Alston J Misquitta

List of Publications by Year
in descending order

53 papers	4,328 citations	186265 28 h-index	197818 49 g-index
53 all docs	53 docs citations	53 times ranked	3366 citing authors

#	Article	IF	Citations
1	High-pressure neutron diffraction study of magnetite, Fe3O4, nanoparticles. Applied Physics Letters, 2022, 120, .	3.3	1
2	Methane hydrate clathrates: effects in the simulation of melting arising from the assumption of simple combining rules in interatomic potentials. Molecular Simulation, 2021, 47, 161-169.	2.0	0
3	Characterization of the fullerene derivative [60]PCBM, by high-field carbon, and two-dimensional NMR spectroscopy, coupled with DFT simulations. Carbon, 2021, 173, 891-900.	10.3	5
4	A non-empirical intermolecular force-field for trinitrobenzene and its application in crystal structure prediction. Journal of Chemical Physics, 2021, 154, 094123.	3.0	6
5	Assessment of SAPT and Supermolecular EDA Approaches for the Development of Separable and Polarizable Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 2759-2774.	5.3	20
6	First-Principles Many-Body Nonadditive Polarization Energies from Monomer and Dimer Calculations Only: A Case Study on Water. Journal of Chemical Theory and Computation, 2020, 16, 224-242.	5.3	7
7	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
8	Ion-Induced Soot Nucleation Using a New Potential for Curved Aromatics. Combustion Science and Technology, 2019, 191, 747-765.	2.3	21
9	Charge Distributions of Nitro Groups Within Organic Explosive Crystals: Effects on Sensitivity and Modeling. ACS Omega, 2019, 4, 8614-8625.	3.5	13
10	X-ray total scattering study of magic-size clusters and quantum dots of cadmium sulphide. Nanoscale, 2019, 11, 21900-21908.	5.6	17
11	Structures of CdSe and CdS Nanoclusters from Ab Initio Random Structure Searching. Journal of Physical Chemistry C, 2019, 123, 29370-29378.	3.1	22
12	New Angles on Standard Force Fields: Toward a General Approach for Treating Atomic-Level Anisotropy. Journal of Chemical Theory and Computation, 2018, 14, 739-758.	5.3	28
13	ISA-Pol: distributed polarizabilities and dispersion models from a basis-space implementation of the iterated stockholder atoms procedure. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	22
14	Intermolecular Interactions. , 2017, , 295-335.		4
15	Multipole Moments in the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2017, 121, 2056-2067.	2.5	7
16	Temporal mapping of photochemical reactions and molecular excited states with carbon specificity. Nature Materials, 2017, 16, 467-473.	27.5	16
17	Molecular dynamics study of CO₂ absorption and desorption in zinc imidazolate frameworks. Molecular Systems Design and Engineering, 2017, 2, 457-469.	3.4	8
18	From dimers to the solid-state: Distributed intermolecular force-fields for pyridine. Journal of Chemical Physics, 2017, 147, 161722.	3.0	16

