Brett I Dunlap

List of Publications by Year
in descending order

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90 papers	2,343 citations	201674 27 h-index	223800 46 g-index
93 all docs	93 docs citations	93 times ranked	1776 citing authors

#	Article	IF	Citations
1	Relating carbon tubules. Physical Review B, 1994, 49, 5643-5651.	3.2	238
2	Ion molecule reactions of carbon cluster ions with D2 and O2. Journal of Chemical Physics, 1987, 86, 715-725.	3.0	154
3	Robust and variational fitting. Physical Chemistry Chemical Physics, 2000, 2, 2113-2116.	2.8	141
4	Symmetry and cluster magnetism. Physical Review A, 1990, 41, 5691-5694.	2.5	114
5	Variational fitting methods for electronic structure calculations. Molecular Physics, 2010, 108, 3167-3180.	1.7	89
6	Catalytic activity of bimetallic nickel alloys for solid-oxide fuel cell anode reactions from density-functional theory. Journal of Power Sources, 2011, 196, 4724-4728.	7.8	84
7	Constraints on small graphitic helices. Physical Review B, 1994, 50, 8134-8137.	3.2	67
8	Asymmetric localization of titanium in carbon molecule (C28). The Journal of Physical Chemistry, 1992, 96, 9095-9097.	2.9	59
9	Electronic structure, vibrational stability, infra-red, and Raman spectra of B24N24 cages. Chemical Physics Letters, 2004, 393, 300-304.	2.6	50
10	Efficient quantum-chemical geometry optimization and the structure of large icosahedral fullerenes. Chemical Physics Letters, 2006, 422, 451-454.	2.6	49
11	Sb@Ni₁₂@Sb₂₀^{â€“/+} and Sb@Pd₁₂@Sb₂₀ⁿ Cluster Anions, Where n = +1, â^'1, â^'3, â^'4: Multi-Oxidation-State Clusters of Interpenetrating Platonic Solids. Journal of the American Chemical Society, 2017, 139, 619-622.	13.7	48
12	Geometry optimization using local density functional methods. The Journal of Physical Chemistry, 1986, 90, 5524-5529.	2.9	47
13	Three-center Gaussian-type-orbital integral evaluation using solid spherical harmonics. Physical Review A, 1990, 42, 1127-1137.	2.5	47
14	Are hemispherical caps of boronâ€“nitride nanotubes possible?. Chemical Physics Letters, 2004, 386, 403-407.	2.6	47
15	On the applicability of LCAO-XÎ± methods to molecules containing transition metal atoms: The nickel atom and nickel hydride. International Journal of Quantum Chemistry, 1977, 12, 81-87.	2.0	42
16	Secondary ion mass spectrometry (SIMS) of metal halides. IV. The envelopes of secondary cluster ion distributions. International Journal of Mass Spectrometry and Ion Processes, 1984, 57, 103-123.	1.8	41
17	Paramagnetism of high nuclearity metal cluster compounds as derived from local density functional calculations. Journal of Chemical Physics, 1991, 95, 7004-7007.	3.0	39
18	Molecular dynamics simulation of yttria-stabilized zirconia (YSZ) crystalline and amorphous solids. Journal of Physics Condensed Matter, 2011, 23, 035401.	1.8	39

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19	Symmetry and Degeneracy in XÎ± and Density Functional Theory. Advances in Chemical Physics, 0, , 287-318.	0.3	39
20	Electronic structure of fullerenelike cages and finite nanotubes of aluminum nitride. Physical Review B, 2005, 72, .	3.2	38
21	Lcao-X? calculations of rotational energy barriers?prototypes of chemical reactions. International Journal of Quantum Chemistry, 1986, 29, 767-777.	2.0	37
22	Bonding in Endohedral Metal-Fullerene Complexes: f-Orbital Covalency in Ce@C28. Angewandte Chemie International Edition in English, 1993, 32, 108-110.	4.4	37
23	ArÃ¨ endohedral metal(IV)C28 compounds hypervalent?. Chemical Physics Letters, 1992, 200, 418-423.	2.6	35
24	The Ïƒ* absorption peak at the oxygen 1sedge of O2: Exchange splitting, ultrafast dissociation, and atomiclike Auger spectra. Journal of Chemical Physics, 1994, 100, 4087-4092.	3.0	35
25	Octahedral C48 and Uniform Strain. The Journal of Physical Chemistry, 1994, 98, 11018-11019.	2.9	34
26	Characterization of cluster ions produced by the sputtering or direct laser vaporization of group 13 metal (Al, Ga, and In) oxides. Journal of Chemical Physics, 1991, 94, 2578-2587.	3.0	32
27	Do the new cluster sources also produce isomers?. International Journal of Quantum Chemistry, 1988, 34, 257-264.	2.0	29
28	Atomic contributions to friction and load for tipâ€“self-assembled monolayers interactions. Physical Review B, 2008, 78, .	3.2	28
29	The role of alternative geometries in alkaliâ€“halide clusters. Journal of Chemical Physics, 1986, 84, 5611-5616.	3.0	27
30	Correlated dynamics in aqueous proton diffusion. Chemical Science, 2018, 9, 7126-7132.	7.4	26
31	Regularities and irregularities in SIMS/FAB spectra of alkali halides analyzed via the bondâ€breaking model. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1983, 1, 432-436.	2.1	25
32	Symmetry and spin density functional theory. Chemical Physics, 1988, 125, 89-97.	1.9	24
33	Theoretical infrared, Raman, and optical spectra of theB36N36cage. Physical Review A, 2005, 71, .	2.5	24
34	SO(2, 1) and the HulthÃ©n Potential. Physical Review A, 1972, 6, 1370-1374.	2.5	22
35	Generalized Gaunt coefficients. Physical Review A, 2002, 66, .	2.5	21
36	Direct quantum chemical integral evaluation. International Journal of Quantum Chemistry, 2001, 81, 373-383.	2.0	20

