

CURRICULUM VITAE

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DEGREES

1981 Doctor of Philosophy, University of Cambridge. Thesis entitled *Aspects of Transformation Behaviour in Olivine, Pyroxenes and Titanomagnetites*
1977 Bachelor of Arts, Clare College, University of Cambridge. 1st Class Honours in both Parts of the Natural Sciences Tripos. Part 2 specialisation in Mineralogy and Petrology. Proceeded in 1981 to the degree of Master of Arts, University of Cambridge

POSITIONS HELD

2007– UCL Vice-Provost (Research)
2006–2007 Executive Dean, UCL Faculty of Mathematical & Physical Sciences
2004–2005 Head of Department, UCL Earth Sciences, and Director of the UCL/Birkbeck Research School of Earth Sciences
2003–2006 Vice-Dean (Research), UCL Faculty of Mathematical & Physical Sciences
1992–2002 Head of Department, UCL Geological Sciences, and Director of the UCL/Birkbeck Research School of Geological & Geophysical Sciences
1991– Professor of Mineral Physics (tenable jointly at UCL and Birkbeck College 1991–2006)
1987–1990 University of London Reader in Mineral Physics, tenable jointly at UCL and Birkbeck College
1983–1987 Royal Society University Research Fellow in UCL Department of Geological Sciences
1981–1983 Natural Environment Research Council Research Fellow, working in the Department of Earth Sciences, University of Cambridge
1980–1981 Fulbright-Hayes Scholar and Research Associate at the Department of the Geophysical Sciences, University of Chicago, working with Prof JV Smith FRS
1977–1980 Natural Environment Research Council Student (by competition), researching the subsolidus behaviour of iron-titanium oxides, having nominated Dr JDC McConnell, of the Department of Mineralogy & Petrology, University of Cambridge, as supervisor
1974 Assistant Scientific Officer at the National Physical Laboratory (Teddington, Middx), researching into dispersive Fourier transform spectroscopy

MEMBERSHIP OF SCIENTIFIC ASSOCIATIONS

Elected Member of the Academia Europaea
Fellow and Past-President of the Mineralogical Society of Great Britain & Ireland

Fellow of the Geological Society of London
Elected Fellow of the Mineralogical Society of America
Elected Fellow of the American Geophysical Union

OTHER APPOINTMENTS

2011– Non-Executive Director, North Middlesex University Hospital NHS Trust
2010– Chair of the UK HEFCE REF2014 Sub-Panel UoA 7: Earth & Environmental Sciences
2010– Chair of Governors, UCL Academy School, Camden
2010– Member of Elsevier's Academic Executive Advisory Board
2010– Co-convenor of the committee of 'Vice-Rectors' of Research of the League of European Research Universities
2010– Chair of Governors of the UCL Academy School, Camden
2010–2011 Member of the Council and Trustee of the Royal Institution
2009 Assessor for the Crafoord Prize Nomination Committee of the Royal Swedish Academy of Sciences
2006–2007 Scientific Consultant for BBC five-part series *Earth: The Power of the Planet*
2005–2008 Member of the UK RAE Sub-Panel 17 for Earth Sciences
2005–2007 Member of the Natural Environment Research Council Peer Review College
2005–2007 Editor of *Earth & Planetary Science Letters*
2004–2008 Member of the Awards Committee of the Geological Society of London
2004–2006 President of the Mineralogical Society of Great Britain & Ireland
2003–2009 Member of the Governing Body and Chair of the Curriculum Committee, La Sainte Union Secondary School, Highgate
2003–2007 Member of the HECToR Science Board (EPSRC)
2003–2007 Member of the Davy Faraday Research Laboratory Committee of the Royal Institution
2003–2006 Member of Council, UCL
2002–2006 Member of the Dana Medal Committee of the Mineralogical Society of America
2001–2008 Member of the High Performance Computing Strategy Board of the Research Councils (RCUK)
2000–2003 Member of the ISIS Facility Access Panel for CCLRC
2000–2003 Member of the HPC(X) Management Board (EPSRC)
1999–2004 Associate Editor, *JGR-Solid Earth*
1998–2002 Secretary of the International Mineralogical Association's Commission on the Physics and Chemistry of Minerals
1996– Member of the Editorial Board of *Physics & Chemistry of Minerals*
1996–1998 Member of the NIREX Geology Review Panel
1996 Member of the Review Group for the Geophysical Laboratory, Washington DC
1995–2001 Chair of the Medals Committee of the European Mineralogical Union
1994–1997 Member of NERC's Earth Science & Technology Board
1993–1996 Member of the SERC's CCP5 committee for the modelling of ionic systems
1992– Member of the editorial board of *Physics of the Earth & Planetary Interiors*
1992–1996 Member of the IASPEI commission on the physical properties of materials of the Earth's interior
1992–1996 Vice-President of the European Mineralogical Union

