Dario Alfè --- Curriculum Vitae

June 2019

Current position : Professor of Physics**,** Department of Earth Sciences, Thomas Young Centre@UCL and London Centre for Nanotechnology, UCL, Gower Street, WC1E 6BT, U.K. and Professore di Fisica della Materia, Dipartimento di Fisica, Universita' degli studi di Napoli Federico II, Monte S. Angelo, 80126 Napoli, Italy.
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Education : *PhD* in Physics (*cum laude*), S.I.S.S.A., Trieste, Italy (1997). *MPhil* in Physics (*cum laude*) S.I.S.S.A (1995). *Laurea in Fisica* (*cum laude*), University of Trieste (1993).

Positions held :

2018 –	Professore di Fisica della Materia (Full Professor), Universita' di Napoli Federico II.
2006 –	Professor of Physics (Full Professor), UCL.
2003 – 2006	Reader in Physics (Associate Professor), UCL.
2006 – 2011	European Young Investigator (EURYI) Research Fellow, UCL.
2000 – 2006	Royal Society University Research Fellow, UCL.
1998 – 2000	Post Doctoral Research Fellow, UCL.
1997 – 1998	Post Doctoral Research Assistant, Department of Physics, University of Keele.
1993 – 1997	Post graduate student, Scuola Internationale di Studi Avanzati (SISSA), Trieste, Italy.
1994 – 1995	Military service (Italian Police).
1993	Scientific consultant, Sincrotrone Trieste.

Research activity :
190 publications (detailed list available at http://www.homepages.ucl.ac.uk/~ucfbdxa/pubs.htm), including 6 in Nature/Science and 4 in Nature Geoscience/Nature Communications/PNAS. Over 8300/11500 citations (Web of Science/Google Scholar), H-index = 50/58. About 140 invited talks; 8 conferences organised or co-organised ; advisory committee of several international conferences. Total research income as Principal Investigator ~ GBP 4.1 million (M); and GBP 0.74 M as co-Investigator. Awarded over 640 M processor hours (PE) of computer time on machines in the UK, Europe and USA, nominally worth over GBP 14 M.

Research interests :

- Development of computer simulation techniques for condensed matter applications, with particular emphasis on new methods for high accuracy (e.g quantum Monte Carlo), and on improving their efficiency on high performance computers.
- Weak interacting systems, molecular adsorption at surfaces. Two dimensional systems.
- Development of statistical mechanics methods for chemical potentials of solids and liquids.
- High pressure-high temperature properties of Earth materials. Stucture, dynamics, melting and solid-solid phase transitions, transport properties.

Supervision : 13 postdocs, 13 PhD students, 4 Masters Students, 2 visiting Professors.

Current group : 2 postdocs, 2 PhD students.

Prizes/Awards (Total value ~ GBP 1,007,000) **:**

2007 – 2012	The Royal Society : *Wolfson Research Merit Award*, GBP 50,000.
2006	Junior Chamber Italy : *The Outstanding Young Person (TOYP) Prize*, *Research*.
2006 – 2011	European Science Foundation (ESF) : *European Young Investigator Award* (*EURYI*), GBP 904,671.
2005	EPSRC : *High Performance Computing Prize*, GBP 2,000.
2002	Study of the Earth Deep Interior (SEDI) : *Doornbos Memorial Prize*, USA, USD 600.
2002	The Leverhulme Trust : *Philip Leverhulme Prize*, GBP 50,000.

Grants as PI (total value ~ GBP 2,780,000):

2018 – 2024 US Air Force Office for Science and Research : *High accuracy simulation methods for realistic materials modelling,* USD 150,000.
2018 – 2021 Natural Environment Research Council (NERC): *Potassium in the Earth's core*, GBP 525,700.
2015 – 2018 NERC: *Chemical Interactions in the Earth's core*, GBP 488,594.
2013 – 2015 EPSRC: *Quantum Monte Carlo made easy*, GBP 216,600.
2011 – 2014 NERC: *Transport properties in the Earth's core*, GBP 448,491.
2011 – 2013 EPSRC: *Quantum Monte Carlo on ten thousand to a million cores*, GBP 292,421.
2011 – 2012 EPSRC: *Doctoral Training*, GBP 46,953.
2011 – 2012 The Leverhulme Trust: *Visiting Professorship*, *E. Hernandez*, GBP 34,000.
2010 – 2012 The Royal Society : *International Research Projects*, GBP 12,000.
2007 The Leverhulme Trust: *Visiting Professorship*, *S Baroni*, GBP 17,000.
2005 – 2009 NERC: *The melting curve of iron from quantum mechanics*, GBP 169,195.
2008 EPSRC: *The temperature of the Earth's core from QMC,* GBP 10,183.
2007 – 2009 The Royal Society: *International Research Projects*, GBP 11,800.
2000 – 2008 The Royal Society: *University Research Fellowship*, GBP 390,000.

Research contracts as PI (total value ~ GBP 320,000):

2013 – 2017 Atomic Weapons Establishment (AWE): *Melting curves of alkaly metals from first principles*, GBP 32,000.
2010 – 2011 Numerical Algorithm Group (NAG): *dCSE support for HECToR*, GBP 127,000.
2006 – 2010 Johnson & Matthey: *Modelling of new catalysts for fuel cells*, GBP 32,000.
2008 – 2009 NAG: *dCSE support for HECToR*, value GBP 90,000.
2004 – 2011 QID S.r.l. (Italy) Various research contracts for *Numerical modelling of nanostructured surfaces in relation to their catalytic activity,* EUR 45,000.

