# Neil Allan

List of Publications by Year
in descending order



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|---|---|---|---|
| 161 papers | 5,556 citations | 109321 35 h-index | 91884 69 g-index |
| 164 all docs | 164 docs citations | 164 times ranked | 6069 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Ab initio study of structural, elastic and thermodynamic properties of Fe3S at high pressure: Implications for planetary cores. American Mineralogist, 2022, 107, 248-256. | 1.9 | 0 |
| 2 | Ab initio study of negative electron affinity on the scandium-terminated diamond (100) surface for electron emission devices. Carbon, 2022, 196, 176-185. | 10.3 | 6 |
| 3 | Hunting the elusive shallow n-type donor â€“ An ab initio study of Li and N co-doped diamond. Carbon, 2021, 171, 857-868. | 10.3 | 9 |
| 4 | Multiple cascade radiation damage simulations of pyrochlore. Molecular Simulation, 2021, 47, 273-283. | 2.0 | 2 |
| 5 | Interatomic forces breaking carbon-carbon bonds. Carbon, 2021, 175, 420-428. | 10.3 | 7 |
| 6 | Improving Hydride Conductivity in Layered Perovskites via Crystal Engineering. Chemistry of Materials, 2021, 33, 177-185. | 6.7 | 8 |
| 7 | Fast-ion conduction and local environments in BIMEVOX. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200430. | 3.4 | 5 |
| 8 | Energy landscapes of perfect and defective solids: from structure prediction to ion conduction. Theoretical Chemistry Accounts, 2021, 140, 1. | 1.4 | 5 |
| 9 | Cooperative excitations in superionic PbF <sub>2</sub>. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20190455. | 3.4 | 7 |
| 10 | Lattice dynamics and thermodynamic properties of Y3Al5O12 (YAG). Journal of Physics and Chemistry of Solids, 2021, 162, 110512. | 4.0 | 6 |
| 11 | Predicted strong spin-phonon interactions in Li-doped diamond. Physical Chemistry Chemical Physics, 2020, 22, 20612-20617. | 2.8 | 5 |
| 12 | GaPâ€“ZnS Multilayer Films: Visible-Light Photoelectrodes by Interface Engineering. Journal of Physical Chemistry C, 2019, 123, 3336-3342. | 3.1 | 7 |
| 13 | Lithium oxide: a quantum-corrected and classical Monte Carlo study. Physical Chemistry Chemical Physics, 2019, 21, 14964-14972. | 2.8 | 3 |
| 14 | Graphene and novel graphitic ZnO and ZnS nanofilms: the energy landscape, non-stoichiometry and water dissociation. Nanoscale Advances, 2019, 1, 1924-1935. | 4.6 | 6 |
| 15 | Ab initio study of negative electron affinity from light metals on the oxygen-terminated diamond (1â€‰1â€‰1) surface. Journal of Physics Condensed Matter, 2019, 31, 295002. | 1.8 | 10 |
| 16 | Calciteâ€“magnesite solid solutions: using genetic algorithms to understand non-ideality. Physics and Chemistry of Minerals, 2019, 46, 193-202. | 0.8 | 3 |
| 17 | Mixing Thermodynamics and Photocatalytic Properties of GaPâ€“ZnS solid solutions. Advanced Theory and Simulations, 2019, 2, 1800146. | 2.8 | 7 |
| 18 | Negative electron affinity from aluminium on the diamond (1â€‰0â€‰0) surface: a theoretical study. Journal of Physics Condensed Matter, 2018, 30, 235002. | 1.8 | 15 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | A theoretical study of substitutional boronâ€“nitrogen clusters in diamond. Journal of Physics Condensed Matter, 2018, 30, 425501. | 1.8 | 10 |
| 20 | Adventures in boron chemistry â€“ the prediction of novel ultra-flexible boron oxide frameworks. Faraday Discussions, 2018, 211, 569-591. | 3.2 | 5 |
| 21 | Super stretchable hexagonal boron nitride Kirigami. Thin Solid Films, 2017, 632, 35-43. | 1.8 | 19 |
| 22 | Simulations of doped CeO2 at finite dopant concentrations. Solid State Ionics, 2017, 299, 32-37. | 2.7 | 19 |