1991–1994	Member of the International Programme Committee for the 1994 IMA General Meeting, Pisa
1989–1993	Co-Convenor of the Steering Committee of the UCL Centre for Materials Research
1989–1992	Member of the NERC Geological Sciences Research Grants & Training Awards Committee
1987–1990	Committee member of the Physical Crystallography Group of the British Crystallographic Association
1986–1992	Officer (Publications Manager) of the Mineralogical Society of Great Britain & Ireland
1986–1990	Chairman of the International Mineralogical Association's Commission on the Physics & Chemistry of Minerals
1985–1986	Council Member of the Mineralogical Society of Great Britain & Ireland

AWARDS, RECOGNITION, etc

2006	Awarded the Louis Néel Medal of the European Geosciences Union for “establishing the importance of computational mineral physics in Earth sciences and for outstanding contributions to the physics of the Earth's core”
2005	Elected Fellow of the American Geophysical Union
2005	Listed in <i>Who's Who</i>
2003	Named one of the Top 10 British Geologists – <i>Independent on Sunday</i> (London), 10 August 2003, Section: Business, p8
2002	Awarded the Murchison Medal of the Geological Society of London
2000	Elected Member of the Academia Europaea
1999	Awarded the Schlumberger Medal of the Mineralogical Society of Great Britain & Ireland
1997–1998	Awarded a Leverhulme Research Fellowship
1997	Elected a Fellow of the Mineralogical Society of America in recognition of significant contributions to the fields of mineralogy, petrology and crystallography
1990–1997	Visiting Research Fellow at the Natural History Museum, London
1990	MacRoberts Lecturer at the Royal Institution
1981–1983	Research Fellow at Clare College, Cambridge
1980–1981	Senior Research Scholar of the Fulbright-Hayes programme
1977	Awarded Clare College Horne Prize
1976	Awarded Clare College Foundation Scholarship
1975	Awarded Clare College Scholarship

RESEARCH GRANTS

2005	NERC grant NE/C515704/1 & NE/C515698/1 <i>E-minerals: Application of GRID-enabled science to understand the environment from the molecular level</i> (with M Dove, Brodholt et al) – £1,335,601
2005	EPSRC grant EP/C534360/1 <i>First-principles thermodynamics of metals under extreme conditions</i> (with M Gillan and D Alfe) – £184,559
2005	NERC grant NE/C519662/1 <i>The structure and anisotropy of the earth's core</i> (with Voadlo and Brodholt) – £163,561
2002	NERC grant NER/T/S/2001/00855 <i>Environment from the molecular level: An e-science project for modelling the atomistic processes involved in environmental issues</i> (with M Dove et al) – £1,657,644
2002	NERC grant NER/O/S/2001/01262 <i>The Deep Earth System</i> (with J Brodholt et al) – £253,000

