Daniel J Cole

List of Publications by Year
in descending order

49 papers	1,487 citations	279487 23 h-index	329751 37 g-index
64 all docs	64 docs citations	64 times ranked	1870 citing authors

#	Article	IF	Citations
1	Exploration and validation of force field design protocols through QM-to-MM mapping. Physical Chemistry Chemical Physics, 2022, 24, 17014-17027.	1.3	4
2	Implementation of the QUBE Force Field in SOMD for High-Throughput Alchemical Free-Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2124-2130.	2.5	5
3	Modeling Molecular Emitters in Organic Light-Emitting Diodes with the Quantum Mechanical Bespoke Force Field. Journal of Chemical Theory and Computation, 2021, 17, 5021-5033.	2.3	6
4	Linear Atomic Cluster Expansion Force Fields for Organic Molecules: Beyond RMSE. Journal of Chemical Theory and Computation, 2021, 17, 7696-7711.	2.3	52
5	Modelling flexible proteinâ€“ligand binding in p38Î± MAP kinase using the QUBE force field. Chemical Communications, 2020, 56, 932-935.	2.2	6
6	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	1.6	2
7	A machine learning based intramolecular potential for a flexible organic molecule. Faraday Discussions, 2020, 224, 247-264.	1.6	22
8	Static Disorder in Excitation Energies of the Fennaâ€“Matthewsâ€“Olson Protein: Structure-Based Theory Meets Experiment. Journal of Physical Chemistry Letters, 2020, 11, 10306-10314.	2.1	16
9	The <scp>ONETEP</scp> linear-scaling density functional theory program. Journal of Chemical Physics, 2020, 152, 174111.	1.2	94
10	ONETEP + TOSCAM: Uniting Dynamical Mean Field Theory and Linear-Scaling Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 4899-4911.	2.3	5
11	Bifunctional Hydrogen Bonding of Imidazole with Water Explored by Rotational Spectroscopy and DFT Calculations. Journal of Physical Chemistry A, 2020, 124, 2649-2659.	1.1	13
12	Superexchange mechanism and quantum many body excitations in the archetypal di-Cu oxo-bridge. Communications Physics, 2020, 3, .	2.0	8
13	Development and Validation of the Quantum Mechanical Bespoke Protein Force Field. ACS Omega, 2019, 4, 14537-14550.	1.6	18
14	The future of force fields in computer-aided drug design. Future Medicinal Chemistry, 2019, 11, 2359-2363.	1.1	17
15	Absolute Free Energy of Binding Calculations for Macrophage Migration Inhibitory Factor in Complex with a Druglike Inhibitor. Journal of Physical Chemistry B, 2019, 123, 8675-8685.	1.2	17
16	New scaling relations to compute atom-in-material polarizabilities and dispersion coefficients: part 1. Theory and accuracy. RSC Advances, 2019, 9, 19297-19324.	1.7	16
17	QUBEKit: Automating the Derivation of Force Field Parameters from Quantum Mechanics. Journal of Chemical Information and Modeling, 2019, 59, 1366-1381.	2.5	68
18	Computation of proteinâ€“ligand binding free energies using quantum mechanical bespoke force fields. MedChemComm, 2019, 10, 1116-1120.	3.5	20

