# Alston J Misquitta

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | Dispersion Energy from Density-Functional Theory Description of Monomers. Physical Review Letters, 2003, 91, 033201. | 7.8 | 333 |
| 6 | Intermolecular forces from asymptotically corrected density functional description of monomers. Chemical Physics Letters, 2002, 357, 301-306. | 2.6 | 266 |
| 7 | Charge-transfer in Symmetry-Adapted Perturbation Theory. Chemical Physics Letters, 2009, 473, 201-205. | 2.6 | 166 |
| 8 | Symmetry-adapted perturbation-theory calculations of intermolecular forces employing density-functional description of monomers. Journal of Chemical Physics, 2005, 122, 214109. | 3.0 | 159 |
| 9 | A quantitative study of the clustering of polycyclic aromatic hydrocarbons at high temperatures. Physical Chemistry Chemical Physics, 2012, 14, 4081. | 2.8 | 147 |
| 10 | Modelling the internal structure of nascent soot particles. Combustion and Flame, 2010, 157, 909-914. | 5.2 | 126 |
| 11 | Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283. | 3.3 | 113 |
| 12 | Atomâ€“atom potentials fromab initiocalculations. International Reviews in Physical Chemistry, 2007, 26, 193-222. | 2.3 | 97 |
| 13 | Distributed polarizabilities obtained using a constrained density-fitting algorithm. Journal of Chemical Physics, 2006, 124, 024111. | 3.0 | 87 |
| 14 | 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 | 2.6 | 79 |
| 15 | 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 |
| 16 | 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 |
| 17 | Charge Transfer from Regularized Symmetry-Adapted Perturbation Theory. Journal of Chemical Theory and Computation, 2013, 9, 5313-5326. | 5.3 | 74 |
| 18 | Accurate Induction Energies for Small Organic Molecules:â€‰ 1. Theory. Journal of Chemical Theory and Computation, 2008, 4, 7-18. | 5.3 | 68 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Spectra of Arâ€“CO2 fromab initiopotential energy surfaces. Journal of Chemical Physics, 2000, 112, 5308-5319. | 3.0 | 67 |
| 20 | 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 |
| 21 | 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 |
| 22 | Is the Induction Energy Important for Modeling Organic Crystals?. Journal of Chemical Theory and Computation, 2008, 4, 522-532. | 5.3 | 55 |
| 23 | Dispersion energies for small organic molecules: first row atoms. Molecular Physics, 2008, 106, 1631-1643. | 1.7 | 54 |
| 24 | Dispersion interactions between semiconducting wires. Physical Review B, 2010, 82, . | 3.2 | 51 |
| 25 | Intermolecular potential energy surfaces and spectra of Neâ€“HCN complex from ab initio calculations. Journal of Chemical Physics, 2001, 114, 764. | 3.0 | 47 |
| 26 | 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 |
| 27 | 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 |
| 28 | A transferable electrostatic model for intermolecular interactions between polycyclic aromatic hydrocarbons. Chemical Physics Letters, 2011, 510, 154-160. | 2.6 | 28 |
| 29 | 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 |
| 30 | 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 |
| 31 | Anomalous nonadditive dispersion interactions in systems of three one-dimensional wires. Physical Review B, 2014, 89, . | 3.2 | 23 |
| 32 | 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 |
| 33 | Structures of CdSe and CdS Nanoclusters from Ab Initio Random Structure Searching. Journal of Physical Chemistry C, 2019, 123, 29370-29378. | 3.1 | 22 |
| 34 | High pressure ionic and molecular crystals of ammonia monohydrate within density functional theory. Journal of Chemical Physics, 2012, 137, 064506. | 3.0 | 21 |
| 35 | Ion-Induced Soot Nucleation Using a New Potential for Curved Aromatics. Combustion Science and Technology, 2019, 191, 747-765. | 2.3 | 21 |
| 36 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Molecular dynamics simulation study of various zeolitic imidazolate framework structures. Dalton Transactions, 2016, 45, 4289-4302. | 3.3 | 19 |
| 38 | X-ray total scattering study of magic-size clusters and quantum dots of cadmium sulphide. Nanoscale, 2019, 11, 21900-21908. | 5.6 | 17 |
| 39 | Temporal mapping of photochemical reactions and molecular excited states with carbon specificity. Nature Materials, 2017, 16, 467-473. | 27.5 | 16 |
| 40 | From dimers to the solid-state: Distributed intermolecular force-fields for pyridine. Journal of Chemical Physics, 2017, 147, 161722. | 3.0 | 16 |
| 41 | Charge Distributions of Nitro Groups Within Organic Explosive Crystals: Effects on Sensitivity and Modeling. ACS Omega, 2019, 4, 8614-8625. | 3.5 | 13 |
| 42 | Molecular dynamics study of CO<sub>2</sub> absorption and desorption in zinc imidazolate frameworks. Molecular Systems Design and Engineering, 2017, 2, 457-469. | 3.4 | 8 |
| 43 | Spintronic and Electronic Phenomena in Organic Molecules Measured with Î¼SR. Journal of the Physical Society of Japan, 2016, 85, 091011. | 1.6 | 7 |
| 44 | Multipole Moments in the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2017, 121, 2056-2067. | 2.5 | 7 |
| 45 | 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 |
| 46 | Intermolecular Interactions. , 2012, , 157-193. | | 6 |
| 47 | 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 |
| 48 | 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 |
| 49 | Localized overlap algorithm for unexpanded dispersion energies. Journal of Chemical Physics, 2014, 140, 114304. | 3.0 | 4 |
| 50 | Intermolecular Interactions. , 2017, , 295-335. | | 4 |
| 51 | Intermolecular Interactions. , 2015, , 1-42. | | 1 |
| 52 | High-pressure neutron diffraction study of magnetite, Fe3O4, nanoparticles. Applied Physics Letters, 2022, 120, . | 3.3 | 1 |
| 53 | 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 |