- 1998 NERC grant GR3/11779 *Computer modelling of grain boundary properties and behaviour in rock forming minerals* (with SC Parker & CRA Catlow) – £111,128
- 1998 NERC grant GR3/12083 *Ab initio study of the free energies and equations of state of liquid and crystalline alloys of Fe at core P and T* (with M Gillan) – £142,822
- 1998 JREI grant JR98UCGI *Advanced computation for quantum studies* (with M Gillan) – £532,325
- 1998 NERC grant GR9/03550 *High performance computing for mineral physics* (with J Brodholt) for four years' access to Cray T3E at CSAR – £1,080,000
- 1996 NERC grant GST/02/1454 *Ab initio study of Fe* (with M Gillan) – £89,292
- 1996 NERC grant GR3/R9627 *Computer modelling of hydrothermal synthesis of minerals* (with CRA Catlow) – £85,140
- 1994 NERC grant GR3/9191 *Experimental and modelling approach to diffusion* (with S Elphick) – £251,286
- 1994 NERC grant GST/02/1002 *HPC Computational Mineral Physics* – £77,791
- 1993 NERC grant GR3/8600 *Rheology of perovskites* – £112,357
- 1993 EC Human mobility grant (with V Saunders et al) – €22,000
- 1993 NERC grant GR3/8816 *Melting and the thermal structure of the Earth* – £148,496
- 1993 SERC grant GR/J31865 *Computational studies of polar and molecular solids* (with CRA Catlow and SL Price) – £233,555
- 1992 NERC grant *Advanced computing* (with CRA Catlow) – £57,200
- 1991 NERC research grant GR3/6970 *Supplement to study computer models of silicates* (with CRA Catlow & SC Parker) – £259,289
- 1991 Birkbeck College grant *High P research* (with RJ Angel) – £8,000
- 1991 British Council Alliance grant – £1,000
- 1990 Guest Research Fellowship grant from the Royal Society (to allow visit of M Matsui, Japan) – £ 8,500
- 1990 SERC Computer Science Initiative grant (with CRA Catlow and SL Price) – £235,000
- 1989 EEC twinning grant (with M Madon, Paris) – €176,000
- 1989 NERC research grant GST/02/435 *High pressure systems* (with Jones, Ross and Angel) – £3,750
- 1988 NERC research grant GR3/6970 *Computer models of silicates* (with CRA Catlow & SC Parker) – £139,859
- 1988 ICI research grant *Zeolite stability* – £61,000
- 1988 University of London Court *High pressure research* – £50,000
- 1988 UCG Earth Science Equipment (FTIR spectrometer) – £160,000
- 1987 NERC research grant GR3/6358 *Lattice dynamics of mantle-forming minerals* – £62,662
- 1987 Royal Society equipment grant – £ 3,600
- 1986 NERC research grant GR3/5993 *Perovskite rheology* – £44,802
- 1985 Grant from ICI *Zeolite research* – £30,000
- 1985 Guest Research Fellowship grant from the Royal Society (for DJ Weidner) – £6,300
- 1983 Research Fellowship from the Royal Society – £66,500

SELECT INVITED PRESENTATIONS

- 2009 Keynote speaker, Goldschmidt Conference, Davos, Switzerland
- 2006 Neel Medal Lecturer, EGS, Vienna
- 2006 Member, the International Advisory Committee, 44th EHPRG, Prague

