Barry D Dunietz

List of Publications by Year
in descending order

100	9,108	145106	45040
papers	citations	33 h-index	94 g-index

105	105	105	10385
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Correlating Interfacial Charge Transfer Rates with Interfacial Molecular Structure in the Tetraphenyldibenzoperiflanthene/C₇₀ Organic Photovoltaic System. Journal of Physical Chemistry Letters, 2022, 13, 763-769.	2.1	4
2	Role of Dielectric Screening in Calculating Excited States of Solvated Azobenzene: A Benchmark Study Comparing Quantum Embedding and Polarizable Continuum Model for Representing the Solvent. Journal of Physical Chemistry Letters, 2022, 13, 4849-4855.	2.1	4
3	Heat flow enhancement in a nanoscale plasmonic junction induced by Kondo resonances and electron-phonon coupling. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 127, 114536.	1.3	1
4	Achieving Predictive Description of Negative Differential Resistance in Molecular Junctions Using a Rangeâ€Separated Hybrid Functional. Advanced Theory and Simulations, 2021, 4, .	1.3	4
5	Cyanide Bridged Platinumâ€Iron Complexes as Cisplatin Prodrug Systems: Design and Computational Study. ChemPhysChem, 2021, 22, 106-111.	1.0	1
6	Simulating energy transfer dynamics in the Fennaâ€“Matthewsâ€“Olson complex via the modified generalized quantum master equation. Journal of Chemical Physics, 2021, 154, 204109.	1.2	19
7	Three-state harmonic models for photoinduced charge transfer. Journal of Chemical Physics, 2021, 154, 174105.	1.2	11
8	CTRAMER: An open-source software package for correlating interfacial charge transfer rate constants with donor/acceptor geometries in organic photovoltaic materials. Journal of Chemical Physics, 2021, 154, 214108.	1.2	4
9	Intersystem Crossing in Tetrapyrrolic Macrocycles. A First-Principles Analysis. Journal of Physical Chemistry C, 2021, 125, 13493-13500.	1.5	12
10	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
11	Electronic Spectra of C₆₀ Films Using Screened Range Separated Hybrid Functionals. Journal of Physical Chemistry A, 2021, 125, 7625-7632.	1.1	5
12	Enhancing fluorescence and lowering the optical gap through C P doping of a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si26.svg"><mml:mi>Ï€</mml:mi></mml:math>-conjugated molecular backbone: A computational-based design approach. Journal of Photochemistry and Photobiology, 2021, 8, 100089.	1.1	5
13	On the Interplay between Electronic Structure and Polarizable Force Fields When Calculating Solution-Phase Charge-Transfer Rates. Journal of Chemical Theory and Computation, 2020, 16, 6481-6490.	2.3	6
14	How Well Does a Solvated Octa-acid Capsule Shield the Embedded Chromophore? A Computational Analysis Based on an Anisotropic Dielectric Continuum Model. Journal of Physical Chemistry B, 2020, 124, 6998-7004.	1.2	4
15	Charge transfer rate constants for the carotenoid-porphyrin-C60 molecular triad dissolved in tetrahydrofuran: The spin-boson model vs the linearized semiclassical approximation. Journal of Chemical Physics, 2020, 153, 044105.	1.2	25
16	Photoinduced charge transfer in Zn(II) and Au(III)-ligated symmetric and asymmetric bacteriochlorin dyads: A computational study. Journal of Chemical Physics, 2020, 153, 134111.	1.2	13
17	Photoinduced Charge Transfer Dynamics in the Carotenoidâ€“Porphyrinâ€“C₆₀ Triad via the Linearized Semiclassical Nonequilibrium Fermiâ€™s Golden Rule. Journal of Physical Chemistry B, 2020, 124, 9579-9591.	1.2	13
18	Molecular-Level Exploration of the Structure-Function Relations Underlying Interfacial Charge Transfer in the Subphthalocyanine/ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math> Organic Photovoltaic System. Physical Review Applied, 2020, 13, .	1.5	14