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19	Harmonic Force Constants for Molecular Mechanics Force Fields via Hessian Matrix Projection. Journal of Chemical Theory and Computation, 2018, 14, 274-281.	2.3	51
20	Role of spin in the calculation of Hubbard <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> and Hund's <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>J</mml:mi></mml:math> parameters from first principles. Physical Review B, 2018, 98, .	1.1	45
21	Evidence of Correlated Static Disorder in the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2017, 8, 2350-2356.	2.1	9
22	Distance dependent photoacoustics revealed through DNA nanostructures. Nanoscale, 2017, 9, 16193-16199.	2.8	15
23	Computationally-guided optimization of small-molecule inhibitors of the Aurora A kinaseâ€“TPX2 proteinâ€“protein interaction. Chemical Communications, 2017, 53, 9372-9375.	2.2	15
24	Nonlinear network model analysis of vibrational energy transfer and localisation in the Fenna-Matthews-Olson complex. Scientific Reports, 2016, 6, 36703.	1.6	7
25	Residue Geometry Networks: A Rigidity-Based Approach to the Amino Acid Network and Evolutionary Rate Analysis. Scientific Reports, 2016, 6, 33213.	1.6	14
26	Biomolecular Force Field Parameterization via Atoms-in-Molecule Electron Density Partitioning. Journal of Chemical Theory and Computation, 2016, 12, 2312-2323.	2.3	104
27	Applications of large-scale density functional theory in biology. Journal of Physics Condensed Matter, 2016, 28, 393001.	0.7	105
28	Molecular dynamics and Monte Carlo simulations for proteinâ€“ligand binding and inhibitor design. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 966-971.	1.1	40
29	Constrained geometric dynamics of the Fennaâ€“Matthewsâ€“Olson complex: the role of correlated motion in reducing uncertainty in excitation energy transfer. Photosynthesis Research, 2014, 122, 275-292.	1.6	18
30	Impact of intracellular domain flexibility upon properties of activated human 5â€•HT 3 receptors. British Journal of Pharmacology, 2014, 171, 1617-1628.	2.7	15
31	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.	2.3	32
32	Enhanced Monte Carlo Sampling through Replica Exchange with Solute Tempering. Journal of Chemical Theory and Computation, 2014, 10, 565-571.	2.3	39
33	Large-Scale Density Functional Theory Transition State Searching in Enzymes. Journal of Physical Chemistry Letters, 2014, 5, 3614-3619.	2.1	49
34	Renormalization of myoglobinâ€“ligand binding energetics by quantum many-body effects. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5790-5795.	3.3	33
35	Constrained geometric simulation of the nicotinic acetylcholine receptor. Journal of Molecular Graphics and Modelling, 2014, 52, 1-10.	1.3	7
36	Toward Ab Initio Optical Spectroscopy of the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2013, 4, 4206-4212.	2.1	45

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37	Natural bond orbital analysis in the ONETEP code: Applications to large protein systems. Journal of Computational Chemistry, 2013, 34, 429-444.	1.5	27
38	Polarized Protein-Specific Charges from Atoms-in-Molecule Electron Density Partitioning. Journal of Chemical Theory and Computation, 2013, 9, 2981-2991.	2.3	35
39	Electrostatic considerations affecting the calculated HOMOâ€“LUMO gap in protein molecules. Journal of Physics Condensed Matter, 2013, 25, 152101.	0.7	48
40	Ligand Discrimination in Myoglobin from Linear-Scaling DFT+U. Journal of Physical Chemistry Letters, 2012, 3, 1448-1452.	2.1	25
41	Ion Adsorption at the Graphene/Electrolyte Interface. Journal of Physical Chemistry Letters, 2011, 2, 1799-1803.	2.1	75
42	Interrogation of the Protein-Protein Interactions between Human BRCA2 BRC Repeats and RAD51 Reveals Atomistic Determinants of Affinity. PLoS Computational Biology, 2011, 7, e1002096.	1.5	35
43	Protein-protein interactions from linear-scaling first-principles quantum-mechanical calculations. Europhysics Letters, 2010, 91, 37004.	0.7	38
44	Multiscale mechanics modeling of direct silicon wafer bonding. Scripta Materialia, 2009, 60, 1125-1128.	2.6	9
45	Water structuring and collagen adsorption at hydrophilic and hydrophobic silicon surfaces. Physical Chemistry Chemical Physics, 2009, 11, 11395.	1.3	50
46	Stress-Driven Oxidation Chemistry of Wet Silicon Surfaces. Journal of Physical Chemistry C, 2008, 112, 12077-12080.	1.5	30
47	Development of a classical force field for the oxidized Si surface: Application to hydrophilic wafer bonding. Journal of Chemical Physics, 2007, 127, 204704.	1.2	68
48	Stress development and impurity segregation during oxidation of the Si(100) surface. Surface Science, 2007, 601, 4888-4898.	0.8	9
49	On assessing functional errors in density functional theory using atomisation energies and electric field gradients. International Journal of Quantum Chemistry, 0, , e26799.	1.0	1