Brett I Dunlap

List of Publications by Citations

90 papers	2,090 citations	27 h-index	43 g-index
93 ext. papers	2,178 ext. citations	3.3 avg, IF	5.04 L-index

#	Paper	IF	Citations
90	Relating carbon tubules. *Physical Review B*, **1994**, 49, 5643-5651	3.3	205
89	Ion molecule reactions of carbon cluster ions with D2 and O2. *Journal of Chemical Physics*, **1987**, 86, 715-725	3.6	141
88	Robust and variational fitting. *Physical Chemistry Chemical Physics*, **2000**, 2, 2113-2116	3.6	126
87	Symmetry and cluster magnetism. *Physical Review A*, **1990**, 41, 5691-5694	2.6	108
86	Variational fitting methods for electronic structure calculations. *Molecular Physics*, **2010**, 108, 3167-3180	1.7	80
85	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	8.9	70
84	Constraints on small graphitic helices. *Physical Review B*, **1994**, 50, 8134-8137	3.3	60
83	Asymmetric localization of titanium in carbon molecule (C28). *The Journal of Physical Chemistry*, **1992**, 96, 9095-9097		52
82	Electronic structure, vibrational stability, infra-red, and Raman spectra of B24N24 cages. *Chemical Physics Letters*, **2004**, 393, 300-304	2.5	47
81	Geometry optimization using local density functional methods. *The Journal of Physical Chemistry*, **1986**, 90, 5524-5529		46
80	Are hemispherical caps of boron□nitride nanotubes possible?. *Chemical Physics Letters*, **2004**, 386, 403-407	2.5	44
79	Three-center Gaussian-type-orbital integral evaluation using solid spherical harmonics. *Physical Review A*, **1990**, 42, 1127-1137	2.6	44
78	Efficient quantum-chemical geometry optimization and the structure of large icosahedral fullerenes. *Chemical Physics Letters*, **2006**, 422, 451-454	2.5	43
77	Sb@Ni@Sb and Sb@Pd@Sb Cluster Anions, Where n = +1, -1, -3, -4: Multi-Oxidation-State Clusters of Interpenetrating Platonic Solids. *Journal of the American Chemical Society*, **2017**, 139, 619-622	16.4	39
76	Electronic structure of fullerenelike cages and finite nanotubes of aluminum nitride. *Physical Review B*, **2005**, 72,	3.3	37
75	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		37
74	The □ absorption peak at the oxygen 1s edge of O2: Exchange splitting, ultrafast dissociation, and atomiclike Auger spectra. *Journal of Chemical Physics*, **1994**, 100, 4087-4092	3.9	35

73	Ar□endohedral metal(IV)C28 compounds hypervalent?. *Chemical Physics Letters*, **1992**, 200, 418-423	2.5	35
72	Bonding in Endohedral Metal□ullerene Complexes: f-Orbital Covalency in Ce@C28. *Angewandte Chemie International Edition in English*, **1993**, 32, 108-110		35
71	On the applicability of LCAO-X□methods to molecules containing transition metal atoms: The nickel atom and nickel hydride. *International Journal of Quantum Chemistry*, **2009**, 12, 81-87	2.1	34
70	Lcao-X□calculations of rotational energy barriers□rototypes of chemical reactions. *International Journal of Quantum Chemistry*, **1986**, 29, 767-777	2.1	34
69	Octahedral C48 and Uniform Strain. *The Journal of Physical Chemistry*, **1994**, 98, 11018-11019		33
68	Paramagnetism of high nuclearity metal cluster compounds as derived from local density functional calculations. *Journal of Chemical Physics*, **1991**, 95, 7004-7007	3.9	33
67	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	3.9	31
66	Molecular dynamics simulation of yttria-stabilized zirconia (YSZ) crystalline and amorphous solids. *Journal of Physics Condensed Matter*, **2011**, 23, 035401	1.8	29
65	Do the new cluster sources also produce isomers?. *International Journal of Quantum Chemistry*, **1988**, 34, 257-264	2.1	28
64	The role of alternative geometries in alkali□alide clusters. *Journal of Chemical Physics*, **1986**, 84, 5611-5616	3.9	27
63	Symmetry and Degeneracy in X□and Density Functional Theory. *Advances in Chemical Physics*,287-318		27
62	Atomic contributions to friction and load for tip□elf-assembled monolayers interactions. *Physical Review B*, **2008**, 78,	3.3	26
61	Regularities and irregularities in SIMS/FAB spectra of alkali halides analyzed via the bond-breaking model. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1983**, 1, 432-436	2.9	23
60	Theoretical infrared, Raman, and optical spectra of the B36N36 cage. *Physical Review A*, **2005**, 71,	2.6	22
59	SO(2, 1) and the Hulth□ Potential. *Physical Review A*, **1972**, 6, 1370-1374	2.6	22
58	Symmetry and spin density functional theory. *Chemical Physics*, **1988**, 125, 89-97	2.3	21
57	Slater□ Exchange Parameters □For Analytic and Variational X□Calculations. *Journal of Chemical Theory and Computation*, **2005**, 1, 1193-200	6.4	19
56	Correlated dynamics in aqueous proton diffusion. *Chemical Science*, **2018**, 9, 7126-7132	9.4	18