Grants as co-I (total value ~ GBP 740,000):

2002 – 2007 NERC: *The deep Earth System*, GBP 253,069.
2006 – 2008 EPSRC-AWE: *First principles thermodynamics at extreme conditions*,GBP 184,559.
2008 – 2010 EPSRC: *Ab-initio path integral of reactions on metal surfaces*, GBP 302,900.

Facilities as PI (computer time, total value ~ 640 M PE, worth ~ GBP 14 M):

2019 – DoE : *Innovative and Novel Computational Impact on Theory and Experiments (INCITE)*, 130 M PE on Titan and Summit (Oak Ridge).
2018 – 2021 NERC: *Potassium in the core*, 25 M PE on ARCHER (GBP 210,000)
2017 – 2018 Department of Energy (DoE), *Director's discretionary* (DD) *award*, 20 M PE on Titan, Rhea, Eos (Oak Ridge, USA).
2016 DoE-DD award, 10 M PE on Titan, Rhea, Eos.
2015 – 2018 NERC: *Chemical interactions in the core*, 22.8 M PE on ARCHER (GBP 270,180).
2011 – 2014 NERC: *Transport properties in the core*, 7.2 M PE on HECToR (GBP 600,000).
2010 – 2015 DoE : *INCITE*, 485 M PE on Titan (Oak Ridge) and Mira (Argonne).
2009 DoE : *Director's discretionary award*, 13 M PE on Jaguar (Oak Ridge).
2009 Distributed European Infrastructure for Supercomputing Applications: 1.7 M PE.
2005 – 2009 NERC: *The melting curve of iron*, 0.5 M PE on HPCx (GBP 600,000).
2008 EPSRC: *Capability challenge*, 6.2 M PE on HPCx (GBP 2,083,000).

Institutional Responsibilities :

2019 – Undergraduate admissions tutor, Department of Earth Sciences, UCL.
2018 – Deputy Undergraduate admissions tutor, Department of Earth Sciences, UCL.
2014 – 2018 Chair, Exam Board, Department of Earth Sciences, UCL
2015 – Chair, Computational Resource Allocation group (CRAG). Distributing computer time allocations on the UCL Institutional machines Legion and Grace.
2012 – 2015 Panel member, CRAG.
2014 – Panel member, Board for the procurement of the UCL computational resources. Overseeing the purchase of the machine "Grace" and its upgrades.
2007 – Panel member, Executive board of the Thomas Young Centre@UCL.

Teaching activities:

2019 – Course organiser – "Termodinamica computazionale", 5th year, Fisica, Università di Napoli Federico II.

2011 – Course organiser – "Deep Earth and Planetary Modelling", 4th year, Earth Sciences, UCL.

2011 – 2014 Course organiser – "Earth and Planetary System Science", 4th year, Earth Sciences, UCL.

2009 – Contributor – "Electronic Structure Methods for Material Modelling", post-graduate course, Physics and Astronomy, UCL.

Other appointments :

2007 – Review panel, ARCHER (the UK National super-computer facility), Computational Science and Engineering (dCSE) support. Assigning approximately 14 full time positions per year to improve the performance of computer codes running on ARCHER (from 2014) and HECToR (2007-2013).

2011 – Review panel, Sandia National Laboratories Z Facility (USA). Assigning approximately 20 days/year of time on the Z machine. This panel meets every 2 years.

2016 Review panel, German Research Foundation.

2014 Review panel, European Science Foundation (ESF) Graphene Flagship call.

2012 Review panel, Philip Leverhulme Prize for Earth, Ocean and Atmospheric science. Assigning 7 prizes worth GBP 100,000 each.

2008 – ESF pool of reviewers.

2012 Reviewer, National Research Assessment (ANVUR), Italy.

2015 – Editorial board, *Physics of the Earth and Planetary Interiors.*

2010 – 2015 National Centre for Computational Science User Council (USA).

2001– 02, 2003, 2004 – 05, 2008 Visiting Professor, S.I.S.S.A.

2001 – 2016 Lectured at over 10 international advanced schools in Austria, China, Finland, France, Germany, Italy, Spain, Switzerland, USA.

2005 – 22 PhD thesis examined worldwide.

Dissemination to the Public :

I have been involved in public dissemination of science events like the BBC Radio 4 program "The material World" (2000), an interview on the Italian RAI television program "Explora" (2006), the RAI International program "Il caffè" (2010), an interview on "Le Scienze" [448, 14 (2005)] (the Italian edition of "Scientific American"), an article in Focus (2006), one in Le Science 2016, and I had various articles on U.K. (The Mirror [1999], The Guardian [2004], The Evening Standard [2005]) and Italian (Il Sole 24 Ore [2005], Il Piccolo [2001, 2005, 2010, 2012, 2016], Trieste News [2012], La voce del Titerno [2005], Il Sannio [2005], Trieste Città [2005], Il Mattino [2005], Io donna [2010], Il fatto quotidiano [2014, 2014]) newspapers. Our work on the conductivity of the Earth's core has been covered in an article in "The New York Times" [2012] and an article in the "Discover" magazine [2014].