| 23 | Piezoelectric effects in boron nitride nanotubes predicted by the atomistic finite element method and molecular mechanics. Nanotechnology, 2017, 28, 355705. | 2.6 | 13 |
| 24 | Perovskite solid solutionsâ€“a Monte Carlo study of the deep earth analogue (K, Na)MgF3. Journal of Structural Chemistry, 2016, 57, 257-266. | 1.0 | 3 |
| 25 | Growth of nano-domains in Gdâ€“CeO<sub>2</sub> mixtures: hybrid Monte Carlo simulations. Journal of Materials Chemistry A, 2016, 4, 4592-4602. | 10.3 | 21 |
| 26 | Light Metals on Oxygen-Terminated Diamond (100): Structure and Electronic Properties. Chemistry of Materials, 2015, 27, 1306-1315. | 6.7 | 26 |
| 27 | Multi-million atom Monte Carlo simulation of oxide materials and solid solutions. Computational Materials Science, 2015, 103, 244-249. | 3.0 | 4 |
| 28 | Three-dimensional kinetic Monte Carlo simulations of diamond chemical vapor deposition. Journal of Chemical Physics, 2015, 142, 214707. | 3.0 | 26 |
| 29 | Order parameter and connectivity topology analysis of crystalline ceramics for nuclear waste immobilization. Journal of Physics Condensed Matter, 2014, 26, 485011. | 1.8 | 6 |
| 30 | Band Gap Modification of ZnO and ZnS through Solid Solution Formation for Applications in Photocatalysis. Energy Procedia, 2014, 60, 32-36. | 1.8 | 15 |
| 31 | Adaptive kinetic Monte Carlo simulation of solid oxide fuel cell components. Journal of Materials Chemistry A, 2014, 2, 13407-13414. | 10.3 | 18 |
| 32 | Towards new binary compounds: Synthesis of amorphous phosphorus carbide by pulsed laser deposition. Journal of Solid State Chemistry, 2013, 198, 466-474. | 2.9 | 53 |
| 33 | Simulation Studies of the Phase Stability of the Ruddlesdenâ€“Popper Phases. Journal of the American Ceramic Society, 2013, 96, 2316-2321. | 3.8 | 14 |
| 34 | Monte Carlo simulation and free energies of mixed oxide nanoparticles. Physical Chemistry Chemical Physics, 2013, 15, 6219. | 2.8 | 5 |
| 35 | GaPâ€ZnS Solid Solutions: Semiconductors for Efficient Visible Light Absorption and Emission. Advanced Materials, 2013, 25, 2989-2993. | 21.0 | 22 |
| 36 | Ultraâ€Flexible Boronâ€Oxygen 3D Solidâ€State Networks. Advanced Functional Materials, 2013, 23, 5887-5892. | 14.9 | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Physisorption of molecular hydrogen in curved carbon nanomaterials: a computational study. WIT Transactions on Engineering Sciences, 2013, , . | 0.0 | 2 |
| 38 | The embedded many-body expansion for energetics of molecular crystals. Journal of Chemical Physics, 2012, 137, 164102. | 3.0 | 102 |
| 39 | Novel potentials for modelling defect formation and oxygen vacancy migration in Gd2Ti2O7 and Gd2Zr2O7 pyrochlores. Journal of Materials Chemistry, 2012, 22, 4675. | 6.7 | 36 |
| 40 | Interfacial storage of noble gases and other trace elements in magmatic systems. Earth and Planetary Science Letters, 2012, 319-320, 287-294. | 4.4 | 21 |
| 41 | Improving density functional theory for crystal polymorph energetics. Physical Chemistry Chemical Physics, 2012, 14, 7739. | 2.8 | 32 |
| 42 | Structure of Nanoclusters on Oxide Substratesâ€"Bi<SUB>2</SUB>O<SUB>3</SUB> on SrTiO<SUB>3</SUB>. Nanoscience and Nanotechnology Letters, 2012, 4, 178-181. | 0.4 | 2 |
| 43 | Solvation of Ti(iv) in aqueous solution under ambient and supercritical conditions. Physical Chemistry Chemical Physics, 2011, 13, 7371. | 2.8 | 10 |
| 44 | Ternary silicon germanium nitrides: A class of tunable band gap materials. Physical Review B, 2011, 84, . | 3.2 | 11 |