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19	Spintronic and Electronic Phenomena in Organic Molecules Measured with Î¼SR. Journal of the Physical Society of Japan, 2016, 85, 091011.	1.6	7
20	Ab Initio Atomâ€“Atom Potentials Using C<scp>am</scp>CASP: Theory and Application to Many-Body Models for the Pyridine Dimer. Journal of Chemical Theory and Computation, 2016, 12, 4184-4208.	5.3	43
21	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
22	Beyond Bornâ€“Mayer: Improved Models for Short-Range Repulsion in ab Initio Force Fields. Journal of Chemical Theory and Computation, 2016, 12, 3851-3870.	5.3	79
23	Molecular dynamics simulation study of various zeolitic imidazolate framework structures. Dalton Transactions, 2016, 45, 4289-4302.	3.3	19
24	Intermolecular Interactions. , 2015, , 1-42.		1
25	Localized overlap algorithm for unexpanded dispersion energies. Journal of Chemical Physics, 2014, 140, 114304.	3.0	4
26	Anomalous nonadditive dispersion interactions in systems of three one-dimensional wires. Physical Review B, 2014, 89, .	3.2	23
27	Distributed Multipoles from a Robust Basis-Space Implementation of the Iterated Stockholder Atoms Procedure. Journal of Chemical Theory and Computation, 2014, 10, 5405-5418.	5.3	58
28	Charge Transfer from Regularized Symmetry-Adapted Perturbation Theory. Journal of Chemical Theory and Computation, 2013, 9, 5313-5326.	5.3	74
29	Simulation study of pressure and temperature dependence of the negative thermal expansion in Zn(CN)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 88, .	3.2	46
30	High pressure ionic and molecular crystals of ammonia monohydrate within density functional theory. Journal of Chemical Physics, 2012, 137, 064506.	3.0	21
31	A quantitative study of the clustering of polycyclic aromatic hydrocarbons at high temperatures. Physical Chemistry Chemical Physics, 2012, 14, 4081.	2.8	147
32	Intermolecular Interactions. , 2012, , 157-193.		6
33	Assessing the Polycyclic Aromatic Hydrocarbon Anisotropic Potential with Application to the Exfoliation Energy of Graphite. Journal of Physical Chemistry A, 2011, 115, 13684-13693.	2.5	24
34	A transferable electrostatic model for intermolecular interactions between polycyclic aromatic hydrocarbons. Chemical Physics Letters, 2011, 510, 154-160.	2.6	28
35	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
36	Modelling the internal structure of nascent soot particles. Combustion and Flame, 2010, 157, 909-914.	5.2	126

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37	A First Principles Development of a General Anisotropic Potential for Polycyclic Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2010, 6, 683-695.	5.3	62
38	Dispersion interactions between semiconducting wires. Physical Review B, 2010, 82, .	3.2	51
39	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
40	Charge-transfer in Symmetry-Adapted Perturbation Theory. Chemical Physics Letters, 2009, 473, 201-205.	2.6	166
41	A first principles prediction of the crystal structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mspace width="0.35em" height="0.8ex" /><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>6</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mrow> Chemical Physics Letters, 2008, 456, 105-109.	2.6	79
42	Accurate Induction Energies for Small Organic Molecules:â€‰ 1. Theory. Journal of Chemical Theory and Computation, 2008, 4, 7-18.	5.3	68
43	Is the Induction Energy Important for Modeling Organic Crystals?. Journal of Chemical Theory and Computation, 2008, 4, 522-532.	5.3	55
44	Accurate Induction Energies for Small Organic Molecules. 2. Development and Testing of Distributed Polarizability Models against SAPT(DFT) Energies. Journal of Chemical Theory and Computation, 2008, 4, 19-32.	5.3	77
45	Dispersion energies for small organic molecules: first row atoms. Molecular Physics, 2008, 106, 1631-1643.	1.7	54
46	Atomâ€“atom potentials fromab initiocalculations. International Reviews in Physical Chemistry, 2007, 26, 193-222.	2.3	97
47	Distributed polarizabilities obtained using a constrained density-fitting algorithm. Journal of Chemical Physics, 2006, 124, 024111.	3.0	87
48	Intermolecular potentials based on symmetry-adapted perturbation theory with dispersion energies from time-dependent density-functional calculations. Journal of Chemical Physics, 2005, 123, 214103.	3.0	454
49	Symmetry-adapted perturbation-theory calculations of intermolecular forces employing density-functional description of monomers. Journal of Chemical Physics, 2005, 122, 214109.	3.0	159
50	Dispersion Energy from Density-Functional Theory Description of Monomers. Physical Review Letters, 2003, 91, 033201.	7.8	333
51	Intermolecular forces from asymptotically corrected density functional description of monomers. Chemical Physics Letters, 2002, 357, 301-306.	2.6	266
52	Intermolecular potential energy surfaces and spectra of Neâ€“HCN complex from ab initio calculations. Journal of Chemical Physics, 2001, 114, 764.	3.0	47
53	Spectra of Arâ€“CO2 fromab initiopotential energy surfaces. Journal of Chemical Physics, 2000, 112, 5308-5319.	3.0	67