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37	The photodissociation of ClCN: A theoretical determination of the rotational state distribution of the CN fragment. Journal of Chemical Physics, 1986, 84, 1391-1396.	3.0	19
38	Slater's Exchange Parameters Î± for Analytic and Variational XÎ± Calculations. Journal of Chemical Theory and Computation, 2005, 1, 1193-1200.	5.3	19
39	Analytic and Variational XÎ± in the Slaterâ˜Roothaan Method. Journal of Physical Chemistry A, 2003, 107, 10082-10089.	2.5	18
40	The limitations of Slaterâ€™s element-dependent exchange functional from analytic density-functional theory. Journal of Chemical Physics, 2006, 124, 044107.	3.0	18
41	Kinetic Monte Carlo simulation of the elementary electrochemistry in a hydrogen-powered solid oxide fuel cell. Journal of Power Sources, 2010, 195, 4177-4184.	7.8	18
42	Accurate density-functional calculations on large systems. International Journal of Quantum Chemistry, 1997, 64, 193-203.	2.0	17
43	Angular momentum in solid-harmonic-Gaussian integral evaluation. Journal of Chemical Physics, 2003, 118, 1036-1043.	3.0	15
44	Angular momentum in molecular quantum mechanical integral evaluation. Computer Physics Communications, 2005, 165, 18-36.	7.5	15
45	Electronic and magnetic properties of organometallic clusters: From the molecular to the metallic state. International Journal of Quantum Chemistry, 1992, 44, 605-619.	2.0	14
46	Accurate molecular energies by extrapolation of atomic energies using an analytic quantum mechanical model. Physical Review B, 2005, 71, .	3.2	14
47	Electronic structure and molecular dynamics of breaking the ROâ€“NO2 bond. Journal of Chemical Physics, 2009, 130, 244110.	3.0	14
48	Lattice dielectric and thermodynamic properties of yttria stabilized zirconia solids. Journal of Physics Condensed Matter, 2009, 21, 145402.	1.8	14
49	Optical excitation energies, Stokes shift, and spin-splitting of C24H72Si14. Journal of Chemical Physics, 2010, 133, 034301.	3.0	14
50	A single-center expansion for H2+ wavefunctions. Chemical Physics Letters, 1975, 30, 39-42.	2.6	13
51	Ammonium Nitrate Cluster Ions. The Journal of Physical Chemistry, 1996, 100, 5281-5285.	2.9	12
52	Cation coordination and interstitial oxygen occupancy in co-doped zirconia from first principles. Solid State Ionics, 2012, 227, 66-72.	2.7	12
53	Kinetic Monte Carlo simulation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si72.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mtext>O</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup></mml:mrow></mml:math> incorporation in the yttria stabilized zirconia (YSZ) fuel cell. Chemical Physics Letters, 2009, 471, 326-330.	2.6	12
54	Thermodynamic and kinetic stabilities of CO2 oligomers. Journal of Chemical Physics, 2013, 138, 134304.	3.0	11