| 45 | Simulations of chemical vapor deposition diamond film growth using a kinetic Monte Carlo model and two-dimensional models of microwave plasma and hot filament chemical vapor deposition reactors. Journal of Applied Physics, 2010, 108, . | 2.5 | 20 |
| 46 | Design of three-dimensional solid-state boron oxide networks:Ab initiocalculations using density functional theory. Physical Review B, 2010, 82, . | 3.2 | 13 |
| 47 | Simulations of chemical vapor deposition diamond film growth using a kinetic Monte Carlo model. Journal of Applied Physics, 2010, 108, . | 2.5 | 33 |
| 48 | Predicting crystal structures ab initio: group 14 nitrides and phosphides. Physical Chemistry Chemical Physics, 2010, 12, 8620. | 2.8 | 12 |
| 49 | Titanium in subduction zone fluids: First insights from ab initio molecular metadynamics simulations. Geochimica Et Cosmochimica Acta, 2010, 74, 2797-2810. | 3.9 | 20 |
| 50 | Oxide and halide nanoclusters on ionic substrates: heterofilm formation and lattice mismatch. Journal of Materials Chemistry, 2010, 20, 10403. | 6.7 | 6 |
| 51 | Bulk and surface energetics of crystalline lithium hydride: Benchmarks from quantum Monte Carlo and quantum chemistry. Physical Review B, 2010, 82, . | 3.2 | 27 |
| 52 | Carbon nitride:Ab initioinvestigation of carbon-rich phases. Physical Review B, 2009, 80, . | 3.2 | 48 |
| 53 | Calculation of properties of crystalline lithium hydride using correlated wave function theory. Physical Review B, 2009, 80, . | 3.2 | 66 |
| 54 | Solid phases of phosphorus carbide: Anab initiostudy. Physical Review B, 2009, 79, . | 3.2 | 37 |

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|---|---|---|---|
| 55 | Simulations of CVD Diamond Film Growth Using a Simplified Monte Carlo Model. Materials Research Society Symposia Proceedings, 2009, 1203, 1. | 0.1 | 1 |
| 56 | QSAR using momentum-space and trivial feature count descriptors â€“ An application to Tetrahymena pyriformis toxicity. Computational and Theoretical Chemistry, 2009, 901, 56-59. | 1.5 | 3 |
| 57 | Simplified Monte Carlo simulations of chemical vapour deposition diamond growth. Journal of Physics Condensed Matter, 2009, 21, 364203. | 1.8 | 24 |
| 58 | Molecular modelling of rare earth element complexation in subduction zone fluids. Geochimica Et Cosmochimica Acta, 2009, 73, 3934-3947. | 3.9 | 16 |
| 59 | Ultrathin oxide films and heterojunctions: CaO layers on BaO and SrO. Physical Chemistry Chemical Physics, 2009, 11, 3217. | 2.8 | 4 |
| 60 | Vibrational analysis of per-fluorinated-triamantane. Chemical Physics Letters, 2008, 460, 237-240. | 2.6 | 2 |
| 61 | Think locally â€“ linking structure, thermodynamics and transport in grossly non-stoichiometric compounds and solid solutions. Journal of Materials Chemistry, 2008, 18, 4124. | 6.7 | 7 |
| 62 | Ultrathin oxide films: CaO layers on BaO and SrO. Materials Research Society Symposia Proceedings, 2008, 1148, 1. | 0.1 | 1 |
| 63 | A Theoretical Study of Ultra-Thin Films with the Wurtzite and Zinc Blende Structures. Materials Research Society Symposia Proceedings, 2007, 1035, 1. | 0.1 | 0 |
| 64 | Activityâ€“composition relations in the system CaCO3â€“MgCO3 predicted from static structure energy calculations and Monte Carlo simulations. Geochimica Et Cosmochimica Acta, 2007, 71, 974-983. | 3.9 | 28 |
| 65 | Modeling of Wetting:Â A Study of Nanowetting at Rough and Heterogeneous Surfaces. Langmuir, 2007, 23, 1187-1194. | 3.5 | 110 |
| 66 | Ba2In2O4(OH)2: Proton sites, disorder and vibrational properties. Journal of Solid State Chemistry, 2007, 180, 3388-3392. | 2.9 | 20 |
| 67 | Investigating the utility of momentum-space descriptors for predicting bloodâ€“brain barrier penetration. Journal of Molecular Graphics and Modelling, 2007, 26, 607-612. | 2.4 | 15 |
