Matt I J Probert

List of Publications by Year in descending order

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58 papers	21,685 citations	430754 18 h-index	149623 56 g-index
76 all docs	76 docs citations	76 times ranked	19812 citing authors

#	Article	IF	Citations
1	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
2	Systematic Comparison of Genetic Algorithm and Basin Hopping Approaches to the Global Optimization of Si(111) Surface Reconstructions. Journal of Physical Chemistry A, 2022, 126, 3043-3056.	1.1	5
3	Electronâ€“phonon interaction and superconductivity in hexagonal ternary carbides Nb₂ AC (A: Al, S, Ge, As and Sn). Electronic Structure, 2021, 3, 045001.	1.0	5
4	Effective modelling of the Seebeck coefficient of Fe₂VAl. Journal of Physics Condensed Matter, 2020, 32, 125401.	0.7	4
5	Anisotropy in antiferromagnets. Journal of Applied Physics, 2020, 128, .	1.1	19
6	The emergence of sequence-dependent structural motifs in stretched, torsionally constrained DNA. Nucleic Acids Research, 2020, 48, 1748-1763.	6.5	21
7	Off-the-shelf DFT-DISPersion methods: Are they now â€œon-trendâ€•for organic molecular crystals?. Journal of Chemical Physics, 2019, 151, 044106.	1.2	11
8	Simultaneous Prediction of the Magnetic and Crystal Structure of Materials Using a Genetic Algorithm. Crystals, 2019, 9, 439.	1.0	8
9	Huge power factor in p-type half-Heusler alloys NbFeSb and TaFeSb. JPhys Materials, 2019, 2, 035002.	1.8	33
10	Quantum diffusion of H/D on Ni(111)â€”A partially adiabatic centroid MD study. Journal of Chemical Physics, 2018, 148, 102339.	1.2	4
11	DL_MG: A Parallel Multigrid Poisson and Poissonâ€“Boltzmann Solver for Electronic Structure Calculations in Vacuum and Solution. Journal of Chemical Theory and Computation, 2018, 14, 1412-1432.	2.3	31
12	Many-body renormalization of forces in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi></mml:math> -electron materials. Physical Review B, 2018, 98, .	1.1	20
13	Atomistic dynamics of sulfur-deficient high-symmetry grain boundaries in molybdenum disulfide. Nanoscale, 2017, 9, 10312-10320.	2.8	18
14	Transverse Fluorescence Microscopy with Magnetic and Optical Tweezers. Biophysical Journal, 2017, 112, 299a.	0.2	0
15	Experimental and density functional study of Mn doped Bi2Te3 topological insulator. APL Materials, 2016, 4, .	2.2	14
16	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
17	Exploring atomic defects in molybdenum disulphide monolayers. Nature Communications, 2015, 6, 6293.	5.8	1,124
18	Theoretical study of core-loss electron energy-loss spectroscopy at graphene nanoribbon edges. Journal of Physics Condensed Matter, 2015, 27, 305301.	0.7	5

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19	The Effect of Cobalt-Sublattice Disorder on Spin Polarisation in Co2FexMn1â^'xSi Heusler Alloys. Materials, 2014, 7, 1473-1482.	1.3	9
20	Density functional theory in the solid state. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130270.	1.6	242
21	4th Workshop on Theory, Modelling and Computational Methods for Semiconductors (TMCSIV). Journal of Physics: Conference Series, 2014, 526, 011001.	0.3	0
22	Quantum simulation of low-temperature metallic liquid hydrogen. Nature Communications, 2013, 4, 2064.	5.8	75
23	Classical and quantum ordering of protons in cold solid hydrogen under megabar pressures. Journal of Physics Condensed Matter, 2013, 25, 085402.	0.7	25
24	3rd Workshop on Theory, Modelling and Computational Methods for Semiconductors (TMCSIII). Journal of Physics: Conference Series, 2012, 367, 011001.	0.3	0
25	Atomistic molecular dynamics simulations of shock compressed quartz. Journal of Chemical Physics, 2011, 135, 044508.	1.2	9
26	Crystal structure prediction for iron as inner core material in heavy terrestrial planets. Earth and Planetary Science Letters, 2011, 312, 237-242.	1.8	32
27	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
28	Hydrogen sorption sites in holmium silicide on silicon(1 1 1). Surface Science, 2010, 604, 686-691.	0.8	0
29	Anab initiostudy of xenon retention in Î±-quartz. Journal of Physics Condensed Matter, 2010, 22, 025501.	0.7	19
30	Quantum Nature of the Proton in Water-Hydroxyl Overlayers on Metal Surfaces. Physical Review Letters, 2010, 104, 066102.	2.9	101
31	The structure and growth direction of rare earth silicide nanowires on Si(100). Applied Physics Letters, 2010, 96, 241903.	1.5	13
32	Theory, Modelling and Computational methods for Semiconductors. Journal of Physics: Conference Series, 2010, 242, 011001.	0.3	0
33	An experiment on the Purcell effect in a wedge cavity. European Journal of Physics, 2009, 30, S81-S88.	0.3	3
34	Improved real-space genetic algorithm for crystal structure and polymorph prediction. Physical Review B, 2008, 77, .	1.1	37
35	Quantitative LEEDIâ^'Vandab initiostudy of theSi(111)â^'3Ã—2â^'Smsurface structure and the missing half-order spots in the3Ã—1diffraction pattern. Physical Review B, 2007, 75, .	1.1	8
36	A periodic genetic algorithm with real-space representation for crystal structure and polymorph prediction. Physical Review B, 2006, 73, .	1.1	145