2006 Invited speaker and session convener, IMA2006-Kobe

2005 Member, Physics and Chemistry of Minerals Programme Group, IASPEI Assembly, Chile

2005 Organiser, the William Smith Meeting of the Geological Society of London on *The Deep Earth*

2003 Invited speaker, Vening Meinesz Research School Integrated Geodynamics Symposium, University of Utrecht

2003 Invited speaker, Spring Meeting American Physical Society, Austin Texas

2003 Keynote speaker, Union Symposium, *The State of the Planet*, IUGG Sapporo Japan

2003 Invited speaker, Department Crystallography, ETH Zurich

2002 Invited speaker, Department of Geological Sciences, Princeton University, New Jersey

2002 Session convenor and speaker, IMA Edinburgh

2002 Invited speaker and session chair, Fall AGU, San Francisco

2001 Invited speaker at ESF meeting on *Ultra-High Pressure Physics*, Corsica

2001 Organiser of CECAM/ESF meeting on *Ab Initio Calculations in Geophysics*, Lyon

2001 Invited speaker, Gordon Conference on *Earth's Deep Interior*, Mt Holyoake College

2001 Invited speaker at the Royal Society Discussion Meeting, *New science from high performance computing*, London

2000 Invited speaker, SEDI 2000, Exeter

1999 Discourse Lecture at the Royal Institution

1999 Session convenor and speaker, EUG 10

1999 Speaker and session chair, IUCr, Glasgow

1999 Invited Speaker at ESF School on the "Deep Earth", Aquafredda, Italy

1998 Plenary lecturer, Toronto IMA

1998 Speaker, NATO ASI *Microscopic processes in minerals*, Lucca, Italy

1996 BCA Cambridge

1994 EMPG-V symposium, UCL

1994 Goldsmidt Conference, Edinburgh

1994 IMA meeting, Pisa

1993 Discourse Lecturer at the Royal Institution

1993 Speaker and symposium convenor, EUG VII

1992 Quo Vadis Meeting, UK Geological Society

1992 4th Int Symp of Expt Min and Pet, Claremont-Ferrand

1991 IUGG, Vienna

1990 IUCr, Bordeaux

1989 EUG V, Strasbourg

1989 28th IGC, Washington

1989 2nd Mineralogical Society Winter Conference, UCL

1988 Royal Society Discussion Meeting, *Seismic tomography and mantle circulation*

1988 European geotraverse workshop, Utrecht

1987 CCP5 Computer simulations meeting, UMIST

1987 EUG IV, Strasbourg

1987 Competing interactions and microstructures, Los Alamos

1987	NATO ASI Thermodynamics of Minerals, Cambridge
1986	14th IMA, Stanford, USA
1985	EUG III, Strasbourg
1985	European Meeting on Modulated structures, Bad Honnef, West Germany.
1982	13th IMA, Varna, Bulgaria
1981	IUCr, Ottawa

PUBLICATIONS

2011

Li, L and Weidner, DJ and Brodholt, J and Alfe, D and Price, GD (2011) *Ab initio molecular dynamic simulation on the elasticity of Mg₃Al₂Si₃O₁₂ pyrope*. J EARTH SCI-CHINA , 22 (2) 169–175. 10.1007/s12583-011-0169-6

Ono, S and Brodholt, JP and David Price, G (2011) *Elastic, thermal and structural properties of platinum*. Journal of Physics and Chemistry of Solids, 72 (3) 169–175

2010

BouDagher-Fadel, MK; Price, GD *Evolution and Paleogeographic Distribution of the Lepidocyclinids*. Journal of Foraminiferal Research, 40, 79–108, 2010

Marcelle K. BouDagher-Fadel and G. David Price, 2010. *American Miogypsinidae: An analysis of their phylogeny and biostratigraphy*. Micropaleontology, 56, 567–586

Marcelle K. BouDagher-Fadel, G. David Price and Eduardo A. M. Koutsoukos. In press. *Foraminiferal biostratigraphy and palaeoenvironments of the Oligocene-Miocene carbonate succession in Campos Basin, southeastern Brazil*. Stratigraphy.

2009

Li, L; Weidner, DJ; Brodholt, J; Alfe D; Price GD. *Ab initio molecular dynamics study of elasticity of akimotoite MgSiO₃ at mantle conditions*. PHYSICS OF THE EARTH AND PLANETARY INTERIORS, 173 (1–2): 115–120 MAR 2009.

