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	Determination of band offsets, hybridization, and exciton binding in 2D semiconductor heterostructures. Science Advances, 2017, 3, e1601832.	10.3	293
2	Supercell size scaling of density functional theory formation energies of charged defects. Physical Review B, 2009, 79, .	3.2	180
3	Tuning the role of charge-transfer states in intramolecular singlet exciton fission through side-group engineering. Nature Communications, 2016, 7, 13622.	12.8	157
4	Vanadium Dioxide: A Peierls-Mott Insulator Stable against Disorder. Physical Review Letters, 2012, 108, 256402.	7.8	156
5	On the growth of Al2O3 scales. Acta Materialia, 2013, 61, 6670-6683.	7.9	140
6	Visualizing electrostatic gating effects in two-dimensional heterostructures. Nature, 2019, 572, 220-223.	27.8	135
7	Multipurpose Black-Phosphorus/hBN Heterostructures. Nano Letters, 2016, 16, 2586-2594.	9.1	127
8	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
9	Applications of large-scale density functional theory in biology. Journal of Physics Condensed Matter, 2016, 28, 393001.	1.8	105
10	The <scp>ONETEP</scp> linear-scaling density functional theory program. Journal of Chemical Physics, 2020, 152, 174111.	3.0	94
11	Anisotropic charge screening and supercell size convergence of defect formation energies. Physical Review B, 2013, 87, .	3.2	91
12	Accurate and efficient method for the treatment of exchange in a plane-wave basis. Journal of Chemical Physics, 2006, 124, 064105.	3.0	87
13	Accurate ionic forces and geometry optimization in linear-scaling density-functional theory with local orbitals. Physical Review B, 2011, 83, .	3.2	75
14	Tensor network simulation of multi-environmental open quantum dynamics via machine learning and entanglement renormalisation. Nature Communications, 2019, 10, 1062.	12.8	74
15	Point Defects and Non-stoichiometry in Li₂TiO₃. Chemistry of Materials, 2014, 26, 1629-1638.	6.7	63
16	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
17	Linear-scaling time-dependent density-functional theory in the linear response formalism. Journal of Chemical Physics, 2013, 139, 064104.	3.0	59
18	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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19	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
20	A molecular movie of ultrafast singlet fission. Nature Communications, 2019, 10, 4207.	12.8	54
21	Calculating optical absorption spectra for large systems using linear-scaling density functional theory. Physical Review B, 2011, 84, .	3.2	52
22	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
23	Dimensionality of Carbon Nanomaterials Determines the Binding and Dynamics of Amyloidogenic Peptides: Multiscale Theoretical Simulations. PLoS Computational Biology, 2013, 9, e1003360.	3.2	49
24	Electrostatic considerations affecting the calculated HOMOâ€“LUMO gap in protein molecules. Journal of Physics Condensed Matter, 2013, 25, 152101.	1.8	48
25	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
26	Toward Ab Initio Optical Spectroscopy of the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2013, 4, 4206-4212.	4.6	45
27	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
28	Pulay forces from localized orbitals optimized in situ using a psinc basis set. Journal of Chemical Physics, 2012, 136, 234101.	3.0	41
29	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
30	Experimental and theoretical analysis of magnetic moment enhancement in oxygen-deficient EuO. Physical Review B, 2010, 81, .	3.2	38
31	Quantum Monte Carlo calculations of the surface energy of an electron gas. Physical Review B, 2007, 76, .	3.2	35
32	Calculating dispersion interactions using maximally localized Wannier functions. Journal of Chemical Physics, 2011, 135, 154105.	3.0	34
33	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
34	Importance of Many-Body Effects in the Kernel of Hemoglobin for Ligand Binding. Physical Review Letters, 2013, 110, 106402.	7.8	29
35	Chemically Selective Alternatives to Photoferroelectrics for Polarizationâ€Enhanced Photocatalysis: The Untapped Potential of Hybrid Inorganic Nanotubes. Advanced Science, 2017, 4, 1600153.	11.2	29
36	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