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19	Discovery and characterization of an acridine radical photoreductant. Nature, 2020, 580, 76-80.	13.7	277
20	Efficient Charge Generation via Hole Transfer in Dilute Organic Donorâ€“Fullerene Blends. Journal of Physical Chemistry Letters, 2020, 11, 2203-2210.	2.1	19
21	On the Role of the Special Pair in Photosystems as a Charge Transfer Rectifier. Journal of Physical Chemistry B, 2020, 124, 1987-1994.	1.2	16
22	Enhancing charge mobilities in self-assembled Nâ‹¯I halogen bonded organic semiconductors: A design approach based on experimental and computational perspectives. Organic Electronics, 2020, 79, 105637.	1.4	3
23	Screened Range-Separated Hybrid Functional with Polarizable Continuum Model Overcomes Challenges in Describing Triplet Excitations in the Condensed Phase Using TDDFT. Journal of Chemical Theory and Computation, 2020, 16, 3287-3293.	2.3	29
24	Combining the mapping Hamiltonian linearized semiclassical approach with the generalized quantum master equation to simulate electronically nonadiabatic molecular dynamics. Journal of Chemical Physics, 2019, 151, 074103.	1.2	30
25	Quantitative Accuracy in Calculating Charge Transfer State Energies in Solvated Molecular Complexes Using a Screened Range Separated Hybrid Functional within a Polarized Continuum Model. Journal of Chemical Theory and Computation, 2019, 15, 4305-4311.	2.3	53
26	Vibronic structure of photosynthetic pigments probed by polarized two-dimensional electronic spectroscopy andab initiocalculations. Chemical Science, 2019, 10, 8143-8153.	3.7	43
27	Explaining Spectral Asymmetries and Excitonic Characters of the Core Pigment Pairs in the Bacterial Reaction Center Using a Screened Range-Separated Hybrid Functional. Journal of Physical Chemistry B, 2019, 123, 8970-8975.	1.2	23
28	A modified approach for simulating electronically nonadiabatic dynamics via the generalized quantum master equation. Journal of Chemical Physics, 2019, 150, 034101.	1.2	38
29	Enhancing charge mobilities in selectively fluorinated oligophenyl organic semiconductors: a design approach based on experimental and computational perspectives. Journal of Materials Chemistry C, 2019, 7, 3881-3888.	2.7	16
30	Computational Study of Charge-Transfer Dynamics in the Carotenoidâ€“Porphyrinâ€“C₆₀ Molecular Triad Solvated in Explicit Tetrahydrofuran and Its Spectroscopic Signature. Journal of Physical Chemistry C, 2018, 122, 11288-11299.	1.5	34
31	Excitonic Interactions in Bacteriochlorin Homo-Dyads Enable Charge Transfer: A New Approach to the Artificial Photosynthetic Special Pair. Journal of Physical Chemistry B, 2018, 122, 4131-4140.	1.2	15
32	A comparative study of different methods for calculating electronic transition rates. Journal of Chemical Physics, 2018, 148, 102304.	1.2	18
33	Fundamental Gaps of Condensed-Phase Organic Semiconductors from Single-Molecule Calculations using Polarization-Consistent Optimally Tuned Screened Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2018, 14, 6287-6294.	2.3	76
34	Controlling the Emissive Activity in Heterocyclic Systems Bearing Câ•P Bonds. Journal of Physical Chemistry Letters, 2018, 9, 3567-3572.	2.1	18
35	Phosphorescence in Bromobenzaldehyde Can Be Enhanced through Intramolecular Heavy Atom Effect. Journal of Physical Chemistry C, 2017, 121, 3771-3777.	1.5	49
36	Modification of Molecular Conductance by in Situ Deprotection of Thiol-Based Porphyrin. ACS Applied Materials & Interfaces, 2017, 9, 15901-15906.	4.0	20

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37	Conductance of Junctions with Acetyl-Functionalized Thiols: A First-Principles-Based Analysis. Journal of Physical Chemistry C, 2017, 121, 10298-10304.	1.5	12