| 68 | Monte Carlo simulation of GaN/AlN and AlN/InN mixtures. Materials Chemistry and Physics, 2007, 105, 179-184. | 4.0 | 9 |
| 69 | Use of massively parallel molecular dynamics simulations for radiation damage in pyrochlores. Journal of Materials Science, 2007, 42, 1920-1930. | 3.7 | 15 |
| 70 | Graphitic Nanofilms as Precursors to Wurtzite Films: Theory. Physical Review Letters, 2006, 96, 066102. | 7.8 | 514 |
| 71 | Simulation of radiation damage in gadolinium pyrochlores. Journal of Physics Condensed Matter, 2006, 18, 2217-2234. | 1.8 | 19 |
| 72 | Raman spectroscopy of nanocrystalline diamond: Anab initioapproach. Physical Review B, 2006, 74, . | 3.2 | 93 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Local cation environments in the pyropeâ€“grossularMg3Al2Si3O12â€“Ca3Al2Si3O12garnet solid solution. Physical Review B, 2006, 74, . | 3.2 | 30 |
| 74 | Simulation of thermodynamic mixing properties of garnet solid solutions at high temperatures and pressures. Chemical Geology, 2006, 225, 336-346. | 3.3 | 17 |
| 75 | Raman spectroscopy of diamondoids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 681-692. | 3.9 | 64 |
| 76 | Monte Carlo simulation of segregation in ceramic thin films: Comparison of the MgO/MnO {100} and {210} surfaces. Journal of Crystal Growth, 2006, 294, 130-136. | 1.5 | 5 |
| 77 | Thin films of wÃ¼rtzite materialsâ€”AlN vs. AlP. Journal of Crystal Growth, 2006, 294, 111-117. | 1.5 | 6 |
| 78 | Sr and Ga substituted Ba2In2O5: Linking ionic conductivity and the potential energy surface. Solid State Ionics, 2006, 177, 223-228. | 2.7 | 16 |
| 79 | Structural forms of fluorides in bone tissue of animals under chronic fluoride intoxication. Journal of Structural Chemistry, 2006, 47, 258-266. | 1.0 | 12 |
| 80 | Order in the disordered state: local structural entities in the fast ion conductor Ba2In2O5. Journal of Solid State Chemistry, 2005, 178, 346-355. | 2.9 | 42 |
| 81 | The use of momentum-space descriptors for predicting octanolâ€“water partition coefficients. Computational and Theoretical Chemistry, 2005, 727, 57-61. | 1.5 | 14 |
| 82 | Similarity in silicate chemistry: trace elements in garnet solid solutions. Computational and Theoretical Chemistry, 2005, 727, 199-204. | 1.5 | 8 |
| 83 | The quantitative use of momentum-space descriptors. Chemical Physics Letters, 2005, 416, 376-380. | 2.6 | 6 |
| 84 | Negative thermal expansion. Journal of Physics Condensed Matter, 2005, 17, R217-R252. | 1.8 | 437 |
| 85 | MgO addimer diffusion on MgO(100): A comparison ofab initioand empirical models. Physical Review B, 2005, 72, . | 3.2 | 64 |
| 86 | Topography of the Potential Energy Hypersurface and Criteria for Fast-Ion Conduction in Perovskite-Related A2B2O5 Oxides. Journal of Physical Chemistry B, 2005, 109, 12362-12365. | 2.6 | 22 |
| 87 | Surface diffusion and surface growth in nanofilms of mixed rocksalt oxides. Physical Chemistry Chemical Physics, 2005, 7, 1839. | 2.8 | 14 |
| 88 | Monte Carlo simulation of segregation in ceramic thin films. Physical Chemistry Chemical Physics, 2005, 7, 3601. | 2.8 | 10 |
| 89 | Size mismatch effects in oxide solid solutions using Monte Carlo and configurational averaging. Physical Chemistry Chemical Physics, 2005, 7, 1127-1135. | 2.8 | 15 |
| 90 | Strikingly Long CÂ·Â·Â·C Distances in 1,2-Disubstitutedortho-Carboranes and Their Dianions. Journal of the American Chemical Society, 2005, 127, 13538-13547. | 13.7 | 178 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Monte Carlo simulation of GaN/InN mixtures. Journal of Materials Chemistry, 2005, 15, 785. | 6.7 | 14 |
