Nicholas D Hine

List of Publications by Year
in descending order

74 papers	3,209 citations	136950 32 h-index	155660 55 g-index
76 all docs	76 docs citations	76 times ranked	4692 citing authors

#	Article	IF	Citations
1	Ultrafast transient absorption spectroelectrochemistry: femtosecond to nanosecond excited-state relaxation dynamics of the individual components of an anthraquinone redox couple. Chemical Science, 2022, 13, 486-496.	7.4	8
2	Atomic and electronic structure of two-dimensional Mo_{(1â^'} _x)W _x S₂ alloys. JPhys Materials, 2021, 4, 025004.	4.2	7
3	Strong in-plane anisotropy in the electronic properties of doped transition metal dichalcogenides exhibited in W1â^'xNbxS2. Physical Review B, 2021, 103, .	3.2	7
4	Ghost anti-crossings caused by interlayer umklapp hybridization of bands in 2D heterostructures. 2D Materials, 2021, 8, 015016.	4.4	8
5	Effects of substituent position on aminobenzoate relaxation pathways in solution. Physical Chemistry Chemical Physics, 2021, 23, 23242-23255.	2.8	3
6	Exploring the Photochemistry of an Ethyl Sinapate Dimer: An Attempt Toward a Better Ultraviolet Filter. Frontiers in Chemistry, 2020, 8, 633.	3.6	9
7	The <scp>ONETEP</scp> linear-scaling density functional theory program. Journal of Chemical Physics, 2020, 152, 174111.	3.0	94
8	ONETEP + TOSCAM: Uniting Dynamical Mean Field Theory and Linear-Scaling Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 4899-4911.	5.3	5
9	Visualizing electrostatic gating effects in two-dimensional heterostructures. Nature, 2019, 572, 220-223.	27.8	135
10	Examining solvent effects on the ultrafast dynamics of catechol. Journal of Chemical Physics, 2019, 151, 084305.	3.0	9
11	Atom-projected and angular momentum resolved density of states in the ONETEP code. Electronic Structure, 2019, 1, 035002.	2.8	7
12	A molecular movie of ultrafast singlet fission. Nature Communications, 2019, 10, 4207.	12.8	54
13	Tensor network simulation of multi-environmental open quantum dynamics via machine learning and entanglement renormalisation. Nature Communications, 2019, 10, 1062.	12.8	74
14	Resolution of the exponent puzzle for the Anderson transition in doped semiconductors. Physical Review B, 2019, 99, .	3.2	10
15	Multifractality of ab initio wave functions in doped semiconductors. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 111, 141-147.	2.7	8
16	Determination of Secondary Species in Solution through Pump-Selective Transient Absorption Spectroscopy and Explicit-Solvent TDDFT. Journal of Physical Chemistry A, 2019, 123, 873-880.	2.5	8
17	Self-assembly of bis-salphen compounds: from semiflexible chains to webs of nanorings. Soft Matter, 2018, 14, 1181-1194.	2.7	9
18	Implicit and explicit host effects on excitons in pentacene derivatives. Journal of Chemical Physics, 2018, 148, 104108.	3.0	12

