Gregory J O Beran

List of Publications by Year
in descending order

101 papers	8,960 citations	101543 36 h-index	40979 93 g-index
108 all docs	108 docs citations	108 times ranked	9375 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
3	Modeling Polymorphic Molecular Crystals with Electronic Structure Theory. Chemical Reviews, 2016, 116, 5567-5613.	47.7	294
4	Computational Investigation of Thermochemistry and Kinetics of Steam Methane Reforming on Ni(111) under Realistic Conditions. Journal of Physical Chemistry C, 2009, 113, 4898-4908.	3.1	220
5	Predicting Organic Crystal Lattice Energies with Chemical Accuracy. Journal of Physical Chemistry Letters, 2010, 1, 3480-3487.	4.6	192
6	Accurate Molecular Crystal Lattice Energies from a Fragment QM/MM Approach with On-the-Fly Ab Initio Force Field Parametrization. Journal of Chemical Theory and Computation, 2011, 7, 3733-3742.	5.3	125
7	Boron Carbides as Efficient, Metalâ€Free, Visibleâ€Lightâ€Responsive Photocatalysts. Angewandte Chemie - International Edition, 2013, 52, 3241-3245.	13.8	117
8	Practical quantum mechanics-based fragment methods for predicting molecular crystal properties. Physical Chemistry Chemical Physics, 2012, 14, 7578.	2.8	110
9	Approximating quantum many-body intermolecular interactions in molecular clusters using classical polarizable force fields. Journal of Chemical Physics, 2009, 130, 164115.	3.0	99
10	Benchmark fragment-based¹H,¹³C,¹⁵N and¹⁷O chemical shift predictions in molecular crystals. Physical Chemistry Chemical Physics, 2016, 18, 21686-21709.	2.8	94
11	Benchmark Calculations of Three-Body Intermolecular Interactions and the Performance of Low-Cost Electronic Structure Methods. Journal of Chemical Theory and Computation, 2015, 11, 3065-3079.	5.3	87
12	How important is thermal expansion for predicting molecular crystal structures and thermochemistry at finite temperatures?. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 514-529.	1.1	75
13	Toward a Comprehensive Model of the Synthesis of TiO₂ Particles from TiCl₄. Industrial & Engineering Chemistry Research, 2007, 46, 6147-6156.	3.7	70
14	First-Principles Thermochemistry for the Production of TiO2from TiCl4. Journal of Physical Chemistry A, 2007, 111, 3560-3565.	2.5	66
15	Fragment-based 13C nuclear magnetic resonance chemical shift predictions in molecular crystals: An alternative to planewave methods. Journal of Chemical Physics, 2015, 143, 102809.	3.0	65
16	Predicting finite-temperature properties of crystalline carbon dioxide from first principles with quantitative accuracy. Chemical Science, 2016, 7, 246-255.	7.4	64
17	Accidental Degeneracy in Crystalline Aspirin: New Insights from High-Level ab Initio Calculations. Crystal Growth and Design, 2012, 12, 2169-2172.	3.0	61
18	Prediction of organic molecular crystal geometries from MP2-level fragment quantum mechanical/molecular mechanical calculations. Journal of Chemical Physics, 2012, 137, 174106.	3.0	60

