 - English: written, proficient. Spoken, proficient.
 - German: written, A2.2 level. Spoken, A2.2 level.