Eduardo Fabiano

List of Publications by Year
in descending order

119	3,898	109137	155451
papers	citations	35 h-index	55 g-index

123	123	123	2935
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Implementation of surface hopping molecular dynamics using semiempirical methods. Chemical Physics, 2008, 349, 334-347.	0.9	219
2	Photoinduced Nonadiabatic Dynamics of Pyrimidine Nucleobases: On-the-Fly Surface-Hopping Study with Semiempirical Methods. Journal of Physical Chemistry B, 2009, 113, 3548-3555.	1.2	209
3	â€œDarker-than-Blackâ€•PbS Quantum Dots: Enhancing Optical Absorption of Colloidal Semiconductor Nanocrystals via Short Conjugated Ligands. Journal of the American Chemical Society, 2015, 137, 1875-1886.	6.6	149
4	Semiclassical Neutral Atom as a Reference System in Density Functional Theory. Physical Review Letters, 2011, 106, 186406.	2.9	117
5	Nonradiative Deexcitation Dynamics of 9H-Adenine: An OM2 Surface Hopping Study. Journal of Physical Chemistry A, 2008, 112, 6859-6863.	1.1	111
6	Photoinduced Nonadiabatic Dynamics of 9Hâ€Guanine. ChemPhysChem, 2009, 10, 1225-1229.	1.0	107
7	Generalized Gradient Approximations of the Noninteracting Kinetic Energy from the Semiclassical Atom Theory: Rationalization of the Accuracy of the Frozen Density Embedding Theory for Nonbonded Interactions. Journal of Chemical Theory and Computation, 2011, 7, 2439-2451.	2.3	83
8	QM/MM Nonadiabatic Decay Dynamics of 9Hâ€Adenine in Aqueous Solution. ChemPhysChem, 2011, 12, 1989-1998.	1.0	79
9	Kineticâ€energyâ€dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	1.0	78
10	Theoretical Study of Singlet and Triplet Excitation Energies in Oligothiophenes. Journal of Physical Chemistry A, 2005, 109, 3078-3085.	1.1	73
11	Colorless to All-Black Full-NIR High-Contrast Switching in Solid Electrochromic Films Prepared with Organic Mixed Valence Systems Based on Dibenzofulvene Derivatives. Chemistry of Materials, 2018, 30, 5610-5620.	3.2	68
12	Semilocal Pauliâ€“Gaussian Kinetic Functionals for Orbital-Free Density Functional Theory Calculations of Solids. Journal of Physical Chemistry Letters, 2018, 9, 4385-4390.	2.1	65
13	Live-Cell-Permeant Thiophene Fluorophores and Cell-Mediated Formation of Fluorescent Fibrils. Journal of the American Chemical Society, 2011, 133, 17777-17785.	6.6	62
14	Laplacian-Level Kinetic Energy Approximations Based on the Fourth-Order Gradient Expansion: Global Assessment and Application to the Subsystem Formulation of Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 164-179.	2.3	62
15	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. Journal of Chemical Theory and Computation, 2013, 9, 2256-2263.	2.3	60
16	Nonuniform Scaling Applied to Surface Energies of Transition Metals. Physical Review Letters, 2012, 108, 126402.	2.9	57
17	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. Bioconjugate Chemistry, 2006, 17, 58-67.	1.8	55
18	Approximate switching algorithms for trajectory surface hopping. Chemical Physics, 2008, 351, 111-116.	0.9	54