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19	Approaching closed-shell accuracy for radicals using coupled cluster theory with perturbative triple substitutions. Physical Chemistry Chemical Physics, 2003, 5, 2488.	2.8	57
20	Electrochemical Reduction of Quinones: Interfacing Experiment and Theory for Defining Effective Radii of Redox Moieties. Journal of Physical Chemistry B, 2010, 114, 14467-14479.	2.6	57
21	Dipole Effects on Electron Transfer are Enormous. Angewandte Chemie - International Edition, 2018, 57, 12365-12369.	13.8	55
22	Crystal Polymorphism in Oxalyl Dihydrazide: Is Empirical DFT-D Accurate Enough?. Journal of Chemical Theory and Computation, 2012, 8, 2698-2705.	5.3	53
23	Predicting Molecular Crystal Properties from First Principles: Finite-Temperature Thermochemistry to NMR Crystallography. Accounts of Chemical Research, 2016, 49, 2501-2508.	15.6	53
24	Ab initioprediction of the polymorph phase diagram for crystalline methanol. Chemical Science, 2018, 9, 4622-4629.	7.4	53
25	Fragment-Based Electronic Structure Approach for Computing Nuclear Magnetic Resonance Chemical Shifts in Molecular Crystals. Journal of Chemical Theory and Computation, 2014, 10, 4862-4872.	5.3	48
26	Dipole-Mediated Rectification of Intramolecular Photoinduced Charge Separation and Charge Recombination. Journal of the American Chemical Society, 2014, 136, 12966-12973.	13.7	48
27	Inaccurate Conformational Energies Still Hinder Crystal Structure Prediction in Flexible Organic Molecules. Crystal Growth and Design, 2020, 20, 4875-4881.	3.0	48
28	Overcoming the difficulties of predicting conformational polymorph energetics in molecular crystals via correlated wavefunction methods. Chemical Science, 2020, 11, 2200-2214.	7.4	48
29	Converging nuclear magnetic shielding calculations with respect to basis and system size in protein systems. Journal of Biomolecular NMR, 2015, 62, 327-340.	2.8	47
30	Spatially Homogeneous QM/MM for Systems of Interacting Molecules with on-the-Fly ab Initio Force-Field Parametrization. Journal of Chemical Theory and Computation, 2010, 6, 155-167.	5.3	45
31	Unrestricted Perfect Pairing:Â The Simplest Wave-Function-Based Model Chemistry beyond Mean Field. Journal of Physical Chemistry A, 2005, 109, 9183-9192.	2.5	42
32	Accurate Noncovalent Interactions via Dispersion-Corrected Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2018, 14, 4711-4721.	5.3	41
33	How many more polymorphs of ROY remain undiscovered. Chemical Science, 2022, 13, 1288-1297.	7.4	41
34	Nitrogen Activation via Three-Coordinate Molybdenum Complexes: Comparison of Density Functional Theory Performance with Wave Function Based Methods. Journal of Physical Chemistry A, 2005, 109, 6762-6772.	2.5	40
35	What Governs the Proton Ordering in Ice XV?. Journal of Physical Chemistry Letters, 2013, 4, 3165-3169.	4.6	40
36	Visible-light-responsive copper(<scp>ii</scp>) borate photocatalysts with intrinsic midgap states for water splitting. Journal of Materials Chemistry A, 2013, 1, 1553-1556.	10.3	38

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37	Improving the accuracy of solid-state nuclear magnetic resonance chemical shift prediction with a simple molecular correction. Physical Chemistry Chemical Physics, 2019, 21, 14992-15000.	2.8	38
38	Predicting Density Functional Theory-Quality Nuclear Magnetic Resonance Chemical Shifts via Î”-Machine Learning. Journal of Chemical Theory and Computation, 2021, 17, 826-840.	5.3	38
39	Conductance switching in diarylethenes bridging carbon nanotubes. Journal of Chemical Physics, 2011, 134, 024524.	3.0	37
40	Fragment and localized orbital methods in electronic structure theory. Physical Chemistry Chemical Physics, 2012, 14, 7559.	2.8	36
41	Accurate and Robust Molecular Crystal Modeling Using Fragment-Based Electronic Structure Methods. Topics in Current Chemistry, 2013, 345, 59-93.	4.0	36
42	The Structure of the Protonated Adenine Dimer by Infrared Multiple Photon Dissociation Spectroscopy and Electronic Structure Calculations. Journal of Physical Chemistry A, 2009, 113, 8099-8107.	2.5	34
43	Enhanced NMR Discrimination of Pharmaceutically Relevant Molecular Crystal Forms through Fragment-Based Ab Initio Chemical Shift Predictions. Crystal Growth and Design, 2016, 16, 6479-6493.	3.0	34
44	Structural switching in self-assembled metalâ€“ligand helicate complexes via ligand-centered reactions. Chemical Science, 2016, 7, 4423-4427.	7.4	33
45	Second-order correction to perfect pairing: An inexpensive electronic structure method for the treatment of strong electron-electron correlations. Journal of Chemical Physics, 2006, 124, 114107.	3.0	32
46	Improved Electrostatic Embedding for Fragment-Based Chemical Shift Calculations in Molecular Crystals. Journal of Chemical Theory and Computation, 2017, 13, 6043-6051.	5.3	32
47	Structures and energetics of electrosprayed uracilnCa2+clusters (n = 14â€“4) in the gas phase. Physical Chemistry Chemical Physics, 2012, 14, 3304-3315.	2.8	31
48	Accelerating MP2C dispersion corrections for dimers and molecular crystals. Journal of Chemical Physics, 2013, 138, 224112.	3.0	30
49	A New Era for abâ€…initio Molecular Crystal Lattice Energy Prediction. Angewandte Chemie - International Edition, 2015, 54, 396-398.	13.8	29
50	Crystal structure of the meta-stable intermediate in the photomechanical, crystal-to-crystal reaction of 9-tert-butyl anthracene ester. CrystEngComm, 2016, 18, 7319-7329.	2.6	29
51	Ab initiothermodynamic properties and their uncertainties for crystalline Î±-methanol. Physical Chemistry Chemical Physics, 2017, 19, 29940-29953.	2.8	29
52	Identifying pragmatic quasi-harmonic electronic structure approaches for modeling molecular crystal thermal expansion. Faraday Discussions, 2018, 211, 181-207.	3.2	29
53	High fidelity sorting of remarkably similar components via metal-mediated assembly. Chemical Science, 2015, 6, 4801-4806.	7.4	27
54	Reliable prediction of three-body intermolecular interactions using dispersion-corrected second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2015, 143, 044113.	3.0	25

