## **Curriculum Vitae Xavier Blase**



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## Education

Undergraduate studies : Ecole Normale Supérieure de Lyon, France Agrégation de physique (1989). PhD at UC Berkeley, Physics Department (December 1994, advisor: Pr. S.G. Louie) Post-doctoral studies: IRRMA, EPFL, Switzerland, 1995-1996 (advisor: Pr. Roberto Car)

## **Professional experience**

Professor (PCC) Ecole Polytechnique, Palaiseau, France (2006-2009). Research director at CNRS, September 2005-present. Associate researcher (Chargé de recherche) CNRS, 1996-2005.

# **Research activity**

I am a condensed matter physicist with a theoretical background aiming at understanding, sometimes predicting, the properties of various systems, from nanotubes to superconducting diamond, DNA nucleobasis or organic photovoltaic cells, using the methodology of *ab initio* quantum simulations, namely *"in silico"* study of real materials based on the basic principles of quantum mechanics. Besides applications to structural, vibrational, electronic, optical, or (super)conducting properties, much emphasis is given to contributing to the development of novel approaches, in particular in the so-called field of many-body perturbation theory, to progress in the computer-aided description of materials, in terms of accuracy, complexity of the systems and of the "physical observables" that can be calculated. My present main activity concerns the development of an efficient embedded many-body perturbation theory (GW/BSE) package using localized real-space Gaussian bases (the FIESTA initiative) in order to study the properties of organic and hybrid systems in complex electrostatic and dielectric environments, at the interface of physics and chemistry.

#### Awards

CNRS Silver medal 2008. Bull-Fourier prize 2014.

# Main research administration duties

Deputy director, "Condensed Matter Low Temperature" department, Néel Institute (2016-2020) Member of the CNRS National Committee section 05 (2012-2015) Head of the French research network "GDR DFT" (2010-2014) Secretary, condensed matter division, French Physical Society (2005-2008).

## **Publications**

Over 165 publications in peer-reviewed journals including *Science*, *Nature (2)*, *Nature Materials*, Review of Modern Physics, Chemical Society Reviews, Physical Review Letters (25), gathering about 17300 citations (WOS). Ten book chapters. H factor=64. Below are 10 selected relevant publications. Publications with a star are related to the more recent line of work (2011-) associated with the development of efficient "embedded" many-body approaches for molecular systems.

(1) Surface segregation and backscattering in doped silicon nanowires M.-V. Fernandez-Serra, C. Adessi, <u>X. Blase</u>, Phys. Rev. Lett. 96, 166805 (2006).

(2) Superconductivity in doped cubic silicon, E. Bustarret, C. Marcenat, P. Achatz, J. Kacmarcik, F. Lévy, A. Huxley, L. Ortéga, E. Bourgeois, <u>X. Blase</u>, D. Débarre, J. Boulmer, *Nature* (London) 444, 465-468 (2006).

(3) Electronic and transport properties of nanotubes, J.-C. Charlier, <u>X. Blase</u> and S. Roche, Rev. Mod. Phys. 79, 677 (2007).

(4) Superconducting Group IV Semiconductors, <u>X. Blase</u>, E. Bustarret, C. Chapelier, T. Klein, C. Marcenat, *Nature Materials* 8, 375-382 (2009).

(5)\* First-principles GW calculations for fullerenes, porphyrins, phtalocyanine, and other molecules of interest for organic photovoltaic applications, <u>X. Blase</u>, C. Attaccalite, V. Olevano, Phys. Rev. B, 2011, 83, 115103.

(6)\* Electron-phonon coupling in the  $C_{60}$  fullerene within the many-body GW approach, Carina Faber, Jonathan Laflamme Janssen, Michel Cote, E. Runge, <u>X. Blase</u>, Phys. Rev. B, 2011, 84, 155104.

(7)\* Short-range to long-range charge-transfer excitations in the zincbacteriochlorin-bacteriochlorin complex: A Bethe-Salpeter study, I. Duchemin, T. Deutsch, <u>X. Blase</u>, Phys. Rev. Lett., 2012, 109, 167801.

(8) Giant osmotic energy conversion measured in a single transmembrane boron nitride nanotube, A. Siria, P. Poncharal, A.-L. Biance, R. Fulcrand, <u>X. Blase</u>, S.T. Purcell and L. Bocquet, *Nature* 494, 455 (2013).

(9)\* The Bethe-Salpeter Formalism with Polarisable Continuum Embedding: Reconciling Linear-Response and State-Specific Features, I. Duchemin, C. A. Guido, D. Jacquemin and <u>X. Blase</u>, Chem. Sci. 2018, **9**, 4430.

(10)\* Cubic-scaling all-electron GW calculations with a separable density-fitting space-time approach", Ivan Duchemin and Xavier Blase, J. Chem. Theory Comput. 2021, **17**, 4, 2383-2393.