BouDagher-Fadel, MK; Price, GD. *Loftusia persica: an Eocene Lazarus occurrence?* MICROPALAEONTOLOGY, 55 (1): 75–85 2009

Bejina, F; Blanchard, M; Wright, K; Price GD. *A computer simulation study of the effect of pressure on Mg diffusion in forsterite*. PHYSICS OF THE EARTH AND PLANETARY INTERIORS, 172 (1–2): 13–19 JAN 2009

2008

Takada A, Richet P, Catlow CRA, Price GD (2008) *Molecular dynamics simulation of temperature-induced structural changes in cristobalite, coesite and amorphous silica*. JOURNAL OF NON-CRYSTALLINE SOLIDS, 354, 181–187.

Ono, S; Brodholt, JP; Price, GD (2008) *Structural phase transitions in IrO₂ at high pressures*. JOURNAL OF PHYSICS-CONDENSED MATTER, 20, Article Number: 045202.

Ono, S; Brodholt, JP; Alfe, D, Price GD (2008) *Ab initio molecular dynamics simulations for thermal equation of state of B2-type NaCl*. JOURNAL OF APPLIED PHYSICS, 103, Article Number: 023510.

Vocadlo L, Wood IG, Alfe D, Price GD (2008) *Ab initio calculations on the free energy and high P-T elasticity of face-centred-cubic iron*. EARTH AND PLANETARY SCIENCE LETTERS, 268, 444–449.

Ono S, Brodholt JP, Price GD (2008) *First-principles simulation of high-pressure polymorphs in MgAl₂O₄*. PHYSICS AND CHEMISTRY OF MINERALS, 35, 381–386.

Knight, KS; Price, GD. *Powder Neutron-Diffraction Studies of Clinopyroxenes. I. The Crystal Structure and Thermoelastic Properties of Jadeite between 1.5 and 270 K*. Canadian Mineralogist, 46: 1593–1622 Part 6 Dec 2008.

Vocadlo, L; Wood, IG; Gillan, MJ; Brodholt J ; Dobson DP; Price GD; Alfe D. *The stability of bcc-Fe at high pressures and temperatures with respect to tetragonal strain*. PHYSICS OF THE EARTH AND PLANETARY INTERIORS, 170 (1–2): 52–59 SEP 2008.

Ono, S; Brodholt, JP; Price, GD. *Phase transitions of BaCO₃ at high pressures*. MINERALOGICAL MAGAZINE, 72 (2): 659–665 APR 2008

Wood, IG; Vocadlo, L; Dobson, DP; Price GD et al. *Thermoelastic properties of magnesiowustite, (Mg_{1-x}Fe_x)O: determination of the Anderson-Gruneisen parameter by time-of-flight neutron powder diffraction at simultaneous high pressures and temperatures*. JOURNAL OF APPLIED CRYSTALLOGRAPHY, 41: 886-896 Part 5 OCT 2008

Ono, S; Oganov, AR; Brodholt, JP; Vocadlo L; Wood IG; Lyakhov A ; Glass CW; Cote AS; Price GD. *High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores*. EARTH AND PLANETARY SCIENCE LETTERS, 272 (1–2): 481–487 JUL 30 2008.

2007

Stackhouse S, Brodholt JP, Price GD (2007) *Electronic spin transitions in iron-bearing MgSiO₃ perovskite*. EARTH AND PLANETARY SCIENCE LETTERS 253 (1–2): 282–290 JAN 15.

Li L, Weidner DJ, Brodholt J, Price GD (2007) *The effect of cation-ordering on the elastic properties of majorite: An ab initio study*. EARTH AND PLANETARY SCIENCE LETTERS 256 (1–2): 28–35 APR 15.

Takada A, Richet P, Catlow CRA, Price GD (2007) *Molecular dynamics simulation of polymorphic and polyamorphic transitions in tetrahedral network glasses: BeF₂ and GeO₂*. JOURNAL OF NON-CRYSTALLINE SOLIDS 353 (18–21): 1892–1898.