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55	Building blocks for bioinspired electrets: molecular-level approach to materials for energy and electronics. Pure and Applied Chemistry, 2015, 87, 779-792.	1.9	24
56	Theoretical predictions suggest carbon dioxide phases III and VII are identical. Chemical Science, 2017, 8, 7374-7382.	7.4	23
57	Bridging photochemistry and photomechanics with NMR crystallography: the molecular basis for the macroscopic expansion of an anthracene ester nanorod. Chemical Science, 2021, 12, 453-463.	7.4	23
58	Symmetry breaking in benzene and larger aromatic molecules within generalized valence bond coupled cluster methods. Journal of Chemical Physics, 2008, 128, 024107.	3.0	22
59	Conductance of a conjugated molecule with carbon nanotube contacts. Physical Review B, 2009, 80, .	3.2	20
60	Solid state photodimerization of 9-tert-butyl anthracene ester produces an exceptionally metastable polymorph according to first-principles calculations. CrystEngComm, 2019, 21, 758-764.	2.6	20
61	Rubrene untwisted: common density functional theory calculations overestimate its deviant tendencies. Journal of Materials Chemistry C, 2021, 9, 2848-2857.	5.5	20
62	Exploiting space-group symmetry in fragment-based molecular crystal calculations. Journal of Computational Chemistry, 2014, 35, 2205-2214.	3.3	19
63	A Fast Implementation of Perfect Pairing and Imperfect Pairing Using the Resolution of the Identity Approximation. Journal of Chemical Theory and Computation, 2006, 2, 300-305.	5.3	18
64	A Springloaded Metal-Ligand Mesocate Allows Access to Trapped Intermediates of Self-Assembly. Inorganic Chemistry, 2018, 57, 4155-4163.	4.0	18
65	Accurate 13-C and 15-N molecular crystal chemical shielding tensors from fragment-based electronic structure theory. Solid State Nuclear Magnetic Resonance, 2018, 96, 10-18.	2.3	17
66	Towards reliable ab initio sublimation pressures for organic molecular crystals â€“ are we there yet?. Physical Chemistry Chemical Physics, 2019, 21, 14799-14810.	2.8	17
67	Measuring and Modeling Highly Accurate 15 N Chemical Shift Tensors in a Peptide.. ChemPhysChem, 2017, 18, 2225-2232.	2.1	16
68	Vibrations of a chelated proton in a protonated tertiary diamine. Physical Chemistry Chemical Physics, 2011, 13, 20380.	2.8	15
69	Can coupled cluster singles and doubles be approximated by a valence active space model?. Journal of Chemical Physics, 2002, 117, 3040-3048.	3.0	14
70	Achieving High-Accuracy Intermolecular Interactions by Combining Coulomb-Attenuated Second-Order MÃ¸llerâ€“Plesset Perturbation Theory with Coupled Kohnâ€“Sham Dispersion. Journal of Chemical Theory and Computation, 2014, 10, 2054-2063.	5.3	14
71	Small Structural Variations Have Large Effects on the Assembly Properties and Spin State of Room Temperature High Spin Fe(II) Iminopyridine Cages. Inorganic Chemistry, 2018, 57, 13386-13396.	4.0	14
72	Effect of halogen substitution on energies and dynamics of reversible photomechanical crystals based on 9-anthracenecarboxylic acid. CrystEngComm, 2021, 23, 5931-5943.	2.6	14