| 92 | Growth of ZnO thin filmsâ€"experiment and theory. Journal of Materials Chemistry, 2005, 15, 139-148. | 6.7 | 364 |
| 93 | Quasiharmonic free energy and derivatives for many-body interactions: The embedded atom method. Physical Review B, 2004, 69, . | 3.2 | 6 |
| 94 | Novel exchange mechanisms in the surface diffusion of oxides. Journal of Physics Condensed Matter, 2004, 16, L187-L192. | 1.8 | 15 |
| 95 | Collective ionic motion in oxide fast-ion-conductors. Physical Chemistry Chemical Physics, 2004, 6, 3052-3055. | 2.8 | 28 |
| 96 | Phosphorus carbides: theory and experiment. Dalton Transactions, 2004, , 3085. | 3.3 | 75 |
| 97 | Simulating surface diffusion and surface growth in ceramics. Dalton Transactions, 2004, , 3071. | 3.3 | 4 |
| 98 | Simulation of mineral solid solutions at zero and high pressure using lattice statics, lattice dynamics and Monte Carlo methods. Journal of Physics Condensed Matter, 2004, 16, S2751-S2770. | 1.8 | 41 |
| 99 | Trace element incorporation into pyrope-grossular solid solutions: an atomistic simulation study. Physics and Chemistry of Minerals, 2003, 30, 217-229. | 0.8 | 31 |
| 100 | Classification of reaction pathways via momentumâ€"space and quantum molecular similarity measures. Chemical Physics Letters, 2003, 367, 207-213. | 2.6 | 12 |
| 101 | Binary phosphorus-carbon compounds: The series P4C3+8n. International Journal of Quantum Chemistry, 2003, 95, 546-553. | 2.0 | 16 |
| 102 | The â€˜zero chargeâ€™ partitioning behaviour of noble gases during mantle melting. Nature, 2003, 423, 738-741. | 27.8 | 107 |
| 103 | Atomistic simulation of mineralâ€"melt trace-element partitioning. Physics of the Earth and Planetary Interiors, 2003, 139, 93-111. | 1.9 | 14 |
| 104 | Atomistic simulations of trace element incorporation into the large site of MgSiO3 and CaSiO3 perovskites. Physics of the Earth and Planetary Interiors, 2003, 139, 113-127. | 1.9 | 24 |
| 105 | Molecular Dynamics Study of Wetting of a Pillar Surface. Langmuir, 2003, 19, 7127-7129. | 3.5 | 87 |
| 106 | Structureâ€"property relationships and momentum space quantities: Hammett Ïƒâ€"constants. Molecular Physics, 2003, 101, 3159-3162. | 1.7 | 20 |
| 107 | Dopant incorporation into garnet solid solutionsâ€"a breakdown of Goldschmidtâ€™s first ruleElectronic supplementary information (ESI) available: (1) comparison between observed and calculated structural parameters of the end-members pyrope and grossular. (2) GULP input file for configuration 1. See http://www.rsc.org/suppdata/cc/b2/b211249c/. Chemical Communications, 2003, , 786-787. | 4.1 | 13 |
| 108 | Beyond the point defect limit: solid solutions, phase diagrams and trace-element partitioning. Physical Chemistry Chemical Physics, 2003, 5, 2190-2196. | 2.8 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Orderâ€“disorder in grossly non-stoichiometric SrFeO2.50â€” a simulation study. Physical Chemistry Chemical Physics, 2003, 5, 2237-2243. | 2.8 | 29 |
| 110 | Ab initio predictions of ferroelectric ternary fluorides with the LiNbO3structure. Chemical Communications, 2003, , 2440-2441. | 4.1 | 8 |
| 111 | Semigrand-canonical ensemble simulations of the phase diagrams of alloys. Modelling and Simulation in Materials Science and Engineering, 2003, 11, 115-126. | 2.0 | 21 |
| 112 | Solid phosphorus carbide?. Chemical Communications, 2002, , 2494-2495. | 4.1 | 16 |
| 113 | Displacement cascades in Gd2Ti2O7 and Gd2Zr2O7: a molecular dynamics study. Journal of Materials Chemistry, 2002, 12, 2923-2926. | 6.7 | 65 |