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37	Ab Initio Path Integral Molecular Dynamics Simulation of Hydrogen in Silicon. AIP Conference Proceedings, 2006, , .	0.3	0
38	STM andab initiostudy of holmium nanowires on a Ge(111) surface. Physical Review B, 2006, 74, .	1.1	6
39	Orientational effects of twisted light on twisted nematic liquid crystals. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, S523-S528.	0.6	2
40	Constant pressure Langevin dynamics: theory and application. Computer Physics Communications, 2005, 169, 322-325.	3.0	13
41	Phase behavior of a three-dimensional core-softened model system. Physical Review E, 2005, 71, 065701.	0.8	16
42	Progression of phase behavior for a sequence of model core-softened potentials. Physical Review E, 2005, 72, 061202.	0.8	4
43	First principles methods using CASTEP. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	9,458
44	Stiffness and thermal expansion of ZrB2: anab initiostudy. Journal of Physics Condensed Matter, 2005, 17, 2233-2241.	0.7	85
45	Langevin dynamics in constant pressure extended systems. Journal of Chemical Physics, 2004, 120, 11432-11441.	1.2	116
46	Improved algorithm for geometry optimisation using damped molecular dynamics. Journal of Computational Physics, 2003, 191, 130-146.	1.9	15
47	Non-equilibrium electron transport in degenerate nitride heterostructuresâ€"dynamic screening effects. Physica E: Low-Dimensional Systems and Nanostructures, 2003, 17, 272-275.	1.3	5
48	Improving the convergence of defect calculations in supercells: Anab initiostudy of the neutral silicon vacancy. Physical Review B, 2003, 67, .	1.1	163
49	Molecular dynamics studies of liquids using a Beowulf computer. Contemporary Physics, 2003, 44, 435-450.	0.8	1
50	Comment on `Checking the influence of numerically induced chaos in the computational study of intramolecular dynamics using trajectory equivalence'. Chemical Physics Letters, 2002, 354, 529-531.	1.2	1
51	First-principles simulation: ideas, illustrations and the CASTEP code. Journal of Physics Condensed Matter, 2002, 14, 2717-2744.	0.7	8,382
52	Comment on â€œAlgorithm for normal random numbersâ€• Physical Review E, 2001, 63, 058701; author reply 058702.	0.8	3
53	Anab initiostudy of muons in ethanal. Journal of Physics Condensed Matter, 1997, 9, 3241-3257.	0.7	6
54	Ab initiostudies of magnetism in the organic radicalp-NPNN. Journal of Physics Condensed Matter, 1997, 9, 3635-3645.	0.7	4

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55	Potential for a novel Î¼SR experiment â€" the results of an ab initio study. Chemical Physics Letters, 1996, 259, 271-275.	1.2	7
56	Theoretical studies of implanted muons in organic magnets. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1996, 37, 247-250.	1.7	3
57	Computer simulations of flux motion in high-temperature superconductors. Physica B: Condensed Matter, 1995, 205, 180-182.	1.3	0
58	Nature of the Irreversibility Line in High-Temperature Superconductors. Physical Review Letters, 1995, 75, 1835-1838.	2.9	14