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19	Band structure interpolation using optimized local orbitals from linear-scaling density functional theory. Physical Review B, 2018, 98, .	3.2	6
20	Photophysics and Photochemistry of DNA Molecules: Electronic Excited States Leading to Thymine Dimerization. Journal of Physical Chemistry C, 2018, 122, 11633-11640.	3.1	4
21	Substituent position effects on sunscreen photodynamics: A closer look at methyl anthranilate. Chemical Physics, 2018, 515, 596-602.	1.9	5
22	Unravelling the Roles of Size, Ligands, and Pressure in the Piezochromic Properties of CdS Nanocrystals. Nano Letters, 2017, 17, 1042-1048.	9.1	17
23	Determination of band offsets, hybridization, and exciton binding in 2D semiconductor heterostructures. Science Advances, 2017, 3, e1601832.	10.3	293
24	Predicting solvatochromic shifts and colours of a solvated organic dye: The example of nile red. Journal of Chemical Physics, 2017, 146, 124504.	3.0	54
25	Evidence of Correlated Static Disorder in the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2017, 8, 2350-2356.	4.6	9
26	Nonradiative Step Facets in Semiconductor Nanowires. Nano Letters, 2017, 17, 2454-2459.	9.1	17
27	Impact of Carbonyl Formation on Cobalt Ripening over Titania Surface. Journal of Physical Chemistry C, 2017, 121, 15880-15887.	3.1	3
28	Linear-scaling density functional theory using the projector augmented wave method. Journal of Physics Condensed Matter, 2017, 29, 024001.	1.8	10
29	Chemically Selective Alternatives to Photoferroelectrics for Polarizationâ€Enhanced Photocatalysis: The Untapped Potential of Hybrid Inorganic Nanotubes. Advanced Science, 2017, 4, 1600153.	11.2	29
30	The potential of imogolite nanotubes as (co-)photocatalysts: a linear-scaling density functional theory study. Journal of Physics Condensed Matter, 2016, 28, 074003.	1.8	28
31	Tuning the role of charge-transfer states in intramolecular singlet exciton fission through side-group engineering. Nature Communications, 2016, 7, 13622.	12.8	157
32	Simulation of electron energy loss spectra of nanomaterials with linear-scaling density functional theory. Journal of Physics Condensed Matter, 2016, 28, 195202.	1.8	13
33	Multipurpose Black-Phosphorus/hBN Heterostructures. Nano Letters, 2016, 16, 2586-2594.	9.1	127
34	Applications of large-scale density functional theory in biology. Journal of Physics Condensed Matter, 2016, 28, 393001.	1.8	105
35	Supercell convergence of charge-transfer energies in pentacene molecular crystals from constrained DFT. Physical Review B, 2016, 93, .	3.2	18
36	Solvent Effects on Electronic Excitations of an Organic Chromophore. Journal of Chemical Theory and Computation, 2016, 12, 1853-1861.	5.3	57

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37	Large-scale density functional theory simulation of inorganic nanotubes: a case study on Imogolite nanotubes. Materials Research Innovations, 2015, 19, S272-S282.	2.3	17
38	Linear-scaling time-dependent density-functional theory beyond the Tamm-Dancoff approximation: Obtaining efficiency and accuracy with in situ optimised local orbitals. Journal of Chemical Physics, 2015, 143, 204107.	3.0	31
39	Energy landscape and band-structure tuning in realistic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></ Physical Review B, 2015, 91, .	3.2	47
40	Elevated Curie temperature and half-metallicity in the ferromagnetic semiconductorLaxEu1â^'xO. Physical Review B, 2015, 92, .	3.2	5
41	Identifying and tracing potential energy surfaces of electronic excitations with specific character via their transition origins: application to oxirane. Physical Chemistry Chemical Physics, 2015, 17, 12065-12079.	2.8	8
42	Pressure-Induced Amorphization and a New High Density Amorphous Metallic Phase in Matrix-Free Ge Nanoparticles. Nano Letters, 2015, 15, 7334-7340.	9.1	26
43	Mapping functional groups on oxidised multi-walled carbon nanotubes at the nanometre scale. Chemical Communications, 2014, 50, 6744-6747.	4.1	12
44	Hybrid MPI-OpenMP Parallelism in the ONETEP Linear-Scaling Electronic Structure Code: Application to the Delamination of Cellulose Nanofibrils. Journal of Chemical Theory and Computation, 2014, 10, 4782-4794.	5.3	50
45	Point Defects and Non-stoichiometry in Li₂TiO₃. Chemistry of Materials, 2014, 26, 1629-1638.	6.7	63
46	Electron Microscopic Characterization of Functionalized Multi-Walled Carbon Nanotubes and Their Interactions with the Blood Brain Barrier. Microscopy and Microanalysis, 2014, 20, 1744-1745.	0.4	0
47	Linear-scaling time-dependent density-functional theory in the linear response formalism. Journal of Chemical Physics, 2013, 139, 064104.	3.0	59
48	Toward Ab Initio Optical Spectroscopy of the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2013, 4, 4206-4212.	4.6	45
49	Importance of Many-Body Effects in the Kernel of Hemoglobin for Ligand Binding. Physical Review Letters, 2013, 110, 106402.	7.8	29
50	On the growth of Al2O3 scales. Acta Materialia, 2013, 61, 6670-6683.	7.9	140
51	Simulations of nanocrystals under pressure: Combining electronic enthalpy and linear-scaling density-functional theory. Journal of Chemical Physics, 2013, 139, 084117.	3.0	7
52	Bromophenyl functionalization of carbon nanotubes: an ab initio study. Nanotechnology, 2013, 24, 375702.	2.6	5
53	Electrostatic considerations affecting the calculated HOMOâ€“LUMO gap in protein molecules. Journal of Physics Condensed Matter, 2013, 25, 152101.	1.8	48
54	Anisotropic charge screening and supercell size convergence of defect formation energies. Physical Review B, 2013, 87, .	3.2	91