| 114 | Wetting of Water and Water/Ethanol Droplets on a Non-Polar Surface:Â A Molecular Dynamics Study. Langmuir, 2002, 18, 10462-10466. | 3.5 | 111 |
| 115 | Ab initio calculation of phase diagrams of ceramics and minerals. Journal of Materials Chemistry, 2001, 11, 63-68. | 6.7 | 48 |
| 116 | Ab Initio Calculation of Phase Diagrams of Oxides. Journal of Physical Chemistry B, 2001, 105, 3594-3599. | 2.6 | 39 |
| 117 | Evaluation of Thermodynamic Properties of Solids by Quasiharmonic Lattice Dynamics. International Journal of Thermophysics, 2001, 22, 535-546. | 2.1 | 11 |
| 118 | Free energy of solid solutions and phase diagrams via quasiharmonic lattice dynamics. Physical Review B, 2001, 63, . | 3.2 | 39 |
| 119 | Sputtering of grains in C-type shocks. Monthly Notices of the Royal Astronomical Society, 2000, 318, 809-816. | 4.4 | 66 |
| 120 | Configurational lattice dynamics and hybrid Monte Carlo approaches to thermodynamic properties of solid solutions. Computational and Theoretical Chemistry, 2000, 506, 45-53. | 1.5 | 4 |
| 121 | Computer simulation of high-temperature, forsterite-melt partitioning. American Mineralogist, 2000, 85, 1087-1091. | 1.9 | 29 |
| 122 | Ionic solids at elevated temperatures and/or high pressures: lattice dynamics, molecular dynamics, Monte Carlo and ab initio studies. Physical Chemistry Chemical Physics, 2000, 2, 1099-1111. | 2.8 | 26 |
| 123 | Simple refinements of Brillouin zone integration. Journal of Physics Condensed Matter, 2000, 12, 549-558. | 1.8 | 28 |
| 124 | Computer simulation of water molecules at kaolinite and silica surfaces. Physical Chemistry Chemical Physics, 2000, 2, 3663-3668. | 2.8 | 87 |
| 125 | Change in the bulk modulus at theB1â€˜B2phase transition. Physical Review B, 1999, 60, 2968-2971. | 3.2 | 9 |
| 126 | Thermodynamics of solid solutions VIA lattice dynamics and hybrid monte carlo simulations. Radiation Effects and Defects in Solids, 1999, 151, 197-202. | 1.2 | 2 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Quasiharmonic free energy and derivatives for slabs:â€ƒOxide surfaces at elevated temperatures. Physical Review B, 1999, 59, 6742-6751. | 3.2 | 35 |
| 128 | Quasiharmonic free energy and derivatives for three-body interactions. Physical Review B, 1999, 59, 353-363. | 3.2 | 12 |
| 129 | Phase transitions in disordered solids via hybrid Monte Carlo: the orthorhombic to cubic phase transition in (Mg,Mn)SiO3 perovskite. Chemical Communications, 1999, , 707-708. | 4.1 | 7 |
| 130 | A study of the electronic, magnetic, structural and dynamic properties of low-dimensional NiO on MgO(100) surfaces. Faraday Discussions, 1999, 114, 105-127. | 3.2 | 15 |
| 131 | Quantum molecular similarity via momentumâ€space indices. Journal of Mathematical Chemistry, 1998, 23, 51-60. | 1.5 | 17 |
| 132 | Hybrid Monte Carlo and lattice dynamics simulations: the enthalpy of mixing of binary oxides. Chemical Communications, 1998, , 627-628. | 4.1 | 15 |
| 133 | Monte Carlo and Hybrid Monte Carlo/Molecular Dynamics Approaches to Orderâ˜'Disorder in Alloys, Oxides, and Silicates. Journal of Physical Chemistry B, 1998, 102, 5202-5207. | 2.6 | 51 |
| 134 | Thermodynamics and mechanism of theB1-B2phase transition in group-I halides and group-II oxides. Physical Review B, 1998, 57, 11164-11172. | 3.2 | 87 |
| 135 | Thermal expansion of polymers: Mechanisms in orthorhombic polyethylene. Physical Review B, 1998, 58, 8416-8427. | 3.2 | 44 |
| 136 | A first-principles Hartree-Fock description of MnO at high pressures. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1998, 77, 1063-1075. | 0.6 | 3 |
