Chris -Kriton Skylaris

List of Publications by Year
in descending order

88 papers	3,495 citations	136940 32 h-index	144002 57 g-index
96 all docs	96 docs citations	96 times ranked	3642 citing authors

#	Article	IF	Citations
1	IntroducingONETEP: Linear-scaling density functional simulations on parallel computers. Journal of Chemical Physics, 2005, 122, 084119.	3.0	550
2	Energy decomposition analysis approaches and their evaluation on prototypical proteinâ€“drug interaction patterns. Chemical Society Reviews, 2015, 44, 3177-3211.	38.1	284
3	Nonorthogonal generalized Wannier function pseudopotential plane-wave method. Physical Review B, 2002, 66, .	3.2	144
4	Preconditioned iterative minimization for linear-scaling electronic structure calculations. Journal of Chemical Physics, 2003, 119, 8842-8848.	3.0	119
5	Field-effect sensors â€“ from pH sensing to biosensing: sensitivity enhancement using streptavidinâ€“biotin as a model system. Analyst, The, 2017, 142, 4173-4200.	3.5	109
6	Perspective: Methods for large-scale density functional calculations on metallic systems. Journal of Chemical Physics, 2016, 145, 220901.	3.0	106
7	Acid-base dissociation mechanisms and energetics at the silicaâ€“water interface: An activationless process. Journal of Colloid and Interface Science, 2015, 451, 231-244.	9.4	96
8	The <scp>ONETEP</scp> linear-scaling density functional theory program. Journal of Chemical Physics, 2020, 152, 174111.	3.0	94
9	Use of the rVV10 Nonlocal Correlation Functional in the B97M-V Density Functional: Defining B97M-rV and Related Functionals. Journal of Physical Chemistry Letters, 2017, 8, 35-40.	4.6	78
10	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	2.6	77
11	Accurate ionic forces and geometry optimization in linear-scaling density-functional theory with local orbitals. Physical Review B, 2011, 83, .	3.2	75
12	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
13	CD1b-restricted GEM T cell responses are modulated byMycobacterium tuberculosismycolic acid meromycolate chains. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10956-E10964.	7.1	58
14	Total-energy calculations on a real space grid with localized functions and a plane-wave basis. Computer Physics Communications, 2002, 147, 788-802.	7.5	57
15	A variational method for density functional theory calculations on metallic systems with thousands of atoms. Journal of Chemical Physics, 2013, 139, 054107.	3.0	51
16	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
17	Large-Scale Density Functional Theory Transition State Searching in Enzymes. Journal of Physical Chemistry Letters, 2014, 5, 3614-3619.	4.6	49
18	Predicting the Oxygen-Binding Properties of Platinum Nanoparticle Ensembles by Combining High-Precision Electron Microscopy and Density Functional Theory. Nano Letters, 2017, 17, 4003-4012.	9.1	47

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19	Achieving plane wave accuracy in linear-scaling density functional theory applied to periodic systems: A case study on crystalline silicon. Journal of Chemical Physics, 2007, 127, 164712.	3.0	46
20	TINKTEP: A fully self-consistent, mutually polarizable QM/MM approach based on the AMOEBA force field. Journal of Chemical Physics, 2016, 145, 124106.	3.0	46
21	Using ONETEP for accurate and efficient density functional calculations. Journal of Physics Condensed Matter, 2005, 17, 5757-5769.	1.8	44
22	Implementation of linear-scaling plane wave density functional theory on parallel computers. Physica Status Solidi (B): Basic Research, 2006, 243, 973-988.	1.5	44
23	Surfactant Proteins A and D: Trimerized Innate Immunity Proteins with an Affinity for Viral Fusion Proteins. Journal of Innate Immunity, 2019, 11, 13-28.	3.8	44
24	Accurate kinetic energy evaluation in electronic structure calculations with localized functions on real space grids. Computer Physics Communications, 2001, 140, 315-322.	7.5	41
25	Pulay forces from localized orbitals optimized in situ using a psinc basis set. Journal of Chemical Physics, 2012, 136, 234101.	3.0	41
26	Cholesteryl esters stabilize human CD1c conformations for recognition by self-reactive T cells. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E1266-75.	7.1	41
27	Fitting EXAFS data using molecular dynamics outputs and a histogram approach. Physical Review B, 2012, 85, .	3.2	40
28	Meta-analysis: the molecular organization of non-fullerene acceptors. Materials Horizons, 2020, 7, 1062-1072.	12.2	38
29	Polarized Protein-Specific Charges from Atoms-in-Molecule Electron Density Partitioning. Journal of Chemical Theory and Computation, 2013, 9, 2981-2991.	5.3	35
30	Including dispersion interactions in the ONETEP program for linear-scaling density functional theory calculations. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2009, 465, 669-683.	2.1	34
31	Largeâ€scale DFT calculations in implicit solventâ€"A case study on the T4 lysozyme L99A/M102Q protein. International Journal of Quantum Chemistry, 2013, 113, 771-785.	2.0	34
32	Density functional theory calculations on entire proteins for free energies of binding: Application to a model polar binding site. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3335-3346.	2.6	34
33	A â€œStepping Stoneâ€•Approach for Obtaining Quantum Free Energies of Hydration. Journal of Physical Chemistry B, 2015, 119, 7030-7040.	2.6	34
34	Machine-Learned Fragment-Based Energies for Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2019, 15, 2743-2758.	5.3	33
35	Expanding the Scope of Density Derived Electrostatic and Chemical Charge Partitioning to Thousands of Atoms. Journal of Chemical Theory and Computation, 2014, 10, 5377-5390.	5.3	32
36	Reconciling Work Functions and Adsorption Enthalpies for Implicit Solvent Models: A Pt (111)/Water Interface Case Study. Journal of Chemical Theory and Computation, 2020, 16, 2703-2715.	5.3	32

