Anthony J Stone

List of Publications by Year
in descending order

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78	5,936	76326	85541
papers	citations	40	71
		h-index	g-index

79	79	79	4683
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Nature and Geometry of Intermolecular Interactions between Halogens and Oxygen or Nitrogen. Journal of the American Chemical Society, 1996, 118, 3108-3116.	13.7	790
2	Distributed Multipole Analysis:â€‰ Stability for Large Basis Sets. Journal of Chemical Theory and Computation, 2005, 1, 1128-1132.	5.3	540
3	Towards an accurate intermolecular potential for water. Molecular Physics, 1992, 77, 439-462.	1.7	267
4	Contribution of Many-Body Terms to the Energy for Small Water Clusters:â€‰ A Comparison of ab Initio Calculations and Accurate Model Potentials. Journal of Physical Chemistry A, 1997, 101, 9163-9168.	2.5	192
5	Are Halogen Bonded Structures Electrostatically Driven?. Journal of the American Chemical Society, 2013, 135, 7005-7009.	13.7	187
6	Revised Anisotropic Site Potentials for the Water Dimer and Calculated Properties. Journal of Physical Chemistry A, 1998, 102, 754-770.	2.5	170
7	Charge-transfer in Symmetry-Adapted Perturbation Theory. Chemical Physics Letters, 2009, 473, 201-205.	2.6	166
8	Computation of charge-transfer energies by perturbation theory. Chemical Physics Letters, 1993, 211, 101-109.	2.6	160
9	Natural Bond Orbitals and the Nature of the Hydrogen Bond. Journal of Physical Chemistry A, 2017, 121, 1531-1534.	2.5	141
10	Exciton coupling in porphyrin dimers. Chemical Physics, 1989, 133, 395-404.	1.9	125
11	Intermolecular Potentials. Science, 2008, 321, 787-789.	12.6	119
12	Applications of the MÃ¶ssbauer effect to silicate mineralogyâ€”II. Iron silicates of unknown and complex crystal structures. Geochimica Et Cosmochimica Acta, 1968, 32, 547-559.	3.9	94
13	Distributed polarizabilities obtained using a constrained density-fitting algorithm. Journal of Chemical Physics, 2006, 124, 024111.	3.0	87
14	Practical schemes for distributed polarizabilities. Molecular Physics, 1993, 78, 1267-1291.	1.7	79
15	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
16	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
17	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
18	The intermolecular potential of chlorine. Molecular Physics, 1988, 63, 173-188.	1.7	72

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19	Distributed dispersion: A new approach. Journal of Chemical Physics, 2003, 119, 4620-4628.	3.0	71
20	MÃ¶ssbauer Spectrum of Fe2+ in a Squareâ€Planar Environment. Journal of Chemical Physics, 1967, 47, 4250-4261.	3.0	68
21	Accurate Induction Energies for Small Organic Molecules:â€‰ 1. Theory. Journal of Chemical Theory and Computation, 2008, 4, 7-18.	5.3	68
22	Transition states from molecular symmetry groups: Analysis of non-rigid acetylene trimer. Molecular Physics, 1991, 72, 33-73.	1.7	66
23	Modeling small hydroniumâ€“water clusters. Journal of Chemical Physics, 1999, 110, 6766-6772.	3.0	64
24	Electrostatic models for polypeptides: can we assume transferability?. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1755.	1.7	61
25	Localization methods for distributed polarizabilities. Molecular Physics, 1994, 83, 293-307.	1.7	61
26	Topography of potential-energy surfaces for Van der Waals complexes. Faraday Discussions, 1994, 97, 243.	3.2	61
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	Theoretical study of rearrangements in boranes. Inorganic Chemistry, 1987, 26, 3845-3850.	4.0	55
29	Is the Induction Energy Important for Modeling Organic Crystals?. Journal of Chemical Theory and Computation, 2008, 4, 522-532.	5.3	55
30	Dispersion energies for small organic molecules: first row atoms. Molecular Physics, 2008, 106, 1631-1643.	1.7	54
31	The induction energy of an assembly of polarizable molecules. Chemical Physics Letters, 1989, 155, 102-110.	2.6	52
32	Dispersion interactions between semiconducting wires. Physical Review B, 2010, 82, .	3.2	51
33	Electrostatic Damping Functions and the Penetration Energy. Journal of Physical Chemistry A, 2011, 115, 7017-7027.	2.5	51
34	Analytical Potentials for HF Dimer and Larger HF Clusters from ab Initio Calculations. Journal of Physical Chemistry A, 1998, 102, 2455-2465.	2.5	50
35	Vibronic Polarization in the Electronic Spectra of Gillespite, a Mineral Containing Iron(II) in Square-Planar Coordination. Inorganic Chemistry, 1966, 5, 1268-1272.	4.0	44
36	Adsorption of water on the NaCl(001) surface. III. Monte Carlo simulations at ambient temperatures. Journal of Chemical Physics, 2000, 112, 6827-6833.	3.0	43

