Andrew Horsfield

List of Publications by Year
in descending order

79 papers	2,922 citations	147801 31 h-index	168389 53 g-index
81 all docs	81 docs citations	81 times ranked	2653 citing authors

#	Article	IF	Citations
1	QM/MM optimization with quantum coupling: Hostâ€“guest interactions in a pentacene-doped p-terphenyl crystal. Journal of Chemical Physics, 2022, 156, 044110.	3.0	4
2	Dissipative Equation of Motion for Electromagnetic Radiation in Quantum Dynamics. Physical Review Letters, 2021, 126, 087401.	7.8	8
3	A simple approximation to the electronâ€“phonon interaction in population dynamics. Journal of Chemical Physics, 2020, 153, 234108.	3.0	6
4	Systematic development of ab initio tight-binding models for hexagonal metals. Physical Review Materials, 2020, 4, .	2.4	3
5	Beyond two-center tight binding: Models for Mg and Zr. Physical Review Materials, 2020, 4, .	2.4	0
6	The microscopic Einstein-de Haas effect. Journal of Chemical Physics, 2019, 150, 224109.	3.0	4
7	Multiple-probe electronic open boundaries with bad contacts. Physical Review B, 2019, 99, .	3.2	1
8	Implicit and explicit host effects on excitons in pentacene derivatives. Journal of Chemical Physics, 2018, 148, 104108.	3.0	12
9	Classical and quantum calculations of the temperature dependence of the free energy of argon. Computational Materials Science, 2018, 144, 36-41.	3.0	5
10	Rectification and negative differential resistance via orbital level pinning. Scientific Reports, 2018, 8, 9120.	3.3	12
11	HOMOâ€“LUMO coupling: the fourth rule for highly effective molecular rectifiers. Nanoscale, 2017, 9, 8119-8125.	5.6	18
12	Non-conservative forces in bulk systems. Materials Science and Technology, 2017, 33, 1442-1446.	1.6	2
13	Efficient local-orbitals based method for ultrafast dynamics. Journal of Chemical Physics, 2017, 147, 044111.	3.0	4
14	Molecular recognition in olfaction. Advances in Physics: X, 2017, 2, 937-977.	4.1	11
15	Molecular Design of a Room-Temperature Maser. Journal of Physical Chemistry C, 2016, 120, 8251-8260.	3.1	31
16	Diversification of MgO//Mg interfacial crystal orientations during oxidation: A density functional theory study. Journal of Alloys and Compounds, 2016, 688, 1233-1240.	5.5	10
17	Gaussian polarizable-ion tight binding. Journal of Chemical Physics, 2016, 145, 144103.	3.0	11
18	Correlation of Local Structure and Diffusion Pathways in the Modulated Anisotropic Oxide Ion Conductor CeNbO_{4.25}. Journal of the American Chemical Society, 2016, 138, 1273-1279.	13.7	34