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37	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.	5.3	31
38	Chemically Selective Alternatives to Photoferroelectrics for Polarizationâ€Enhanced Photocatalysis: The Untapped Potential of Hybrid Inorganic Nanotubes. Advanced Science, 2017, 4, 1600153.	11.2	29
39	The Role of Electrostatics in Enzymes: Do Biomolecular Force Fields Reflect Protein Electric Fields?. Journal of Chemical Information and Modeling, 2020, 60, 3131-3144.	5.4	29
40	Computational prediction of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml spectra of gold nanoparticles from classical molecular dynamics simulations. Physical Review B, 2011, 83, .	3.2	28
41	Performance of the AMOEBA Water Model in the Vicinity of QM Solutes: A Diagnosis Using Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2017, 13, 1963-1979.	5.3	28
42	Natural bond orbital analysis in the ONETEP code: Applications to large protein systems. Journal of Computational Chemistry, 2013, 34, 429-444.	3.3	27
43	A benchmark for materials simulation. Science, 2016, 351, 1394-1395.	12.6	26
44	Performance of extended Lagrangian schemes for molecular dynamics simulations with classical polarizable force fields and density functional theory. Journal of Chemical Physics, 2017, 146, 124115.	3.0	26
45	Lithium intercalation edge effects and doping implications for graphite anodes. Journal of Materials Chemistry A, 2020, 8, 7947-7955.	10.3	25
46	ParaMol: A Package for Automatic Parameterization of Molecular Mechanics Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 2026-2047.	5.4	22
47	Evaluation of Methods for Viscosity Simulations of Lubricants at Different Temperatures and Pressures: A Case Study on PAO-2. Tribology Transactions, 2021, 64, 1138-1148.	2.0	22
48	Anharmonic Infrared Spectroscopy through the Fourier Transform of Time Correlation Function Formalism in O<scp>NETEP</scp>. Journal of Chemical Theory and Computation, 2015, 11, 3321-3332.	5.3	20
49	Proteinâ€“ligand free energies of binding from full-protein DFT calculations: convergence and choice of exchangeâ€“correlation functional. Physical Chemistry Chemical Physics, 2021, 23, 9381-9393.	2.8	20
50	Recent progress in linear-scaling density functional calculations with plane waves and pseudopotentials: the ONETEP code. Journal of Physics Condensed Matter, 2008, 20, 064209.	1.8	19
51	First Principles-Based Calculations of Free Energy of Binding: Application to Ligand Binding in a Self-Assembling Superstructure. Journal of Chemical Theory and Computation, 2011, 7, 1102-1108.	5.3	19
52	What Is the Price of Open-Source Software?. Journal of Physical Chemistry Letters, 2015, 6, 2751-2754.	4.6	19
53	Porting ONETEP to graphical processing unitâ€based coprocessors. 1. FFT box operations. Journal of Computational Chemistry, 2013, 34, 2446-2459.	3.3	18
54	Self-consistent implementation of meta-GGA functionals for the ONETEP linear-scaling electronic structure package. Journal of Chemical Physics, 2016, 145, 204114.	3.0	18