55	Analytic and Variational X□n the Slater□Roothaan Method. *Journal of Physical Chemistry A*, **2003**, 107, 10082-10089	2.8	18
54	Kinetic Monte Carlo simulation of the elementary electrochemistry in a hydrogen-powered solid oxide fuel cell. *Journal of Power Sources*, **2010**, 195, 4177-4184	8.9	17
53	Accurate density-functional calculations on large systems. *International Journal of Quantum Chemistry*, **1997**, 64, 193-203	2.1	16
52	Direct quantum chemical integral evaluation. *International Journal of Quantum Chemistry*, **2001**, 81, 373-383	2.1	16
51	Generalized Gaunt coefficients. *Physical Review A*, **2002**, 66,	2.6	16
50	The photodissociation of ClCN: A theoretical determination of the rotational state distribution of the CN fragment. *Journal of Chemical Physics*, **1986**, 84, 1391-1396	3.9	16
49	The limitations of Slater□ element-dependent exchange functional from analytic density-functional theory. *Journal of Chemical Physics*, **2006**, 124, 044107	3.9	15
48	Optical excitation energies, Stokes shift, and spin-splitting of C24H72Si14. *Journal of Chemical Physics*, **2010**, 133, 034301	3.9	14
47	Electronic structure and molecular dynamics of breaking the RO-NO2 bond. *Journal of Chemical Physics*, **2009**, 130, 244110	3.9	14
46	Accurate molecular energies by extrapolation of atomic energies using an analytic quantum mechanical model. *Physical Review B*, **2005**, 71,	3.3	13
45	Angular momentum in molecular quantum mechanical integral evaluation. *Computer Physics Communications*, **2005**, 165, 18-36	4.2	12
44	Cation coordination and interstitial oxygen occupancy in co-doped zirconia from first principles. *Solid State Ionics*, **2012**, 227, 66-72	3.3	11
43	Kinetic Monte Carlo simulation of O2- incorporation in the yttria stabilized zirconia (YSZ) fuel cell. *Chemical Physics Letters*, **2009**, 471, 326-330	2.5	11
42	Lattice dielectric and thermodynamic properties of yttria stabilized zirconia solids. *Journal of Physics Condensed Matter*, **2009**, 21, 145402	1.8	11
41	Ammonium Nitrate Cluster Ions. *The Journal of Physical Chemistry*, **1996**, 100, 5281-5285		11
40	A single-center expansion for H2+ wavefunctions. *Chemical Physics Letters*, **1975**, 30, 39-42	2.5	11
39	Angular momentum in solid-harmonic-Gaussian integral evaluation. *Journal of Chemical Physics*, **2003**, 118, 1036-1043	3.9	10
38	Electronic and magnetic properties of organometallic clusters: From the molecular to the metallic state. *International Journal of Quantum Chemistry*, **1992**, 44, 605-619	2.1	10