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55	The magic number nine-atom alkali halide cluster ion. Is the nine-atom planar structure the most stable?. Organic Mass Spectrometry, 1986, 21, 221-224.	1.3	10
56	Accurate density functional calculations on large systems. International Journal of Quantum Chemistry, 1996, 58, 123-132.	2.0	10
57	Quantum chemical molecular dynamics. International Journal of Quantum Chemistry, 1998, 69, 317-325.	2.0	10
58	Effects of dopant clustering in cubic zirconia stabilized by yttria and scandia from molecular dynamics. Solid State Ionics, 2013, 253, 130-136.	2.7	9
59	Proton transport through hydrated chitosanâ€based polymer membranes under electric fields. Journal of Polymer Science, Part B: Polymer Physics, 2017, 55, 1103-1109.	2.1	9
60	Variational, V-representable, and variable-occupation-number perturbation theories. Journal of Chemical Physics, 2008, 129, 244109.	3.0	8
61	On the optimal value of Î± for the Hartreeâ€“Fockâ€“Slater method. Chemical Physics Letters, 2004, 399, 417-421.	2.6	7
62	A Combined Hartree-Fock and Local-Density-Functional Method To Calculate Linear and Nonlinear Optical Properties of Molecules. ACS Symposium Series, 1996, , 164-173.	0.5	6
63	Self-consistent, constrained linear-combination-of-atomic-potentials approach to quantum mechanics. Journal of Chemical Physics, 2011, 134, 044122.	3.0	6
64	Quantum Chemical Molecular Dynamics. Advances in Quantum Chemistry, 1998, 33, 167-187.	0.8	5
65	Chip Scale Module Package for WLAN Module Application. , 2007, , .		5
66	Alternative perspective on density-functional perturbation theory. Physical Review A, 2007, 76, .	2.5	5
67	Smooth scaling of valence electronic properties in fullerenes: From one carbon atom, to C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>, to graphene. Physical Review A, 2013, 87, .	2.5	5
68	Density perturbation theory. Journal of Chemical Physics, 2015, 143, 044115.	3.0	5
69	Symmetry and Local Potential Methods. , 1991, , 49-60.		5
70	Optimization of analytic density functionals by parallel genetic algorithm. Chemical Physics Letters, 2008, 463, 278-282.	2.6	4
71	Kinetic Monte Carlo Simulation of AC Impedance on the Cathode Side of a Solid Oxide Fuel Cell. Journal of the Electrochemical Society, 2010, 157, B90.	2.9	4
72	Electrical characterization of wafer level fan-out (WLFO) using film substrate for low cost millimeter wave application. , 2010, , .		4

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73	Dipole moments from atomic-number-dependent potentials in analytic density-functional theory. Journal of Chemical Physics, 2006, 125, 214104.	3.0	3
74	Three-center molecular integrals and derivatives using solid harmonic Gaussian orbital and Kohnâ€“Sham potential basis sets. Canadian Journal of Chemistry, 2013, 91, 907-915.	1.1	3
75	Variationally fitting the total electron-electron interaction. Physical Review B, 2016, 93, .	3.2	3
76	Symmetry and density-functional exchange and correlation. Theoretical and Computational Chemistry, 1995, , 151-167.	0.4	2
77	Atomistic Modeling of Solid Oxide Fuel Cells. Annual Reports in Computational Chemistry, 2010, , 201-234.	1.7	2
78	Degenerate density perturbation theory. Physical Review B, 2016, 94, .	3.2	2
79	Orbital angular momentum eigenfunctions for fast and numerically stable evaluations of closed-form pseudopotential matrix elements. Journal of Chemical Physics, 2017, 147, 074102.	3.0	2
80	Direct quantum chemical integral evaluation. International Journal of Quantum Chemistry, 2001, 81, 373-383.	2.0	2
81	Fully Analytic Implementation of Density Functional Theory for Efficient Calculations on Large Molecules. , 0, , 157-168.		1
82	General degeneracy in density functional perturbation theory. Physical Review B, 2017, 96, .	3.2	1
83	Jahn-Teller effect in density-functional theory. Physical Review A, 2019, 99, .	2.5	1
84	Accurate densityâ€functional calculations on large systems. International Journal of Quantum Chemistry, 1997, 64, 193-203.	2.0	1
85	Constraints on Small Fullerene Helices. Materials Research Society Symposia Proceedings, 1994, 359, 169.	0.1	0
86	Shattering dissociation in high-energy molecular collisions between nitrate esters. Journal of Chemical Physics, 2011, 135, 114306.	3.0	0
87	Self-Consistent-Field Electrochemistry. ECS Transactions, 2011, 35, 1055-1063.	0.5	0
88	Dopant Clustering and Correlated Oxygen Migration in Conditionally Stabilized Zirconia Electrolytes. Journal of Fuel Cell Science and Technology, 2015, 12, .	0.8	0
89	Designing Fullerene Materials with Heptagonal and Pentagonal Defects. , 1996, , 437-457.		0
90	Density Functional Calculations on Special Clusters. , 1996, , 97-121.		0