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	Jahn-Teller effect in density-functional theory. Physical Review A, 2019, 99, .	2.5	1
2	Correlated dynamics in aqueous proton diffusion. Chemical Science, 2018, 9, 7126-7132.	7.4	26
3	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
4	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
5	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
6	General degeneracy in density functional perturbation theory. Physical Review B, 2017, 96, .	3.2	1
7	Degenerate density perturbation theory. Physical Review B, 2016, 94, .	3.2	2
8	Variationally fitting the total electron-electron interaction. Physical Review B, 2016, 93, .	3.2	3
9	Dopant Clustering and Correlated Oxygen Migration in Conditionally Stabilized Zirconia Electrolytes. Journal of Fuel Cell Science and Technology, 2015, 12, .	0.8	0
10	Density perturbation theory. Journal of Chemical Physics, 2015, 143, 044115.	3.0	5
11	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
12	Thermodynamic and kinetic stabilities of CO2 oligomers. Journal of Chemical Physics, 2013, 138, 134304.	3.0	11
13	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
14	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
15	Cation coordination and interstitial oxygen occupancy in co-doped zirconia from first principles. Solid State Ionics, 2012, 227, 66-72.	2.7	12
16	Molecular dynamics simulation of yttria-stabilized zirconia (YSZ) crystalline and amorphous solids. Journal of Physics Condensed Matter, 2011, 23, 035401.	1.8	39
17	Shattering dissociation in high-energy molecular collisions between nitrate esters. Journal of Chemical Physics, 2011, 135, 114306.	3.0	0
18	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

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19	Self-Consistent-Field Electrochemistry. ECS Transactions, 2011, 35, 1055-1063.	0.5	0
20	Self-consistent, constrained linear-combination-of-atomic-potentials approach to quantum mechanics. Journal of Chemical Physics, 2011, 134, 044122.	3.0	6
21	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
22	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
23	Variational fitting methods for electronic structure calculations. Molecular Physics, 2010, 108, 3167-3180.	1.7	89
24	Optical excitation energies, Stokes shift, and spin-splitting of C24H72Si14. Journal of Chemical Physics, 2010, 133, 034301.	3.0	14
25	Atomistic Modeling of Solid Oxide Fuel Cells. Annual Reports in Computational Chemistry, 2010, , 201-234.	1.7	2
26	Electrical characterization of wafer level fan-out (WLFO) using film substrate for low cost millimeter wave application. , 2010, , .		4
27	Electronic structure and molecular dynamics of breaking the ROâ€“NO2 bond. Journal of Chemical Physics, 2009, 130, 244110.	3.0	14
28	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:m incorporation in the yttria stabilized zirconia (YSZ) fuel cell. Chemical Physics Letters, 2009, 471, 326-330.	2.6	12
29	Lattice dielectric and thermodynamic properties of yttria stabilized zirconia solids. Journal of Physics Condensed Matter, 2009, 21, 145402.	1.8	14
30	Optimization of analytic density functionals by parallel genetic algorithm. Chemical Physics Letters, 2008, 463, 278-282.	2.6	4
31	Atomic contributions to friction and load for tipâ€“self-assembled monolayers interactions. Physical Review B, 2008, 78, .	3.2	28
32	Variational, V-representable, and variable-occupation-number perturbation theories. Journal of Chemical Physics, 2008, 129, 244109.	3.0	8
33	Chip Scale Module Package for WLAN Module Application. , 2007, , .		5
34	Alternative perspective on density-functional perturbation theory. Physical Review A, 2007, 76, .	2.5	5
35	Efficient quantum-chemical geometry optimization and the structure of large icosahedral fullerenes. Chemical Physics Letters, 2006, 422, 451-454.	2.6	49
36	Dipole moments from atomic-number-dependent potentials in analytic density-functional theory. Journal of Chemical Physics, 2006, 125, 214104.	3.0	3