Price GD (2007) *Mineral Physics: Past, Present, and Future*. In Schubert G (editor in chief) Treatise on Geophysics: *Mineral Physics* (ed: GD Price), 2, 1–6.

Price GD (ed) (2007) *Mineral Physics*. Treatise on Geophysics (Schubert G (editor in chief)), 2, p642.

Takada A, Richet P, Catlow CRA, Price GD (2007) *A molecular dynamics simulation of complex structural changes in amorphous silica at high temperatures*. PHYSICS AND CHEMISTRY OF GLASSES-EUROPEAN JOURNAL OF GLASS SCIENCE AND TECHNOLOGY PART B, 48, 182–187.

Alfredsson M, Cora F, Dobson DP, Davy J, Brodholt JP, Parker, SC, Price, GD (2007) *Dopant control over the crystal morphology of ceramic materials*. SURFACE SCIENCE, 601, 4793–4800.

Alfe, D; Gillan, MJ; Price, GD (2007) *Temperature and composition of the Earth's core*. CONTEMPORARY PHYSICS, 48, 63–80.

2006

Stackhouse, S., J. P. Brodholt, and G. D. Price (2006), *Elastic anisotropy of FeSiO₃ end-members of the perovskite and post-perovskite phases*, Geophys. Res. Lett., 33, L01304, doi:10.1029/2005GL023887

Ostanin S, Alfe D, Dobson D, Vocadlo L, Brodholt JP, Price GD (2006) *Ab initio study of the phase separation of argon in molten iron at high pressures*. GEOPHYSICAL RESEARCH LETTERS 33 (6): Art. No. L06303.

Stackhouse S, Brodholt JP, Dobson DP, Price GD (2006) *Electronic spin transitions and the seismic properties of ferrous iron-bearing MgSiO₃ post-perovskite*. GEOPHYSICAL RESEARCH LETTERS 33 (12): Art. No. L12S03.

Li L, Weidner DJ, Brodholt J, Alfe D, Price GD, Caracas R, Wentzcovitch R (2006) *Phase stability of CaSiO₃ perovskite at high pressure and temperature: Insights from ab initio molecular dynamics*. PHYSICS OF THE EARTH AND PLANETARY INTERIORS 155 (3–4): 260–268.

Li L, Weidner DJ, Brodholt J, Alfe D, Price GD, Caracas R, Wentzcovitch R (2006) *Elasticity of CaSiO₃ perovskite at high pressure and high temperature*. PHYSICS OF THE EARTH AND PLANETARY INTERIORS 155 (3–4): 249–259.

Gillan MJ, Alfe D, Brodholt J, Vocadlo, L., Price, G. D. (2006) *First-principles modelling of Earth and planetary materials at high pressures and temperatures*. REPORTS ON PROGRESS IN PHYSICS 69 (8): 2365–2441.

Li L, Weidner DJ, Brodholt J, Alfe D, Price GD (2006) *Elasticity of Mg₂SiO₄ ringwoodite at mantle conditions*. PHYSICS OF THE EARTH AND PLANETARY INTERIORS 157 (3–4): 181–187.

Mehta S, Price GD, Alfe D (2006) *Ab initio thermodynamics and phase diagram of solid magnesium: A comparison of the LDA and GGA*. JOURNAL OF CHEMICAL PHYSICS 125 (19): Art. No. 194507 NOV 21.