38	Enhancing charge mobilities in organic semiconductors by selective fluorination: a design approach based on a quantum mechanical perspective. Chemical Science, 2017, 8, 6947-6953.	3.7	20
39	What Is the Optoelectronic Effect of the Capsule on the Guest Molecule in Aqueous Host/Guest Complexes? A Combined Computational and Spectroscopic Perspective. Journal of Physical Chemistry C, 2017, 121, 15481-15488.	1.5	17
40	Photoinduced Homolytic Bond Cleavage of the Central Siâ€“C Bond in Porphyrin Macrocycles Is a Charge Polarization Driven Process. Journal of Physical Chemistry A, 2016, 120, 7634-7640.	1.1	6
41	Achieving Predictive Description of Molecular Conductance by Using a Range-Separated Hybrid Functional. Nano Letters, 2016, 16, 6092-6098.	4.5	21
42	Deleterious Effects of Exact Exchange Functionals on Predictions of Molecular Conductance. Journal of Chemical Theory and Computation, 2016, 12, 3431-3435.	2.3	10
43	The Effect of Interfacial Geometry on Charge-Transfer States in the Phthalocyanine/Fullerene Organic Photovoltaic System. Journal of Physical Chemistry A, 2016, 120, 2970-2975.	1.1	20
44	Unraveling the Mechanism of Photoinduced Charge Transfer in Carotenoidâ€“Porphyrinâ€“C₆₀ Molecular Triad. Journal of Physical Chemistry Letters, 2015, 6, 1231-1237.	2.1	48
45	Calculating High Energy Charge Transfer States Using Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2015, 11, 1110-1117.	2.3	51
46	Ultrafast Charge-Transfer Dynamics at the Boron Subphthalocyanine Chloride/C₆₀ Heterojunction: Comparison between Experiment and Theory. Journal of Physical Chemistry Letters, 2015, 6, 569-575.	2.1	41
47	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
48	Communication: Charge-transfer rate constants in zinc-porphyrin-porphyrin-derived dyads: A Fermi golden rule first-principles-based study. Journal of Chemical Physics, 2014, 141, 121102.	1.2	31
49	Molecular Structure, Spectroscopy, and Photoinduced Kinetics in Trinuclear Cyanide Bridged Complex in Solution: A First-Principles Perspective. Journal of the American Chemical Society, 2014, 136, 16954-16957.	6.6	13
50	Donor-to-Donor vs Donor-to-Acceptor Interfacial Charge Transfer States in the Phthalocyanineâ€“Fullerene Organic Photovoltaic System. Journal of Physical Chemistry Letters, 2014, 5, 3810-3816.	2.1	68
51	Calculation from First-Principles of Golden Rule Rate Constants for Photoinduced Subphthalocyanine/Fullerene Interfacial Charge Transfer and Recombination in Organic Photovoltaic Cells. Journal of Physical Chemistry C, 2014, 118, 9780-9789.	1.5	58
52	Orbital gap predictions for rational design of organic photovoltaic materials. Organic Electronics, 2014, 15, 1509-1520.	1.4	110
53	Active control of thermal transport in molecular spin valves. Physical Review B, 2013, 88, .	1.1	5
54	End-Group Influence on Frontier Molecular Orbital Reorganization and Thermoelectric Properties of Molecular Junctions. Journal of Physical Chemistry Letters, 2013, 4, 3825-3833.	2.1	12

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55	Calculation from First Principles of Intramolecular Golden-Rule Rate Constants for Photo-Induced Electron Transfer in Molecular Donorâ€“Acceptor Systems. Journal of Physical Chemistry C, 2013, 117, 23391-23401.	1.5	77
56	Solvated Charge Transfer States of Functionalized Anthracene and Tetracyanoethylene Dimers: A Computational Study Based on a Range Separated Hybrid Functional and Charge Constrained Self-Consistent Field with Switching Gaussian Polarized Continuum Models. Journal of Chemical Theory and Computation, 2013, 9, 1125-1131.	2.3	71