#	Article	IF	Citations
19	[1]Benzothieno[3,2-b]benzothiophene-Based Organic Dyes for Dye-Sensitized Solar Cells. Journal of Organic Chemistry, 2016, 81, 3235-3245.	1.7	52
20	Semiclassical atom theory applied to solid-state physics. Physical Review B, 2016, 93, .	1.1	51
21	Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces. Physical Review B, 2010, 82, .	1.1	50
22	Design and synthesis of fluorenone-based dyes: two-photon excited fluorescent probes for imaging of lysosomes and mitochondria in living cells. Journal of Materials Chemistry B, 2015, 3, 3315-3323.	2.9	50
23	Frozen density embedding with hybrid functionals. Journal of Chemical Physics, 2010, 133, 164111.	1.2	49
24	Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdewâ€“Burkeâ€“Ernzerhof-Like Enhancement Factor. Journal of Chemical Theory and Computation, 2011, 7, 3548-3559.	2.3	49
25	Kohn-Sham kinetic energy density in the nuclear and asymptotic regions: Deviations from the von WeizsÃcker behavior and applications to density functionals. Physical Review B, 2015, 91, .	1.1	49
26	Semilocal dynamical correlation with increased localization. Physical Review B, 2012, 86, .	1.1	45
27	Laplacian-dependent models of the kinetic energy density: Applications in subsystem density functional theory with meta-generalized gradient approximation functionals. Journal of Chemical Physics, 2017, 146, 064105.	1.2	44
28	Relevance of coordinate and particle-number scaling in density-functional theory. Physical Review A, 2013, 87, .	1.0	42
29	Semilocal density functional theory with correct surface asymptotics. Physical Review B, 2016, 93, .	1.1	41
30	Interfacial Electronic Structure of the Dipolar Vanadyl Naphthalocyanine on Au(111): â€œPush-Backâ€•vs Dipolar Effects. Journal of Physical Chemistry C, 2011, 115, 21128-21138.	1.5	40
31	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. Physical Review B, 2013, 88, .	1.1	40
32	Correlation energy functional from jellium surface analysis. Physical Review B, 2011, 84, .	1.1	39
33	High-Performance Electrofluorochromic Switching Devices Using a Novel Arylamine-Fluorene Redox-Active Fluorophore. ACS Applied Materials & Interfaces, 2019, 11, 12202-12208.	4.0	38
34	Self-Assembled Monolayers of Cobalt(II)â^' (4-tert-Butylphenyl)-Porphyrins:Â The Influence of the Electronic Dipole on Scanning Tunneling Microscopy Images. Journal of the American Chemical Society, 2004, 126, 16951-16958.	6.6	37
35	Performance of Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory. Journal of Chemical Theory and Computation, 2019, 15, 3044-3055.	2.3	37
36	Torsional potential of Ï€-conjugated molecules using the localized Hartreeâ€“Fock Kohnâ€“Sham exchange potential. Chemical Physics Letters, 2006, 418, 496-501.	1.2	35