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37	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
38	An ab Initio and Diffusion Monte Carlo Study of the Potential Energy Surface of the CO Dimer. Journal of Physical Chemistry A, 1998, 102, 434-445.	2.5	42
39	Intermolecular interactions in halogens: Bromine and iodine. Chemical Physics Letters, 1988, 145, 365-370.	2.6	41
40	Instability of Ice Films. Langmuir, 2002, 18, 4632-4636.	3.5	41
41	Conformational dependence of the molecular charge distribution and its influence on intermolecular interactions. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 1701.	1.7	40
42	Adsorption of water on NaCl(001). I. Intermolecular potentials and low temperature structures. Journal of Chemical Physics, 1999, 110, 12089-12096.	3.0	36
43	A perturbation theory study of adlayer CO on NaCl(100). Journal of Chemical Physics, 1996, 104, 3058-3070.	3.0	35
44	Adsorption of water on the MgO(001) surface. Surface Science, 1999, 437, 239-248.	1.9	35
45	Atomic anisotropy and the structure of liquid chlorine. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1689.	1.1	33
46	Stationary points on the potential energy surfaces of (SO2)2and (SO2)3. Journal of Chemical Physics, 1992, 96, 8390-8410.	3.0	31
47	Induced dipole moments in acetylene complexes. The Journal of Physical Chemistry, 1991, 95, 3519-3522.	2.9	29
48	Transferability of topologically partitioned polarizabilities: the case of n-alkanes. Molecular Physics, 1996, 89, 595-605.	1.7	29
49	Developments in computational studies of crystallization and morphology applied to urea. Physical Chemistry Chemical Physics, 2000, 2, 3017-3027.	2.8	29
50	Potential energy surfaces of van der Waals complexes of water and hydrogen halides modeled using distributed multipoles. Journal of Chemical Physics, 1995, 102, 5551-5565.	3.0	28
51	Adsorption of water on the BaF2(111) surface. Journal of Chemical Physics, 2002, 117, 800-807.	3.0	27
52	Intermolecular perturbation theory for Van der Waals molecules. Faraday Discussions of the Chemical Society, 1982, 73, 19.	2.2	26
53	An OHD-RIKES and simulation study comparing a benzylmethylimidazolium ionic liquid with an equimolar mixture of dimethylimidazolium and benzene. Physical Chemistry Chemical Physics, 2015, 17, 9973-9983.	2.8	26
54	H ï¿½ï¿½ï¿½ H model potential for exchange-repulsion energy of methane dimer. Journal of Computational Chemistry, 1998, 19, 847-857.	3.3	25

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55	Assessment of multipolar approximations to the induction energy. Chemical Physics Letters, 1989, 155, 111-118.	2.6	24
56	Anomalous nonadditive dispersion interactions in systems of three one-dimensional wires. Physical Review B, 2014, 89, .	3.2	23
57	Temperature variation of proton hyperfine splittings in amino groups. Transactions of the Faraday Society, 1965, 61, 2593.	0.9	22
58	A new representation of the dispersion interaction. Molecular Physics, 2000, 98, 275-286.	1.7	22
59	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
60	Water from First Principles. Science, 2007, 315, 1228-1229.	12.6	21
61	Potential energy surfaces of several van der Waals complexes modelled using distributed multipoles. Chemical Physics Letters, 1995, 240, 89-96.	2.6	20
62	Reply to â€œComment on â€˜Natural Bond Orbitals and the Nature of the Hydrogen Bondâ€™â€• Journal of Physical Chemistry A, 2018, 122, 733-736.	2.5	19
63	Bonding in transition-metal clusters. Inorganic Chemistry, 1989, 28, 3120-3127.	4.0	16
64	Ice Nucleation on a Model Hexagonal Surface. Langmuir, 2004, 20, 8715-8720.	3.5	15
65	Classical Electrostatics in Molecular Interactions. , 1991, , 103-131.		15
66	Using monomer properties to obtain integrated intensities for vibrational transitions of van der Waals complexes. Molecular Physics, 1992, 77, 823-835.	1.7	12
67	Transferable polarizabilities for the alkanes. Molecular Physics, 2004, 102, 985-991.	1.7	12
68	Stereoselectivity and regioselectivity in Dielsâ€“Alder reactions studied by intermolecular perturbation theory. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1663-1668.	1.7	9
69	The dielectric virial coefficient and model intermolecular potentials. Physical Chemistry Chemical Physics, 2000, 2, 429-434.	2.8	8
70	Physical Basis of Intermolecular Interactions. , 2017, , 3-26.		8
71	An amorphous monolayer: Infrared spectroscopic and theoretical studies of SO2 on NaCl (100). Journal of Chemical Physics, 1996, 104, 6843-6855.	3.0	6
72	A model with charges and polarizability for CS2 in an ionic liquid. Journal of Chemical Sciences, 2017, 129, 883-890.	1.5	6

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73	Theoretical studies of the interface between water and Langmuir films of aliphatic alcohols. Journal of Chemical Physics, 2003, 119, 5670-5679.	3.0	5
74	Classical Electrostatics in Molecular Interactions. , 1991, , 103-131.		4
75	A Classical Model for 3-body Interactions in Aqueous Ionic Systems. Journal of Chemical Physics, 0, , .	3.0	3
76	Universal Models of Hydrogen Bonding. , 2000, , 25-34.		1
77	On the search for solutions. Nature, 1988, 335, 465-465.	27.8	0
78	Lattice sums and their derivatives for surface adlayers. Molecular Physics, 2005, 103, 2477-2481.	1.7	0