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73	The interplay of intra- and intermolecular errors in modeling conformational polymorphs. Journal of Chemical Physics, 2022, 156, 104112.	3.0	14
74	Spin-component-scaled and dispersion-corrected second-order MÃ¸llerâ€“Plesset perturbation theory: a path toward chemical accuracy. Physical Chemistry Chemical Physics, 2022, 24, 3695-3712.	2.8	13
75	Theoretical assessment of the structure and stability of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î»</mml:mi></mml:math> phase of nitrogen. Physical Review Materials, 2019, 3, .	2.4	12
76	Dipole Effects on Electron Transfer are Enormous. Angewandte Chemie, 2018, 130, 12545-12549.	2.0	11
77	Improving Predicted Nuclear Magnetic Resonance Chemical Shifts Using the Quasi-Harmonic Approximation. Journal of Chemical Theory and Computation, 2019, 15, 5259-5274.	5.3	11
78	Polarizable continuum models provide an effective electrostatic embedding model for fragmentâ€based chemical shift prediction in challenging systems. Journal of Computational Chemistry, 2020, 41, 2251-2265.	3.3	11
79	Extracting dominant pair correlations from many-body wave functions. Journal of Chemical Physics, 2004, 121, 78.	3.0	10
80	The localizability of valence space electronâ€“electron correlations in pair-based coupled cluster models. Molecular Physics, 2006, 104, 1191-1206.	1.7	10
81	Designed and then realized. Nature Materials, 2017, 16, 602-604.	27.5	10
82	Massively Parallel Implementation of Divide-and-Conquer Jacobi Iterations Using Particle-Mesh Ewald for Force Field Polarization. Journal of Chemical Theory and Computation, 2018, 14, 3633-3642.	5.3	10
83	Fast divide-and-conquer algorithm for evaluating polarization in classical force fields. Journal of Chemical Physics, 2017, 146, 114103.	3.0	8
84	Reduced-cost supercell approach for computing accurate phonon density of states in organic crystals. Journal of Chemical Physics, 2020, 153, 224105.	3.0	8
85	Noncovalent Interactions in Molecular Crystals. , 2017, , 303-331.		7
86	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
87	Modeling the Î± - and Î² -resorcinol phase boundary via combination of density functional theory and density functional tight-binding. Journal of Chemical Physics, 2021, 154, 134109.	3.0	7
88	Combining crystal structure prediction and simulated spectroscopy in pursuit of the unknown nitrogen phase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î¶</mml:mi></mml:math> crystal structure. Physical Review Materials, 2020, 4, .	2.4	7
89	Averaged Condensed Phase Model for Simulating Molecules in Complex Environments. Journal of Chemical Theory and Computation, 2017, 13, 1117-1129.	5.3	6
90	Search for Stratospheric Bromine Reservoir Species:Â Theoretical Study of the Photostability of Mono-, Tri-, and Pentacoordinated Bromine Compounds. Journal of Physical Chemistry A, 2005, 109, 8133-8139.	2.5	5

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91	On the Nature of Unrestricted Orbitals in Variational Active Space Wave Functions. Journal of Physical Chemistry A, 2006, 110, 9915-9920.	2.5	5
92	Communication: Constructing an implicit quantum mechanical/molecular mechanics solvent model by coarse-graining explicit solvent. Journal of Chemical Physics, 2013, 139, 081103.	3.0	5
93	Leveraging Electron Transfer Dissociation for Site Selective Radical Generation: Applications for Peptide Epimer Analysis. Journal of the American Society for Mass Spectrometry, 2017, 28, 1365-1373.	2.8	5
94	Modeling Small Structural and Environmental Differences in Solids with ¹⁵Nâ€...NMR Chemical Shift Tensors. ChemPhysChem, 2021, 22, 1008-1017.	2.1	5
95	Partitioning Techniques in Coupled-Cluster Theory. , 2003, , 433-457.		5
96	Fast electronic structure methods for strongly correlated molecular systems. Journal of Physics: Conference Series, 2005, 16, 233-242.	0.4	3
97	Calculation of Complex Bio- and Organic Systems: From Ground-State Reactivity and Spectroscopy to Excited-State Dynamics. ChemPhysChem, 2014, 15, 3139-3140.	2.1	3
98	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	3.2	3
99	Reduced computational cost of polarizable force fields by a modification of the always stable predictor-corrector. Journal of Chemical Physics, 2019, 150, 151103.	3.0	3
100	Compressive Sensing in Quantum Chemistry: A Little Computation Goes a Long Way. ACS Central Science, 2015, 1, 14-15.	11.3	1
101	Titelbild: Dipole Effects on Electron Transfer are Enormous (Angew. Chem. 38/2018). Angewandte Chemie, 2018, 130, 12357-12357.	2.0	0