2005

- S. Stackhouse, J.P. Brodholt, J. Wookey, J-M. Kendall and G.D. Price; (2005) *The effect of temperature on acoustic anisotropy of the perovskite and post-perovskite polymorphs of MgSiO₃*. Earth Planet Sci. Lett. 230(1–2) 1–10.
- Alfredsson M, Brodholt JP, Dobson DP, Oganov AR, Catlow CRA, Parker SC, Price GD (2005) *Crystal morphology and surface structures of orthorhombic MgSiO₃ perovskite*. Physics and Chemistry of Minerals, 31 (10): 671–682.
- Oganov AR, Price GD (2005) *Ab initio thermodynamics of MgSiO₃ perovskite at high pressures and temperatures*. J CHEM PHYS 122 (12): art. no. 124501.
- Caracas R, Wentzcovitch R, Price GD, Brodholt J (2005) *CaSiO₃ perovskite at lower mantle pressures*. GEOPHYS RES LETT 32 (6): art. no. L06306.
- Oganov AR, Gillan MJ, Price GD (2005) *Structural stability of silica at high pressures and temperatures*. PHYS REV B 71 (6): art. no. 064104.
- M. Alfredsson, F. Cora, J. P. Brodholt P.B. Wilson and G. D. Price (2005) *Magnetic and Structural Phase Transitions using hybrid functionals*, Mol. Sim., 31, 367–377.
- S. Wells, D. Alfe, L. Blanchard, J. Brodholt, M. Calleja, C.R.A. Catlow, G.D. Price, R. Tyler, K. Wright (2005) *Ab-initio simulations of magnetic iron sulphides*, Mol. Sim., 31, 379–384.
- Dove, M. T., Calleja, M., Bruin, R., Wakelin, J., Tucker, M. G., Lewis, G. J., Mehmood Hasan, S., Alexandrov, V. N., Keegan, M., Ballard, S., Tyer, R. P., Todorov, I., Wilson, P. B., Alfredsson, M., Price, G.D., Chapman, C., Emmerich, W., Wells, S. A., Marmier, A., Parker, S. C., Du, Z. (2005) *The Minerals laboratory tools and experience*. Mol. Sim. 31, 329–337.
- S. Stackhouse, J. P. Brodholt, and G. D. Price (2005) *High temperature elastic anisotropy of the perovskite and post-perovskite polymorphs of Al₂O₃*, GEOPHYSICAL RESEARCH LETTERS, 32 (13): art. no. L13305.
- Oganov AR, Price GD, Scandolo S (2005) *Ab initio theory of planetary materials*. Z Kristallogr., 220 531–548.
- L. Li, J. Brodholt, S. Stackhouse, D. J. Weidner, M. Alfredsson, and G. D. Price (2005) *Electronic spin state of ferric iron in Al-bearing perovskite in the lower mantle*, GEOPHYSICAL RESEARCH LETTERS 32 (17): Art. No. L17307.
- Alfredsson M, Cora F, Brodholt JP, Parker SC, Price GD (2005) *Crystal morphology and surface structures of orthorhombic MgSiO₃ in the presence of divalent impurity ions*. PHYSICS AND CHEMISTRY OF MINERALS 32 (5–6): 379–387.
- Blanchard M, Alfredsson M, Brodholt J, Price GD, Wright K, Catlow CRA (2005) *Electronic structure study of the high-pressure vibrational spectrum of FeS₂ pyrite* JOURNAL OF PHYSICAL CHEMISTRY B 109 (46): 22067–22073.
- Wookey J, Stackhouse S, Kendall JM, Brodholt J, Price GD (2005) *Efficacy of the post-perovskite phase as an explanation for lowermost-mantle seismic properties* NATURE 438 (7070): 1004–1007.
- Adrian P. Jones, Kai Wünemann, G. David Price (2005) *Modeling impact volcanism as a possible origin for the Ontong Java Plateau*. Geological Society of America, Special Paper 388, 711–720.
- Li L, Brodholt JP, Stackhouse S, Weidner DJ, Alfredsson M, Price GD *Elasticity of (Mg, Fe)(Si, Al)O₃-perovskite at high pressure*. EARTH AND PLANETARY SCIENCE LETTERS 240 (2): 529–536 DEC 1 2005.