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19	Hubbard-like Hamiltonians for interacting electrons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>s</mml:mi><mml:mo>,</mml:mo><mml:mi>p</mml:mi></mml:math> and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>orbitals. Physical Review B, 2016, 93, .	3.2	26
20	Which wets TiB2 inoculant particles: Al or Al3Ti?. Journal of Alloys and Compounds, 2016, 664, 460-468.	5.5	44
21	First-principles calculation of Mg/MgO interfacial free energies. Journal of Alloys and Compounds, 2015, 650, 228-238.	5.5	26
22	Why Ni is absent from the surface of La₂NiO_{4+Î´}?. Journal of Materials Chemistry A, 2015, 3, 23760-23767.	10.3	37
23	Electron spin changes during general anesthesia in Drosophila. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E3524-33.	7.1	51
24	Electron-Energy Loss Study of Nonlocal Effects in Connected Plasmonic Nanoprisms. ACS Nano, 2013, 7, 6287-6296.	14.6	62
25	Nonlocal propagation and tunnelling of surface plasmons in metallic hourglass waveguides. Optics Express, 2013, 21, 27509.	3.4	12
26	Quantumâ€“classical simulations of the electronic stopping force and charge on slow heavy channelling ions in metals. Journal of Physics Condensed Matter, 2013, 25, 125501.	1.8	13
27	Nonlocal Effects in the Nanofocusing Performance of Plasmonic Tips. Nano Letters, 2012, 12, 3308-3314.	9.1	131
28	The Swipe Card Model of Odorant Recognition. Sensors, 2012, 12, 15709-15749.	3.8	40
29	Where does tight binding go from here?. Physica Status Solidi (B): Basic Research, 2012, 249, 231-236.	1.5	8
30	Plasmonic Sinks for the Selective Removal of Long-Lived States. ACS Nano, 2011, 5, 9958-9965.	14.6	44
31	A multiconfigurational time-dependent Hartree-Fock method for excited electronic states. I. General formalism and application to open-shell states. Journal of Chemical Physics, 2011, 134, 244101.	3.0	48
32	A multiconfigurational time-dependent Hartree-Fock method for excited electronic states. II. Coulomb interaction effects in single conjugated polymer chains. Journal of Chemical Physics, 2011, 134, 244102.	3.0	18
33	Analog of Rabi oscillations in resonant electron-ion systems. Journal of Chemical Physics, 2011, 134, 194105.	3.0	8
34	Nonconservative current-induced forces: A physical interpretation. Beilstein Journal of Nanotechnology, 2011, 2, 727-733.	2.8	21
35	Modelling non-adiabatic processes using correlated electron-ion dynamics. European Physical Journal B, 2010, 77, 305-329.	1.5	33
36	The treatment of electronic excitations in atomistic models of radiation damage in metals. Reports on Progress in Physics, 2010, 73, 116501.	20.1	109

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37	Odour character differences for enantiomers correlate with molecular flexibility. Journal of the Royal Society Interface, 2009, 6, 75-86.	3.4	48
38	Inelastic quantum transport in nanostructures: The self-consistent Born approximation and correlated electron-ion dynamics. Physical Review B, 2008, 78, .	3.2	27
39	Robust nonadiabatic molecular dynamics for metals and insulators. Journal of Chemical Physics, 2007, 127, 214104.	3.0	21
40	Could Humans Recognize Odor by Phonon Assisted Tunneling?. Physical Review Letters, 2007, 98, 038101.	7.8	136
41	Dynamical simulation of inelastic quantum transport. Journal of Physics Condensed Matter, 2007, 19, 196201.	1.8	61
42	Density functional calculations of surface free energies. Journal of Chemical Physics, 2006, 124, 134709.	3.0	10
43	The transfer of energy between electrons and ions in solids. Reports on Progress in Physics, 2006, 69, 1195-1234.	20.1	77
44	Molecular conduction: Do time-dependent simulations tell you more than the Landauer approach?. Journal of Chemical Physics, 2006, 124, 214708.	3.0	75
45	Self-interstitial atom defects in bcc transition metals: Group-specific trends. Physical Review B, 2006, 73, .	3.2	360
46	Hyperfine structure of Sc@C82from ESR and DFT. Nanotechnology, 2005, 16, 2469-2473.	2.6	24
47	Correlated electronâ€“ion dynamics with open boundaries: formalism. Journal of Physics Condensed Matter, 2005, 17, 3985-3995.	1.8	14
48	Correlated electronâ€“ion dynamics: the excitation of atomic motion by energetic electrons. Journal of Physics Condensed Matter, 2005, 17, 4793-4812.	1.8	57
49	Open-boundary Ehrenfest molecular dynamics: towards a model of current induced heating in nanowires. Journal of Physics Condensed Matter, 2004, 16, L65-L72.	1.8	32
50	Power dissipation in nanoscale conductors: classical, semi-classical and quantum dynamics. Journal of Physics Condensed Matter, 2004, 16, 3609-3622.	1.8	79
51	Beyond Ehrenfest: correlated non-adiabatic molecular dynamics. Journal of Physics Condensed Matter, 2004, 16, 8251-8266.	1.8	86
52	Many-site expansion for correcting approximate density functionals. Physical Review B, 2000, 61, 12560-12561.	3.2	0
53	Transferable atomic-type orbital basis sets for solids. Physical Review B, 2000, 62, 4899-4905.	3.2	121
54	Electromigration of vacancies in copper. Physical Review B, 2000, 62, 8568-8571.	3.2	37