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55	Dimensionality of Carbon Nanomaterials Determines the Binding and Dynamics of Amyloidogenic Peptides: Multiscale Theoretical Simulations. PLoS Computational Biology, 2013, 9, e1003360.	3.2	49
56	Linear-scaling density functional theory simulations of polar semiconductor nanorods. Journal of Physics: Conference Series, 2012, 367, 012002.	0.4	10
57	Linear-scaling DFTâ€‰+â€‰Uwith full local orbital optimization. Physical Review B, 2012, 85, .	3.2	24
58	Fermi-level pinning can determine polarity in semiconductor nanorods. Physical Review B, 2012, 85, .	3.2	15
59	Pulay forces from localized orbitals optimized in situ using a psinc basis set. Journal of Chemical Physics, 2012, 136, 234101.	3.0	41
60	Vanadium Dioxide: A Peierls-Mott Insulator Stable against Disorder. Physical Review Letters, 2012, 108, 256402.	7.8	156
61	Calculating optical absorption spectra for large systems using linear-scaling density functional theory. Physical Review B, 2011, 84, .	3.2	52
62	Accurate ionic forces and geometry optimization in linear-scaling density-functional theory with local orbitals. Physical Review B, 2011, 83, .	3.2	75
63	Thickness-dependent magnetic properties of oxygen-deficient EuO. Physical Review B, 2011, 84, .	3.2	22
64	Factors influencing the distribution of charge in polar nanocrystals. Physical Review B, 2011, 83, .	3.2	17
65	Calculating dispersion interactions using maximally localized Wannier functions. Journal of Chemical Physics, 2011, 135, 154105.	3.0	34
66	Electrostatic interactions in finite systems treated with periodic boundary conditions: Application to linear-scaling density functional theory. Journal of Chemical Physics, 2011, 135, 204103.	3.0	61
67	Projector self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>DFT</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> nonorthogonal generalized Wannier functions. Physical Review B, 2010, 82, .	3.2	42
68	Linear-scaling density-functional simulations of charged point defects in Al2O3 using hierarchical sparse matrix algebra. Journal of Chemical Physics, 2010, 133, 114111.	3.0	38
69	Experimental and theoretical analysis of magnetic moment enhancement in oxygen-deficient EuO. Physical Review B, 2010, 81, .	3.2	38
70	Linear-scaling density-functional theory with tens of thousands of atoms: Expanding the scope and scale of calculations with ONETEP. Computer Physics Communications, 2009, 180, 1041-1053.	7.5	119
71	Supercell size scaling of density functional theory formation energies of charged defects. Physical Review B, 2009, 79, .	3.2	180
72	Localization lengths over metal to band insulator transitions. Journal of Physics Condensed Matter, 2007, 19, 506212.	1.8	11

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73	Quantum Monte Carlo calculations of the surface energy of an electron gas. Physical Review B, 2007, 76, .	3.2	35
74	Accurate and efficient method for the treatment of exchange in a plane-wave basis. Journal of Chemical Physics, 2006, 124, 064105.	3.0	87