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37	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
38	Linear-scaling DFTâ€‰+â€‰Uwith full local orbital optimization. Physical Review B, 2012, 85, .	3.2	24
39	Thickness-dependent magnetic properties of oxygen-deficient EuO. Physical Review B, 2011, 84, .	3.2	22
40	Supercell convergence of charge-transfer energies in pentacene molecular crystals from constrained DFT. Physical Review B, 2016, 93, .	3.2	18
41	Factors influencing the distribution of charge in polar nanocrystals. Physical Review B, 2011, 83, .	3.2	17
42	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
43	Unravelling the Roles of Size, Ligands, and Pressure in the Piezochromic Properties of CdS Nanocrystals. Nano Letters, 2017, 17, 1042-1048.	9.1	17
44	Nonradiative Step Facets in Semiconductor Nanowires. Nano Letters, 2017, 17, 2454-2459.	9.1	17
45	Fermi-level pinning can determine polarity in semiconductor nanorods. Physical Review B, 2012, 85, .	3.2	15
46	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
47	Mapping functional groups on oxidised multi-walled carbon nanotubes at the nanometre scale. Chemical Communications, 2014, 50, 6744-6747.	4.1	12
48	Implicit and explicit host effects on excitons in pentacene derivatives. Journal of Chemical Physics, 2018, 148, 104108.	3.0	12
49	Localization lengths over metal to band insulator transitions. Journal of Physics Condensed Matter, 2007, 19, 506212.	1.8	11
50	Linear-scaling density functional theory simulations of polar semiconductor nanorods. Journal of Physics: Conference Series, 2012, 367, 012002.	0.4	10
51	Linear-scaling density functional theory using the projector augmented wave method. Journal of Physics Condensed Matter, 2017, 29, 024001.	1.8	10
52	Resolution of the exponent puzzle for the Anderson transition in doped semiconductors. Physical Review B, 2019, 99, .	3.2	10
53	Evidence of Correlated Static Disorder in the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2017, 8, 2350-2356.	4.6	9
54	Self-assembly of bis-salphen compounds: from semiflexible chains to webs of nanorings. Soft Matter, 2018, 14, 1181-1194.	2.7	9

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55	Examining solvent effects on the ultrafast dynamics of catechol. Journal of Chemical Physics, 2019, 151, 084305.	3.0	9
56	Exploring the Photochemistry of an Ethyl Sinapate Dimer: An Attempt Toward a Better Ultraviolet Filter. Frontiers in Chemistry, 2020, 8, 633.	3.6	9
57	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
58	Multifractality of ab initio wave functions in doped semiconductors. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 111, 141-147.	2.7	8
59	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
60	Ghost anti-crossings caused by interlayer umklapp hybridization of bands in 2D heterostructures. 2D Materials, 2021, 8, 015016.	4.4	8
61	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
62	Simulations of nanocrystals under pressure: Combining electronic enthalpy and linear-scaling density-functional theory. Journal of Chemical Physics, 2013, 139, 084117.	3.0	7
63	Atom-projected and angular momentum resolved density of states in the ONETEP code. Electronic Structure, 2019, 1, 035002.	2.8	7
64	Atomic and electronic structure of two-dimensional Mo_{(1â^'} _x)W _x S₂ alloys. JPhys Materials, 2021, 4, 025004.	4.2	7
65	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
66	Band structure interpolation using optimized local orbitals from linear-scaling density functional theory. Physical Review B, 2018, 98, .	3.2	6
67	Bromophenyl functionalization of carbon nanotubes: an ab initio study. Nanotechnology, 2013, 24, 375702.	2.6	5
68	Elevated Curie temperature and half-metallicity in the ferromagnetic semiconductorLaxEu1â^'xO. Physical Review B, 2015, 92, .	3.2	5
69	Substituent position effects on sunscreen photodynamics: A closer look at methyl anthranilate. Chemical Physics, 2018, 515, 596-602.	1.9	5
70	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
71	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
72	Impact of Carbonyl Formation on Cobalt Ripening over Titania Surface. Journal of Physical Chemistry C, 2017, 121, 15880-15887.	3.1	3

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73	Effects of substituent position on aminobenzoate relaxation pathways in solution. Physical Chemistry Chemical Physics, 2021, 23, 23242-23255.	2.8	3
74	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