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55	Ab initiotight binding. Journal of Physics Condensed Matter, 2000, 12, R1-R24.	1.8	45
56	Hydrogen diffusion on Si(001) studied with the local density approximation and tight binding. Journal of Physics Condensed Matter, 1998, 10, 3719-3730.	1.8	31
57	Carbon vacancies in titanium carbide. Modelling and Simulation in Materials Science and Engineering, 1998, 6, 335-335.	2.0	2
58	A simplified density functional theory study of triboelectronic lubricant degradation. Modelling and Simulation in Materials Science and Engineering, 1997, 5, 311-315.	2.0	1
59	Efficientab initiotight binding. Physical Review B, 1997, 56, 6594-6602.	3.2	98
60	Carbon vacancies in titanium carbide. Modelling and Simulation in Materials Science and Engineering, 1997, 5, 187-198.	2.0	37
61	Bond order potentials and other efficient tight binding methods. Radiation Effects and Defects in Solids, 1997, 142, 93-105.	1.2	0
62	A comparison of linear scaling tight-binding methods. Modelling and Simulation in Materials Science and Engineering, 1997, 5, 199-222.	2.0	82
63	Bond order potentials for covalent systems. Journal of Phase Equilibria and Diffusion, 1997, 18, 573-579.	0.3	0
64	Tight-binding bond order potential a forces for atomistic simulations. Journal of Phase Equilibria and Diffusion, 1997, 18, 614-623.	0.3	18
65	Bond-order potentials: Can they bridge the electronic-atomistic length-scale gap?. Journal of Computer-Aided Materials Design, 1996, 3, 149-156.	0.7	0
66	Tight-Binding Theory and Computational Materials Synthesis. MRS Bulletin, 1996, 21, 42-48.	3.5	16
67	Computational materials synthesis. III. Synthesis of hydrogenated amorphous carbon from molecular precursors. Physical Review B, 1996, 54, 15785-15794.	3.2	12
68	Computational materials synthesis. I. A tight-binding scheme for hydrocarbons. Physical Review B, 1996, 54, 15773-15775.	3.2	55
69	O(N) tight-binding methods with finite electronic temperature. Physical Review B, 1996, 53, 15381-15384.	3.2	19
70	Bond-order potentials: Theory and implementation. Physical Review B, 1996, 53, 12694-12712.	3.2	175
71	Theory for the(1Ã—1)Rumpled Relaxations at TiC(001) and TaC(001) Surfaces. Physical Review Letters, 1996, 76, 90-93.	7.8	18
72	Puckering models for the Si(113) surface reconstruction. Physical Review B, 1996, 54, 13744-13747.	3.2	19

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73	Bond-order potential and cluster recursion for the description of chemical bonds: Efficient real-space methods for tight-binding molecular dynamics. Physical Review B, 1996, 53, 1656-1666.	3.2	80
74	Computational materials synthesis. II. A study of polymerization. Physical Review B, 1996, 54, 15776-15784.	3.2	7
75	Tight-binding parameters for silicon-boron interactions with application to boron-defect pairs in crystalline silicon. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1996, 73, 71-84.	0.6	7
76	A tight-binding molecular dynamics simulation of the melting and solidification of silicon. Modelling and Simulation in Materials Science and Engineering, 1994, 2, 277-294.	2.0	15
77	The Fermi surface and pseudopotentials of aluminium. Journal of Physics Condensed Matter, 1993, 5, 3925-3936.	1.8	4
78	Ordered silicon-tin structures on a silicon (111) substrate. Journal of Physics Condensed Matter, 1992, 4, 7333-7340.	1.8	4
79	Structure and Interactions at the Mg(0001)/Water Interface: An ab initio Study. Journal of Chemical Physics, 0, , .	3.0	2