| 137 | Ionic solids at elevated temperatures and high pressures: MgF2. Journal of Chemical Physics, 1997, 107, 4337-4344. | 3.0 | 41 |
| 138 | Free-energy derivatives and structure optimization within quasiharmonic lattice dynamics. Physical Review B, 1997, 56, 14380-14390. | 3.2 | 83 |
| 139 | Impurity cations in the bulk and the {001} surface of muscovite: an atomistic simulation study. Journal of Materials Chemistry, 1997, 7, 1947-1951. | 6.7 | 19 |
| 140 | Free energy of formation of defects in polar solids. Faraday Discussions, 1997, 106, 377-387. | 3.2 | 38 |
| 141 | Potentials for B-metal compounds: The stannates ASnO<sub>3</sub> (A = Ca, Sr or Ba) and SnO<sub>2</sub>. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1996, 73, 33-39. | 0.6 | 10 |
| 142 | Momentum-space electron densities?localized orbitals in hydrocarbons, boranes, and transition metal complexes. International Journal of Quantum Chemistry, 1996, 60, 579-592. | 2.0 | 4 |
| 143 | The zero static internal stress approximation in lattice dynamics, and the calculation of isotope effects on molar volumes. Journal of Chemical Physics, 1996, 105, 8300-8303. | 3.0 | 62 |
| 144 | Momentum-space similarity. Advances in Molecular Similarity, 1996, , 61-87. | 0.5 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 145 | Applications of momentum-space similarity. Journal of Computer-Aided Molecular Design, 1995, 9, 331-340. | 2.9 | 20 |
| 146 | Momentum-space electron densities and quantum molecular similarity. Topics in Current Chemistry, 1995, , 85-111. | 4.0 | 25 |
| 147 | Oxygen Interstitial Defects in High-Tc Oxides. Molecular Simulation, 1994, 12, 89-100. | 2.0 | 9 |
| 148 | Ab initiostudy of MnO and NiO. Physical Review B, 1994, 50, 5041-5054. | 3.2 | 441 |
| 149 | Density functional theory and interionic potentials. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 871-878. | 0.6 | 18 |
| 150 | Ionic halides and oxides at high pressure: calculated Hugoniots, isotherms and thermal pressures. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 4369. | 1.7 | 18 |
| 151 | Molecular similarity of anti-HIV phospholipids. Journal of the American Chemical Society, 1993, 115, 12615-12616. | 13.7 | 36 |
| 152 | Differences Between High-T<sub>c</sub>Oxides Containing Six-, Five-, Four- And Two-Fold Coordinated Copper. Molecular Simulation, 1992, 9, 115-128. | 2.0 | 5 |
| 153 | Polar Solids at High Pressure: NaF. Molecular Simulation, 1992, 9, 161-169. | 2.0 | 10 |
| 154 | Atomistic lattice simulations of the ternary fluorides AMF3(A = Li, Na, K, Rb, Cs; M = Mg, Ca, Sr, Ba). Journal of Materials Chemistry, 1991, 1, 1035. | 6.7 | 23 |
| 155 | Oxygen ion migration in La<sub>2</sub>CuO<sub>4</sub>. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1991, 64, 1129-1132. | 0.6 | 34 |
| 156 | Ionic solids at high pressures and elevated temperatures: MgO (periclase). Journal of Chemical Physics, 1991, 95, 6792-6799. | 3.0 | 26 |
| 157 | Atomistic Simulation of High-Tc Oxides. Journal of the American Ceramic Society, 1990, 73, 3175-3184. | 3.8 | 20 |
| 158 | Theoretical studies of fluorocarbons. Part I. Small perfluoroalkane molecules. Journal of Fluorine Chemistry, 1990, 46, 317-337. | 1.7 | 12 |
| 159 | The Practical Calculation of Interionic Potentials in Solids using Electron Gas Theory. Molecular Simulation, 1990, 4, 269-283. | 2.0 | 16 |
| 160 | Momentum space studies of large polyenes. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1519. | 1.1 | 7 |
| 161 | Momentum space properties and local density approximations in small molecules: A critical appraisal. Journal of Chemical Physics, 1986, 84, 5594-5605. | 3.0 | 30 |