



# Paulo Medeiros

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## Experience

- 2018-Present **Scientific Programmer, SMHI**, Sweden.  
Numerical Weather Prediction Group. Scientific software development and optimisation in collaboration with local, national and international groups and consortia.
- 2015-2017 **Postdoctoral Research Associate, University of Cambridge**, UK.  
Theory of Condensed Matter (TCM) Group, Physics Department (Cavendish Lab.).  
Development, implementation and application of methods for 1D materials search.
- 2010-2011 **Guest Research Fellow, Linköping University**, Linköping, Sweden.  
Computational Physics Division, Department of Physics, Chemistry and Biology, IFM.  
Computational studies of low-dimensional atomic clusters interacting with graphene.
- 2007-2008 **Technical Specialist, Institute of Physics**, Salvador, Brazil.  
Management and maintenance of the computer systems (mainly Linux) at use in the research premises of the Surfaces and Materials Physics Group (GSUMA).

## Selected open-Source Software development

- Since 2014 **BandUP**, *Band Unfolding code for Plane-wave based calculations*.  
Free and open-source code that unfolds the band and spin electronic structures of periodic quantum systems. For more information and downloads, please visit <http://www.ifm.liu.se/theomod/compphys/band-unfolding>.
- Since 2017 **Unlimited Polymorphic Lists in Fortran 2008**.  
A test module that explores object-oriented features that are part of the Fortran 2008 standard, and, in particular, the use of unlimited polymorphic entities. Available in my GitHub page (@paulovcmedeiros).

## Education

- 2011-2015 **Ph.D. in Physics, Linköping University**, Linköping, Sweden.  
Specialization in **Theoretical and Computational Physics**  
Thesis: *Electronic properties of complex interfaces and nanostructures*  
Supervisor: Sven Stafström
- 2008-2010 **MSc. in Physics, Federal University of Bahia**, Salvador, Brazil.  
Specialization in **Solid State and Materials Physics**  
Thesis: *Density functional theory study of the adsorption of alkali and halogen atoms on graphene*.  
Supervisor: Caio Mario Castro de Castilho
- 2004-2008 **BSc. in Physics, Federal University of Bahia**, Salvador, Brazil.

SMHI – Swedish Meteorological and Hydrological Institute  
Folkborgsvägen 17, 601 76 Norrköping, Sweden

☎ +46(0)11 495 83 43 • ✉ paulo.medeiros@smhi.se

🌐 paulovcmedeiros • 🌐 paulovcmedeiros

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## Selected courses and workshops attended

### Technical

- *Programming: Modern Fortran*. NAG & University of Cambridge, UK (2016)
- *Introduction to OpenMP 4.0 (Webinar)*. ARCHER National Supercomputing Service, UK (2016)
- *CASTEP Developer Workshop*. University of Oxford, Oxford, UK (2015)
- *Basic techniques and tools for development and maintenance of atomic-scale software*. CECAM-HQ-EPFL, Lausanne, Switzerland (2014)
- *Shared Memory Programming With OpenMP*. National Supercomputer Centre (NSC), Sweden (2013)
- *KCSE Winter School in Multiscale Modeling*. KTH, Sweden (2012)
- *Brazil-Argentine School of Computer Simulation on Nanomaterials*. UFABC, Brazil (2009)

### Others

- *An Initial Guide to Leadership*. University of Cambridge, UK (2017)
- *Lecturing: An Introduction (Sciences)*. University of Cambridge, UK (2017)
- *Assisting with PhD Supervision*. University of Cambridge, UK (2016)

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## Selected publications\*

- [1] P. V. C. Medeiros et al., “Single-atom scale structural selectivity in the nanowires encapsulated inside ultranarrow, single-walled carbon nanotubes”, *ACS Nano* **11**, 6178–6185 (2017).
- [2] P. V. C. Medeiros, S. S. Tsirkin, S. Stafström, and J. Björk, “Unfolding spinor wavefunctions and expectation values of general operators: Introducing the unfolding-density operator”, *Phys. Rev. B* **91**, 041116(R) (2015).
- [3] P. V. C. Medeiros, S. Stafström, and J. Björk, “Effects of extrinsic and intrinsic perturbations on the electronic structure of graphene: Retaining an effective primitive cell band structure by band unfolding”, *Phys. Rev. B* **89**, 041407(R) (2014).

\*For a full list of publications and citation stats, please visit my Google Scholar profile at <https://scholar.google.se/citations?user=R--GyM4AAAAJ&hl=en>.

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