# Brett I Dunlap

List of Publications by Year
in descending order



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|---|---|---|---|
| 90 papers | 2,343 citations | 230014 27 h-index | 252626 46 g-index |
| 93 all docs | 93 docs citations | 93 times ranked | 2042 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Jahn-Teller effect in density-functional theory. Physical Review A, 2019, 99, . | 1.0 | 1 |
| 2 | Correlated dynamics in aqueous proton diffusion. Chemical Science, 2018, 9, 7126-7132. | 3.7 | 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. | 2.4 | 9 |
| 4 | Sb@Ni<sub>12</sub>@Sb<sub>20</sub><sup>â€“/+</sup> and Sb@Pd<sub>12</sub>@Sb<sub>20</sub><sup>n</sup> 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. | 6.6 | 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. | 1.2 | 2 |
| 6 | General degeneracy in density functional perturbation theory. Physical Review B, 2017, 96, . | 1.1 | 1 |
| 7 | Degenerate density perturbation theory. Physical Review B, 2016, 94, . | 1.1 | 2 |
| 8 | Variationally fitting the total electron-electron interaction. Physical Review B, 2016, 93, . | 1.1 | 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. | 1.2 | 5 |
| 11 | Effects of dopant clustering in cubic zirconia stabilized by yttria and scandia from molecular dynamics. Solid State Ionics, 2013, 253, 130-136. | 1.3 | 9 |
| 12 | Thermodynamic and kinetic stabilities of CO2 oligomers. Journal of Chemical Physics, 2013, 138, 134304. | 1.2 | 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. | 0.6 | 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, . | 1.0 | 5 |
| 15 | Cation coordination and interstitial oxygen occupancy in co-doped zirconia from first principles. Solid State Ionics, 2012, 227, 66-72. | 1.3 | 12 |
| 16 | Molecular dynamics simulation of yttria-stabilized zirconia (YSZ) crystalline and amorphous solids. Journal of Physics Condensed Matter, 2011, 23, 035401. | 0.7 | 39 |
| 17 | Shattering dissociation in high-energy molecular collisions between nitrate esters. Journal of Chemical Physics, 2011, 135, 114306. | 1.2 | 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. | 4.0 | 84 |