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37	Orbital-dependent second-order scaled-opposite-spin correlation functionals in the optimized effective potential method. Journal of Chemical Physics, 2014, 141, 024113.	1.2	35
38	Exchange-correlation generalized gradient approximation for gold nanostructures. Journal of Chemical Physics, 2011, 134, 194112.	1.2	34
39	Interaction-Strength Interpolation Method for Main-Group Chemistry: Benchmarking, Limitations, and Perspectives. Journal of Chemical Theory and Computation, 2016, 12, 4885-4896.	2.3	34
40	Testing the broad applicability of the PBEint GGA functional and its oneâ€parameter hybrid form. International Journal of Quantum Chemistry, 2013, 113, 673-682.	1.0	33
41	Modified Fourth-Order Kinetic Energy Gradient Expansion with Hartree Potential-Dependent Coefficients. Journal of Chemical Theory and Computation, 2017, 13, 4228-4239.	2.3	33
42	Localized exchange-correlation potential from second-order self-energy for accurate Kohn-Sham energy gap. Journal of Chemical Physics, 2007, 126, 214102.	1.2	31
43	New organic dyes based on a dibenzofulvene bridge for highly efficient dye-sensitized solar cells. Journal of Materials Chemistry A, 2014, 2, 14181-14188.	5.2	31
44	Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory. Physical Review B, 2015, 91, .	1.1	31
45	Nonlocal kinetic energy functional from the jellium-with-gap model: Applications to orbital-free density functional theory. Physical Review B, 2018, 97, .	1.1	31
46	First disubstituted dibenzothiophene-5,5-dioxide monodispersed molecular materials for efficient blue-electroluminescence. Journal of Materials Chemistry, 2010, 20, 1012-1018.	6.7	29
47	Assessment of interaction-strength interpolation formulas for gold and silver clusters. Journal of Chemical Physics, 2018, 148, 134106.	1.2	28
48	Optical Properties ofN-Succinimidyl Bithiophene and the Effects of the Binding to Biomolecules:Â Comparison between Coupled-Cluster and Time-Dependent Density Functional Theory Calculations and Experiments. Journal of Physical Chemistry B, 2006, 110, 18651-18660.	1.2	26
49	Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis. Physical Review B, 2011, 84, .	1.1	26
50	Optimized effective potential method based on spin-resolved components of the second-order correlation energy in density functional theory. Physical Review B, 2013, 87, .	1.1	26
51	Synthesis and characterization of a new series of dibenzofulvene based organic dyes for DSSCs. Dyes and Pigments, 2016, 130, 79-89.	2.0	26
52	Jellium-with-gap model applied to semilocal kinetic functionals. Physical Review B, 2017, 95, .	1.1	26
53	Restoring Size Consistency of Approximate Functionals Constructed from the Adiabatic Connection. Journal of Physical Chemistry Letters, 2018, 9, 3137-3142.	2.1	26
54	Investigation of the Exchange-Correlation Potentials of Functionals Based on the Adiabatic Connection Interpolation. Journal of Chemical Theory and Computation, 2019, 15, 1006-1015.	2.3	26

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55	Fluorineâ€“thiophene-substituted organic dyes for dye sensitized solar cells. Journal of Materials Chemistry A, 2013, 1, 11909.	5.2	25
56	A density difference based analysis of orbital-dependent exchange-correlation functionals. Molecular Physics, 2014, 112, 700-710.	0.8	25
57	Improving the Propertyâ€“Function Tuning Range of Thiophene Materials via Facile Synthesis of Oligo/Polythiopheneâ€Sâ€Oxides and Mixed Oligo/Polythiopheneâ€Sâ€Oxides/Oligo/Polythiopheneâ€S,Sâ€Dioxides. Advanced Functional Materials, 2016, 26, 6970-6984.	7.8	25
58	Communication: Strong-interaction limit of an adiabatic connection in Hartree-Fock theory. Journal of Chemical Physics, 2018, 149, 241101.	1.2	25
59	Ab initiodepolarization in self-assembled molecular monolayers: Beyond conventional density-functional theory. Physical Review B, 2009, 80, .	1.1	24
60	Accurate Kohnâ€“Sham ionization potentials from scaledâ€oppositeâ€spin secondâ€order optimized effective potential methods. Journal of Computational Chemistry, 2016, 37, 2081-2090.	1.5	24
61	Towards an accurate description of the electronic properties of the biphenylthiol/gold interface: The role of exact exchange. Journal of Chemical Physics, 2009, 131, 234101.	1.2	23
62	Spin-dependent gradient correction for more accurate atomization energies of molecules. Journal of Chemical Physics, 2012, 137, 194105.	1.2	23
63	Generalized Gradient Approximation Correlation Energy Functionals Based on the Uniform Electron Gas with Gap Model. Journal of Chemical Theory and Computation, 2014, 10, 2016-2026.	2.3	23
64	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. Journal of Chemical Theory and Computation, 2014, 10, 3151-3162.	2.3	23
65	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. Journal of Chemical Physics, 2015, 142, 154121.	1.2	23
66	Accuracy of basis-set extrapolation schemes for DFT-RPA correlation energies in molecular calculations. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	22
67	Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. Journal of Chemical Theory and Computation, 2015, 11, 122-131.	2.3	22
68	Nonradiative Relaxation in Thiophene-S,S-dioxide Derivatives:Â The Role of the Environment. Journal of Physical Chemistry B, 2005, 109, 6004-6011.	1.2	21
69	Polymorphism in Crystalline Microfibers of Achiral Octithiophene: The Effect on Charge Transport, Supramolecular Chirality and Optical Properties. Advanced Functional Materials, 2014, 24, 4943-4951.	7.8	21
70	Controlling the Functional Properties of Oligothiophene Crystalline Nano/Microfibers via Tailoring of the Selfâ€Assembling Molecular Precursors. Advanced Functional Materials, 2018, 28, 1801946.	7.8	21
71	Frozen density embedding calculations with the orbital-dependent localized Hartreeâ€“Fock Kohnâ€“Sham potential. Chemical Physics Letters, 2011, 518, 114-118.	1.2	20
72	On the accuracy of frozen density embedding calculations with hybrid and orbital-dependent functionals for non-bonded interaction energies. Journal of Chemical Physics, 2012, 137, 014102.	1.2	20