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37	The limitations of Slaterâ€™s element-dependent exchange functional from analytic density-functional theory. Journal of Chemical Physics, 2006, 124, 044107.	3.0	18
38	Angular momentum in molecular quantum mechanical integral evaluation. Computer Physics Communications, 2005, 165, 18-36.	7.5	15
39	Accurate molecular energies by extrapolation of atomic energies using an analytic quantum mechanical model. Physical Review B, 2005, 71, .	3.2	14
40	Theoretical infrared, Raman, and optical spectra of theB36N36cage. Physical Review A, 2005, 71, .	2.5	24
41	Slater's Exchange Parameters Î± for Analytic and Variational XÎ± Calculations. Journal of Chemical Theory and Computation, 2005, 1, 1193-1200.	5.3	19
42	Electronic structure of fullerenelike cages and finite nanotubes of aluminum nitride. Physical Review B, 2005, 72, .	3.2	38
43	Are hemispherical caps of boronâ€“nitride nanotubes possible?. Chemical Physics Letters, 2004, 386, 403-407.	2.6	47
44	Electronic structure, vibrational stability, infra-red, and Raman spectra of B24N24 cages. Chemical Physics Letters, 2004, 393, 300-304.	2.6	50
45	On the optimal value of Î± for the Hartreeâ€“Fockâ€“Slater method. Chemical Physics Letters, 2004, 399, 417-421.	2.6	7
46	Analytic and Variational XÎ± in the Slaterâˆ’Roothaan Method. Journal of Physical Chemistry A, 2003, 107, 10082-10089.	2.5	18
47	Angular momentum in solid-harmonic-Gaussian integral evaluation. Journal of Chemical Physics, 2003, 118, 1036-1043.	3.0	15
48	Generalized Gaunt coefficients. Physical Review A, 2002, 66, .	2.5	21
49	Direct quantum chemical integral evaluation. International Journal of Quantum Chemistry, 2001, 81, 373-383.	2.0	20
50	Direct quantum chemical integral evaluation. International Journal of Quantum Chemistry, 2001, 81, 373-383.	2.0	2
51	Robust and variational fitting. Physical Chemistry Chemical Physics, 2000, 2, 2113-2116.	2.8	141
52	Quantum chemical molecular dynamics. International Journal of Quantum Chemistry, 1998, 69, 317-325.	2.0	10
53	Quantum Chemical Molecular Dynamics. Advances in Quantum Chemistry, 1998, 33, 167-187.	0.8	5
54	Accurate density-functional calculations on large systems. International Journal of Quantum Chemistry, 1997, 64, 193-203.	2.0	17

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55	Accurate densityâ€functional calculations on large systems. International Journal of Quantum Chemistry, 1997, 64, 193-203.	2.0	1
56	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
57	Accurate density functional calculations on large systems. International Journal of Quantum Chemistry, 1996, 58, 123-132.	2.0	10
58	Ammonium Nitrate Cluster Ions. The Journal of Physical Chemistry, 1996, 100, 5281-5285.	2.9	12
59	Designing Fullerene Materials with Heptagonal and Pentagonal Defects. , 1996, , 437-457.		0
60	Density Functional Calculations on Special Clusters. , 1996, , 97-121.		0
61	Symmetry and density-functional exchange and correlation. Theoretical and Computational Chemistry, 1995, , 151-167.	0.4	2
62	Constraints on small graphitic helices. Physical Review B, 1994, 50, 8134-8137.	3.2	67
63	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
64	Octahedral C48 and Uniform Strain. The Journal of Physical Chemistry, 1994, 98, 11018-11019.	2.9	34
65	Relating carbon tubules. Physical Review B, 1994, 49, 5643-5651.	3.2	238
66	Constraints on Small Fullerene Helices. Materials Research Society Symposia Proceedings, 1994, 359, 169.	0.1	0
67	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
68	Asymmetric localization of titanium in carbon molecule (C28). The Journal of Physical Chemistry, 1992, 96, 9095-9097.	2.9	59
69	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
70	ArÃ¨ endohedral metal(IV)C28 compounds hypervalent?. Chemical Physics Letters, 1992, 200, 418-423.	2.6	35
71	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
72	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

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73	Symmetry and Local Potential Methods. , 1991, , 49-60.		5
74	Symmetry and cluster magnetism. Physical Review A, 1990, 41, 5691-5694.	2.5	114
75	Three-center Gaussian-type-orbital integral evaluation using solid spherical harmonics. Physical Review A, 1990, 42, 1127-1137.	2.5	47
76	Do the new cluster sources also produce isomers?. International Journal of Quantum Chemistry, 1988, 34, 257-264.	2.0	29
77	Symmetry and spin density functional theory. Chemical Physics, 1988, 125, 89-97.	1.9	24
78	Ion molecule reactions of carbon cluster ions with D2 and O2. Journal of Chemical Physics, 1987, 86, 715-725.	3.0	154
79	Geometry optimization using local density functional methods. The Journal of Physical Chemistry, 1986, 90, 5524-5529.	2.9	47
80	The role of alternative geometries in alkaliâ€“halide clusters. Journal of Chemical Physics, 1986, 84, 5611-5616.	3.0	27
81	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
82	Lcao-X? calculations of rotational energy barriers?prototypes of chemical reactions. International Journal of Quantum Chemistry, 1986, 29, 767-777.	2.0	37
83	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
84	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
85	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
86	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
87	A single-center expansion for H2+ wavefunctions. Chemical Physics Letters, 1975, 30, 39-42.	2.6	13
88	SO(2, 1) and the HulthÃ©n Potential. Physical Review A, 1972, 6, 1370-1374.	2.5	22
89	Fully Analytic Implementation of Density Functional Theory for Efficient Calculations on Large Molecules. , 0, , 157-168.		1
90	Symmetry and Degeneracy in Xî± and Density Functional Theory. Advances in Chemical Physics, 0, , 287-318.	0.3	39