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|---|---|---|---|
| 19 | Self-Consistent-Field Electrochemistry. ECS Transactions, 2011, 35, 1055-1063. | 0.3 | 0 |
| 20 | Self-consistent, constrained linear-combination-of-atomic-potentials approach to quantum mechanics. Journal of Chemical Physics, 2011, 134, 044122. | 1.2 | 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. | 4.0 | 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. | 1.3 | 4 |
| 23 | Variational fitting methods for electronic structure calculations. Molecular Physics, 2010, 108, 3167-3180. | 0.8 | 89 |
| 24 | Optical excitation energies, Stokes shift, and spin-splitting of C24H72Si14. Journal of Chemical Physics, 2010, 133, 034301. | 1.2 | 14 |
| 25 | Atomistic Modeling of Solid Oxide Fuel Cells. Annual Reports in Computational Chemistry, 2010, , 201-234. | 0.9 | 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. | 1.2 | 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:mn></mml:m incorporation in the yttria stabilized zirconia (YSZ) fuel cell. Chemical Physics Letters, 2009, 471, 326-330. | 1.2 | 12 |
| 29 | Lattice dielectric and thermodynamic properties of yttria stabilized zirconia solids. Journal of Physics Condensed Matter, 2009, 21, 145402. | 0.7 | 14 |
| 30 | Optimization of analytic density functionals by parallel genetic algorithm. Chemical Physics Letters, 2008, 463, 278-282. | 1.2 | 4 |
| 31 | Atomic contributions to friction and load for tipâ€“self-assembled monolayers interactions. Physical Review B, 2008, 78, . | 1.1 | 28 |
| 32 | Variational, V-representable, and variable-occupation-number perturbation theories. Journal of Chemical Physics, 2008, 129, 244109. | 1.2 | 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, . | 1.0 | 5 |
| 35 | Efficient quantum-chemical geometry optimization and the structure of large icosahedral fullerenes. Chemical Physics Letters, 2006, 422, 451-454. | 1.2 | 49 |
| 36 | Dipole moments from atomic-number-dependent potentials in analytic density-functional theory. Journal of Chemical Physics, 2006, 125, 214104. | 1.2 | 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. | 1.2 | 18 |
| 38 | Angular momentum in molecular quantum mechanical integral evaluation. Computer Physics Communications, 2005, 165, 18-36. | 3.0 | 15 |
| 39 | Accurate molecular energies by extrapolation of atomic energies using an analytic quantum mechanical model. Physical Review B, 2005, 71, . | 1.1 | 14 |
| 40 | Theoretical infrared, Raman, and optical spectra of theB36N36cage. Physical Review A, 2005, 71, . | 1.0 | 24 |
| 41 | Slater's Exchange Parameters Î± for Analytic and Variational XÎ± Calculations. Journal of Chemical Theory and Computation, 2005, 1, 1193-1200. | 2.3 | 19 |
| 42 | Electronic structure of fullerenelike cages and finite nanotubes of aluminum nitride. Physical Review B, 2005, 72, . | 1.1 | 38 |
| 43 | Are hemispherical caps of boronâ€“nitride nanotubes possible?. Chemical Physics Letters, 2004, 386, 403-407. | 1.2 | 47 |
| 44 | Electronic structure, vibrational stability, infra-red, and Raman spectra of B24N24 cages. Chemical Physics Letters, 2004, 393, 300-304. | 1.2 | 50 |
| 45 | On the optimal value of Î± for the Hartreeâ€“Fockâ€“Slater method. Chemical Physics Letters, 2004, 399, 417-421. | 1.2 | 7 |
| 46 | Analytic and Variational XÎ± in the Slaterâˆ’Roothaan Method. Journal of Physical Chemistry A, 2003, 107, 10082-10089. | 1.1 | 18 |
| 47 | Angular momentum in solid-harmonic-Gaussian integral evaluation. Journal of Chemical Physics, 2003, 118, 1036-1043. | 1.2 | 15 |
| 48 | Generalized Gaunt coefficients. Physical Review A, 2002, 66, . | 1.0 | 21 |
| 49 | Direct quantum chemical integral evaluation. International Journal of Quantum Chemistry, 2001, 81, 373-383. | 1.0 | 20 |
| 50 | Direct quantum chemical integral evaluation. International Journal of Quantum Chemistry, 2001, 81, 373-383. | 1.0 | 2 |
| 51 | Robust and variational fitting. Physical Chemistry Chemical Physics, 2000, 2, 2113-2116. | 1.3 | 141 |
| 52 | Quantum chemical molecular dynamics. International Journal of Quantum Chemistry, 1998, 69, 317-325. | 1.0 | 10 |
| 53 | Quantum Chemical Molecular Dynamics. Advances in Quantum Chemistry, 1998, 33, 167-187. | 0.4 | 5 |
| 54 | Accurate density-functional calculations on large systems. International Journal of Quantum Chemistry, 1997, 64, 193-203. | 1.0 | 17 |

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| 55 | Accurate densityâ€functional calculations on large systems. International Journal of Quantum Chemistry, 1997, 64, 193-203. | 1.0 | 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. | 1.0 | 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. | 0.2 | 2 |
| 62 | Constraints on small graphitic helices. Physical Review B, 1994, 50, 8134-8137. | 1.1 | 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. | 1.2 | 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. | 1.1 | 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. | 1.0 | 14 |
| 70 | ArÃ¨ endohedral metal(IV)C28 compounds hypervalent?. Chemical Physics Letters, 1992, 200, 418-423. | 1.2 | 35 |
| 71 | Paramagnetism of high nuclearity metal cluster compounds as derived from local density functional calculations. Journal of Chemical Physics, 1991, 95, 7004-7007. | 1.2 | 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. | 1.2 | 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. | 1.0 | 114 |
| 75 | Three-center Gaussian-type-orbital integral evaluation using solid spherical harmonics. Physical Review A, 1990, 42, 1127-1137. | 1.0 | 47 |
| 76 | Do the new cluster sources also produce isomers?. International Journal of Quantum Chemistry, 1988, 34, 257-264. | 1.0 | 29 |
| 77 | Symmetry and spin density functional theory. Chemical Physics, 1988, 125, 89-97. | 0.9 | 24 |
| 78 | Ion molecule reactions of carbon cluster ions with D2 and O2. Journal of Chemical Physics, 1987, 86, 715-725. | 1.2 | 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. | 1.2 | 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. | 1.0 | 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. | 1.2 | 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. | 1.9 | 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. | 0.9 | 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. | 1.0 | 42 |
| 87 | A single-center expansion for H2+ wavefunctions. Chemical Physics Letters, 1975, 30, 39-42. | 1.2 | 13 |
| 88 | SO(2, 1) and the HulthÃ©n Potential. Physical Review A, 1972, 6, 1370-1374. | 1.0 | 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 |