57	On the suppression and significance of ghost transmission in electron transport modeling of single molecule junctions. Journal of Chemical Physics, 2012, 137, 194104.	1.2	12
58	Length dependence of frontier orbital alignment in aromatic molecular junctions. Applied Physics Letters, 2012, 101, .	1.5	44
59	Ab Initio Study of the Emissive Charge-Transfer States of Solvated Chromophore-Functionalized Silsesquioxanes. Journal of the American Chemical Society, 2012, 134, 6944-6947.	6.6	72
60	Ab Initio Calculation of the Electronic Absorption of Functionalized Octahedral Silsesquioxanes via Time-Dependent Density Functional Theory with Range-Separated Hybrid Functionals. Journal of Physical Chemistry A, 2012, 116, 1137-1145.	1.1	52
61	Calculating Off-Site Excitations in Symmetric Donorâ€“Acceptor Systems via Time-Dependent Density Functional Theory with Range-Separated Density Functionals. Journal of Chemical Theory and Computation, 2012, 8, 2661-2668.	2.3	34
62	End-Group-Induced Charge Transfer in Molecular Junctions: Effect on Electronic-Structure and Thermopower. Journal of Physical Chemistry Letters, 2012, 3, 1962-1967.	2.1	57
63	Effect of Length and Contact Chemistry on the Electronic Structure and Thermoelectric Properties of Molecular Junctions. Journal of the American Chemical Society, 2011, 133, 8838-8841.	6.6	156
64	Bias effects on the electronic spectrum of a molecular bridge. Journal of Chemical Physics, 2011, 134, 054708.	1.2	3
65	Photoinduced absolute negative current in a symmetric molecular electronic bridge. Physical Review B, 2010, 82, .	1.1	6
66	On the conditions for enhanced transport through molecular junctions based on metal centres ligated by pairs of pyridazino-derived ligands. Molecular Physics, 2010, 108, 2591-2599.	0.8	2
67	Contact Geometry Symmetry Dependence of Field Effect Gating in Single-Molecule Transistors. Journal of the American Chemical Society, 2010, 132, 2914-2918.	6.6	12
68	Beyond 7-Azaindole: Conjugation Effects on Intermolecular Double Hydrogen-Atom Transfer Reactions. Journal of Physical Chemistry A, 2009, 113, 4862-4867.	1.1	16
69	Multiadsorption and Coadsorption of Hydrogen on Model Conjugated Systems. Journal of Physical Chemistry C, 2009, 113, 12571-12579.	1.5	22
70	On the Electronic Spectra of a Molecular Bridge Under Non-Equilibrium Electric Potential Conditions. Progress in Theoretical Chemistry and Physics, 2009, , 265-277.	0.2	1
71	Accessing Metalâ"Carbide Chemistry. A Computational Analysis of Thermodynamic Considerations. Organometallics, 2008, 27, 814-826.	1.1	21
72	Gating of single molecule transistors: Combining field-effect and chemical control. Journal of Chemical Physics, 2008, 128, 154706.	1.2	26

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73	Conductance of a Cobalt(II) Terpyridine Complex Based Molecular Transistor:â€‰ A Computational Analysis. Journal of Physical Chemistry A, 2008, 112, 2043-2048.	1.1	22
74	Synthetic, Mechanistic, and Computational Investigations of Nitrile-Alkyne Cross-Metathesis. Journal of the American Chemical Society, 2008, 130, 8984-8999.	6.6	74
75	Modeling time-dependent current through electronic open channels using a mixed time-frequency solution to the electronic equations of motion. Physical Review B, 2008, 78, .	1.1	34
76	Ab initio study of charge transport of hydrogen functionalized palladium wires. Journal of Chemical Physics, 2008, 129, 024702.	1.2	5
77	Enhanced Conductance via Induced Î-Stacking Interactions in Cobalt(II) Terpyridine Bridged Complexes. Journal of Physical Chemistry B, 2008, 112, 16070-16075.	1.2	12
78	Carbonyl mediated conductance through metal bound peptides: a computational study. Nanotechnology, 2007, 18, 424003.	1.3	12