37	Accurate density functional calculations on large systems. *International Journal of Quantum Chemistry*, **1996**, 58, 123-132	2.1	9
36	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		9
35	Proton transport through hydrated chitosan-based polymer membranes under electric fields. *Journal of Polymer Science, Part B: Polymer Physics*, **2017**, 55, 1103-1109	2.6	8
34	Thermodynamic and kinetic stabilities of CO2 oligomers. *Journal of Chemical Physics*, **2013**, 138, 134304	3.9	8
33	Quantum chemical molecular dynamics. *International Journal of Quantum Chemistry*, **1998**, 69, 317-325	2.1	8
32	Variational, V-representable, and variable-occupation-number perturbation theories. *Journal of Chemical Physics*, **2008**, 129, 244109	3.9	8
31	On the optimal value of □ for the Hartree□Fock□Slater method. *Chemical Physics Letters*, **2004**, 399, 417-421	2.5	7
30	Effects of dopant clustering in cubic zirconia stabilized by yttria and scandia from molecular dynamics. *Solid State Ionics*, **2013**, 253, 130-136	3.3	6
29	Self-consistent, constrained linear-combination-of-atomic-potentials approach to quantum mechanics. *Journal of Chemical Physics*, **2011**, 134, 044122	3.9	6
28	A Combined Hartree-Fock and Local-Density-Functional Method To Calculate Linear and Nonlinear Optical Properties of Molecules. *ACS Symposium Series*, **1996**, 164-173	0.4	6
27	Density perturbation theory. *Journal of Chemical Physics*, **2015**, 143, 044115	3.9	5
26	Smooth scaling of valence electronic properties in fullerenes: From one carbon atom, to C60, to graphene. *Physical Review A*, **2013**, 87,	2.6	5
25	Alternative perspective on density-functional perturbation theory. *Physical Review A*, **2007**, 76,	2.6	5
24	Quantum Chemical Molecular Dynamics. *Advances in Quantum Chemistry*, **1998**, 33, 167-187	1.4	5
23	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	3.9	4
22	Optimization of analytic density functionals by parallel genetic algorithm. *Chemical Physics Letters*, **2008**, 463, 278-282	2.5	4
21	Symmetry and Local Potential Methods **1991**, 49-60		4
20	Variationally fitting the total electron-electron interaction. *Physical Review B*, **2016**, 93,	3.3	3

19	Kinetic Monte Carlo Simulation of Electrochemical Systems. *Reviews in Computational Chemistry*, **2015**, 175-204		3
18	Dipole moments from atomic-number-dependent potentials in analytic density-functional theory. *Journal of Chemical Physics*, **2006**, 125, 214104	3.9	3
17	Chip Scale Module Package for WLAN Module Application **2007**,		3
16	Degenerate density perturbation theory. *Physical Review B*, **2016**, 94,	3.3	2
15	Orbital angular momentum eigenfunctions for fast and numerically stable evaluations of closed-form pseudopotential matrix elements. *Journal of Chemical Physics*, **2017**, 147, 074102	3.9	2
14	Three-center molecular integrals and derivatives using solid harmonic Gaussian orbital and Kohn‐Sham potential basis sets. *Canadian Journal of Chemistry*, **2013**, 91, 907-915	0.9	2
13	Atomistic Modeling of Solid Oxide Fuel Cells. *Annual Reports in Computational Chemistry*, **2010**, 201-234	1.8	2
12	Symmetry and density-functional exchange and correlation. *Theoretical and Computational Chemistry*, **1995**, 151-167		2
11	Isomerization and Icosahedral Fullerenes **1992**, 1295-1303		2
10	Direct quantum chemical integral evaluation **2001**, 81, 373		2
9	Jahn-Teller effect in density-functional theory. *Physical Review A*, **2019**, 99,	2.6	1
8	General degeneracy in density functional perturbation theory. *Physical Review B*, **2017**, 96,	3.3	1
7	Electrical characterization of wafer level fan-out (WLFO) using film substrate for low cost millimeter wave application **2010**,		1
6	Accurate density-functional calculations on large systems **1997**, 64, 193		1
5	Shattering dissociation in high-energy molecular collisions between nitrate esters. *Journal of Chemical Physics*, **2011**, 135, 114306	3.9	
4	Fully Analytic Implementation of Density Functional Theory for Efficient Calculations on Large Molecules		157-168
3	Constraints on Small Fullerene Helices. *Materials Research Society Symposia Proceedings*, **1994**, 359, 169		
2	Designing Fullerene Materials with Heptagonal and Pentagonal Defects **1996**, 437-457		

List of Publications

1 Density Functional Calculations on Special Clusters **1996**, 97-121