2004

- Gubbins D, Alfè D, Masters G, Price GD, Gillan MJ (2004) *Gross thermodynamics of 2-component core convection*. Geophysical Journal International, 157, 1407–1414.
- Vočadlo L, Alfè D, Price GD, Gillan MJ (2004) *Ab initio melting curve of copper by the phase co-existence approach*. J Chem Phys 120: 2872–2878.
- F. Nimmo, G.D. Price, J. Brodholt, D. Gubbins (2004) *The influence of potassium on core and geodynamo evolution* Geophysical Journal International, 156: 363–376.
- I. G. Wood, Lidunka Vočadlo, K. S. Knight, David P. Dobson, W. G. Marshall, G. David Price and John Brodholt (2004) *Thermal expansion and crystal structure of cementite, Fe₃C, between 4K and 600K determined by time-of-flight neutron powder diffraction*. J Appl Cryst, 37: 82–90.

Alfe D, Vocadlo L, Price GD, Gillan MJ (2004) *Melting curve of materials: theory versus experiments*. J Phys-Condens Mat 16: S973–S982.

Alfe D, Price GD, Gillan MJ (2004) *The melting curve of iron from quantum mechanics calculations*. J Phys Chem Solids 65: 1573–1580.

Martin, P., Vočadlo, L., Alfè, D., and Price, G. D. (2004) *An Ab Initio Study of the Relative Stabilities and Equations of State of Fe₃S Polymorphs*. Mineralogical Magazine, 68, 813–817.

Takada A, Richet P, Catlow CRA, Price GD. (2004) *Molecular dynamics simulations of vitreous silica structures*. J NON-CRYST SOLIDS 345–46: 224–229.

Alfredsson M, Price GD, Catlow CRA, Parker SC, Orlando R, Brodholt JP (2004). *Electronic structure of the antiferromagnetic B1-structured FeO*. PHYS REV B 70 (16): art. no. 165111.

G. D. Price, D. Alfè, L. Vocadlo, M. J. Gillan, (2004) *The Earth's core: an approach from first principles*, in "The State of the Planet: Frontiers and Challenges in Geophysics" (Editors R. S. J. Sparks and C. J. Hawkesworth), AGU Geophysical Monograph Series 150, 1–12.

2003

Jones AP, Price GD, De Carli, PS, Price, NJ, Clegg, RA (2003) *Impact decompression melting: a possible trigger for impact induced volcanism and mantle hotspots?* In: Impact markers in the Stratigraphic Record (eds C Koeberl and F Martinez-Ruiz), Springer, Berlin, p91–120.

Alfe D, Gillan MJ, Price GD (2003) *Thermodynamics from first principles: temperature and composition of the Earth's core*. Mineral Mag 67 (1): 113–123.

Oganov AR, Gillan MJ, Price GD (2003) *Ab initio lattice dynamics and structural stability of MgO*. J Chem Phys. 118 10174–10182.

Jones A P, Mutanen T, Tuisku P, Hanski E and Price G D (2003) *The Pechenga structure, Russia: giant Ni-Cu mineralisation related to large meteorite impact?* Applied Earth Science (Trans. Inst. Min. Metall. B), Vol. 112, B149–150.

Vočadlo L, Alfè D, Gillan MJ, Wood IG, Brodholt JP, Price, GD (2003) *Possible thermal and chemical stabilisation of body-centred-cubic iron in the Earth's core?* Nature, 424: 536–539.

Takada A, Catlow CRA, Price GD (2003) *'Computer synthesis' of B₂O₃ polymorphs*. Phys Chem Glasses 44: 147–149.

Vočadlo L, Alfè D, Gillan MJ, Price GD (2003) *The properties of iron under Core conditions from first principles calculations*, Physics of the Earth and Planetary Interiors, 140, 101–125.

Gubbins D, Alfè D, Masters G, Price GD, Gillan MJ (2003) *Can the Earth's Dynamo run on Heat Alone?* Geophysical Journal International, 155, 609–622.

2002

Alfe, D, Gillan, MJ, Price, GD (2002) *Composition and temperature of the Earth's core constrained by combining ab initio calculations and seismic data*. Earth Planet. Sci. Lett. 195, 91–98.

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