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55	Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. Journal of Chemical Physics, 2016, 145, 044109.	3.0	16
56	Mutually polarizable QM/MM model with in situ optimized localized basis functions. Journal of Chemical Physics, 2019, 150, 074103.	3.0	16
57	Practical Approach to Large-Scale Electronic Structure Calculations in Electrolyte Solutions via Continuum-Embedded Linear-Scaling Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 7860-7872.	3.1	16
58	Strain effects in coreâ€“shell PtCo nanoparticles: a comparison of experimental observations and computational modelling. Physical Chemistry Chemical Physics, 2020, 22, 24784-24795.	2.8	15
59	Electronic annealing Fermi operator expansion for DFT calculations on metallic systems. Journal of Chemical Physics, 2018, 148, 074107.	3.0	14
60	Linear-scaling density functional simulations of the effect of crystallographic structure on the electronic and optical properties of fullerene solvates. Physical Chemistry Chemical Physics, 2017, 19, 5617-5628.	2.8	13
61	Insights into the Charge-Transfer Mechanism of Organic Photovoltaics: Effect of Domain Size. Journal of Physical Chemistry C, 2018, 122, 17024-17034.	3.1	13
62	A computational chemistry approach to modelling conducting polymers in ionic liquids for next generation batteries. Energy Reports, 2020, 6, 198-208.	5.1	13
63	Mechanism of Li nucleation at graphite anodes and mitigation strategies. Journal of Materials Chemistry A, 2021, 9, 16798-16804.	10.3	13
64	Pushing the boundaries of lithium battery research with atomistic modelling on different scales. Progress in Energy, 2022, 4, 012002.	10.9	12
65	Effect of Polymerization Statistics on the Electronic Properties of Copolymers for Organic Photovoltaics. Journal of Physical Chemistry C, 2017, 121, 2529-2538.	3.1	11
66	Modification of O and CO binding on Pt nanoparticles due to electronic and structural effects of titania supports. Journal of Chemical Physics, 2019, 151, 114702.	3.0	11
67	Electrochemistry from first-principles in the grand canonical ensemble. Journal of Chemical Physics, 2021, 155, 024114.	3.0	11
68	Li nucleation on the graphite anode under potential control in Li-ion batteries. Journal of Materials Chemistry A, 2022, 10, 11426-11436.	10.3	11
69	Electronically Excited States in Solution via a Smooth Dielectric Model Combined with Equation-of-Motion Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2017, 13, 5572-5581.	5.3	10
70	Electron localisation descriptors in ONETEP: a tool for interpreting localisation and bonding in large-scale DFT calculations. Electronic Structure, 2020, 2, 027001.	2.8	10
71	Electronic structure calculations in electrolyte solutions: Methods for neutralization of extended charged interfaces. Journal of Chemical Physics, 2020, 153, 124101.	3.0	8
72	A Monte Carlo Resampling Approach for the Calculation of Hybrid Classical and Quantum Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 415-424.	5.3	7

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73	Atom-projected and angular momentum resolved density of states in the ONETEP code. Electronic Structure, 2019, 1, 035002.	2.8	7
74	Understanding Adsorption of Organics on Pt(111) in the Aqueous Phase: Insights from DFT Based Implicit Solvent and Statistical Thermodynamics Models. Journal of Chemical Theory and Computation, 2022, 18, 1849-1861.	5.3	7
75	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
76	Mechanism of Os-Catalyzed Oxidative Cyclization of 1,5-Dienes. Journal of Organic Chemistry, 2019, 84, 15173-15183.	3.2	6
77	Analysis of DNA interactions and GC content with energy decomposition in large-scale quantum mechanical calculations. Physical Chemistry Chemical Physics, 2021, 23, 8891-8899.	2.8	6
78	Classical molecular dynamics simulations of the complex between the RAD51 protein and the BRC hairpin loops of the BRCA2 protein. Molecular Simulation, 2008, 34, 749-759.	2.0	4
79	How Does Polymorphism Affect the Interfacial Charge-Transfer States in Organic Photovoltaics?. Journal of Physical Chemistry C, 2019, 123, 25585-25595.	3.1	2
80	Generation of Quantum Configurational Ensembles Using Approximate Potentials. Journal of Chemical Theory and Computation, 2021, 17, 7021-7042.	5.3	2
81	Massively parallel linear-scaling Hartreeâ€“Fock exchange and hybrid exchangeâ€“correlation functionals with plane wave basis set accuracy. Journal of Chemical Physics, 2021, 155, 224106.	3.0	2
82	Energy decomposition analysis method for metallic systems. Physical Chemistry Chemical Physics, 2022, 24, 1702-1711.	2.8	2
83	Towards Statistically Representative Atomic Resolution 3D Nano-metrology for Materials Modelling and Catalyst Design. Microscopy and Microanalysis, 2015, 21, 2197-2198.	0.4	1
84	Translocation of flexible and tensioned ssDNA through in silico designed hydrophobic nanopores with two constrictions. Nanoscale, 2021, 13, 1673-1679.	5.6	1
85	Atomistic level characterisation of ssDNA translocation through the E. coli proteins CsgG and CsgF for nanopore sequencing. Computational and Structural Biotechnology Journal, 2021, 19, 6417-6430.	4.1	1
86	Spectroscopic chemical insights leading to the design of versatile sustainable composites for enhanced marine application. RSC Advances, 2015, 5, 101221-101231.	3.6	0
87	Ab initio molecular dynamics study of AlCl4â^' adsorption on PEDOT conducting polymer chains. Energy Reports, 2021, 7, 111-119.	5.1	0
88	Intercalation voltages for spinel LixMn2O4 (0â‰xâ‰2) cathode materials: Calibration of calculations with the ONETEP linear-scaling DFT code. Materials Today Communications, 2021, 27, 102380.	1.9	0