79	Theoretical Studies of Conjugation Effects on Excited State Intramolecular Hydrogen-Atom Transfer Reactions in Model Systems. Journal of Physical Chemistry A, 2007, 111, 10139-10143.	1.1	11
80	Electron Transport through Heterogeneous Intermolecular Tunnel Junctions. Journal of Physical Chemistry C, 2007, 111, 1535-1540.	1.5	7
81	Single-molecule field-effect transistors: A computational study of the effects of contact geometry and gating-field orientation on conductance-switching properties. Physical Review B, 2007, 75, .	1.1	18
82	Fragmentation pathways and mechanisms of aromatic compounds in atmospheric pressure studied by GCâ€“DMS and DMSâ€“MS. International Journal of Mass Spectrometry, 2007, 263, 137-147.	0.7	28
83	Metathesis-Enabled Formation of a Terminal Ruthenium Carbide Complex:Â A Computational Study. Organometallics, 2006, 25, 4756-4762.	1.1	15
84	Hydrogen Physisorption on the Organic Linker in Metal Organic Frameworks:Â Ab Initio Computational Study. Journal of Physical Chemistry B, 2006, 110, 10479-10484.	1.2	39
85	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
86	Benchmarking the performance of density functional theory based Greenâ€™s function formalism utilizing different self-energy models in calculating electronic transmission through molecular systems. Journal of Chemical Physics, 2006, 125, 204717.	1.2	27
87	Spin-dependent electronic transport through a porphyrin ring ligating anFe(II)atom: Anab initiostudy. Physical Review B, 2006, 74, .	1.1	41
88	The Spin Dependence of the Spatial Size of Fe(II) and of the Structure of Fe(II)-Porphyrins. Journal of Physical Chemistry A, 2004, 108, 4653-4657.	1.1	36
89	Initiation of Electro-Oxidation of CO on Pt Based Electrodes at Full Coverage Conditions Simulated by Ab Initio Electronic Structure Calculations. Journal of Physical Chemistry B, 2004, 108, 9888-9892.	1.2	16
90	Electro-oxidation of CO on Pt-based electrodes simulated by electronic structure calculations. Journal of Electroanalytical Chemistry, 2003, 554-555, 459-465.	1.9	18

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91	Manifestations of Symmetry Breaking in Self-consistent Field Electronic Structure Calculations. Journal of Physical Chemistry A, 2003, 107, 9160-9167.	1.1	13
92	Initial Steps of the Photodissociation of the CO Ligated Heme Group. Journal of Physical Chemistry B, 2003, 107, 5623-5629.	1.2	68
93	GEOMETRIC DIRECT MINIMIZATION OF HARTREEâ€“FOCK CALCULATIONS INVOLVING OPEN SHELL WAVEFUNCTIONS WITH SPIN RESTRICTED ORBITALS. Journal of Theoretical and Computational Chemistry, 2002, 01, 255-261.	1.8	10
94	Characterization of the Relevant Excited States in the Photodissociation of CO-Ligated Hemoglobin and Myoglobin. Journal of the American Chemical Society, 2002, 124, 12070-12071.	6.6	81
95	Large-Scale ab Initio Quantum Chemical Calculations on Biological Systems. Accounts of Chemical Research, 2001, 34, 351-358.	7.6	101
96	Application and development of multiconfigurational localized perturbation theory. Journal of Chemical Physics, 2001, 115, 11052-11067.	1.2	19
97	Activation of the Câ”H Bond of Methane by Intermediate Q of Methane Monooxygenase:Â A Theoretical Study. Journal of the American Chemical Society, 2001, 123, 3836-3837.	6.6	108
98	Large Scale ab Initio Quantum Chemical Calculation of the Intermediates in the Soluble Methane Monooxygenase Catalytic Cycle. Journal of the American Chemical Society, 2000, 122, 2828-2839.	6.6	176
99	Calculation of atomization energies by a multiconfigurational localized perturbation theoryâ€”Application for closed shell cases. Journal of Chemical Physics, 1999, 110, 1921-1930.	1.2	14
100	Correlated ab Initio Electronic Structure Calculations for Large Molecules. Journal of Physical Chemistry A, 1999, 103, 1913-1928.	1.1	274