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73	Kinetic and Exchange Energy Densities near the Nucleus. Computation, 2016, 4, 19.	1.0	20
74	Nanoscale Characterization and Unexpected Photovoltaic Behavior of Low Band Gap Sulfur-Overrich-Thiophene/Benzothiadiazole Decamers and Polymers. Journal of Physical Chemistry C, 2015, 119, 27200-27211.	1.5	19
75	Orthogonal electronic coupling in multicentre arylamine mixed-valence compounds based on a dibenzofulveneâ€“thiophene conjugated bridge. Chemical Communications, 2017, 53, 8960-8963.	2.2	19
76	The ab initio density functional theory applied for spin-polarized calculations. Journal of Chemical Physics, 2020, 152, 054109.	1.2	19
77	Semilocal and hybrid density embedding calculations of ground-state charge-transfer complexes. Journal of Chemical Physics, 2013, 138, 124112.	1.2	18
78	Frozen density embedding with non-integer subsystemsâ€™ particle numbers. Journal of Chemical Physics, 2014, 140, 114101.	1.2	17
79	A series of diphenylamine-fluorenone derivatives as potential fluorescent probes for neuroblastoma cell staining. Tetrahedron, 2016, 72, 2920-2928.	1.0	17
80	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. Computation, 2018, 6, 7.	1.0	17
81	Arylamino-fluorene derivatives: Optically induced electron transfer investigation, redox-controlled modulation of absorption and fluorescence. Dyes and Pigments, 2020, 177, 108325.	2.0	17
82	The role of exactâ€exchange in the theoretical description of organicâ€metal interfaces. International Journal of Quantum Chemistry, 2010, 110, 2162-2171.	1.0	16
83	Hartree potential dependent exchange functional. Journal of Chemical Physics, 2016, 145, 084110.	1.2	15
84	Noncovalent Interactions from Models for the MÃ¸llerâ€“Plesset Adiabatic Connection. Journal of Physical Chemistry Letters, 2021, 12, 4867-4875.	2.1	15
85	Methods to generate reference total and Pauli kinetic potentials. Physical Review B, 2020, 101, .	1.1	14
86	Monodispersed molecular donors for bulk hetero-junction solar cells: from molecular properties to device performances. Chemical Communications, 2010, 46, 6273.	2.2	13
87	Accurate singlet and triplet excitation energies using the Localized Hartreeâ€“Fock Kohnâ€“Sham potential. Chemical Physics, 2011, 391, 19-26.	0.9	13
88	A simple non-empirical procedure for spin-component-scaled MP2 methods applied to the calculation of the dissociation energy curve of noncovalently-interacting systems. Physical Chemistry Chemical Physics, 2013, 15, 15485.	1.3	13
89	Accurate ionization potential of gold anionic clusters from density functional theory and many-body perturbation theory. European Physical Journal B, 2013, 86, 1.	0.6	13
90	The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development. Computation, 2019, 7, 65.	1.0	13

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91	Nonlocal kinetic energy functionals in real space using a Yukawa-potential kernel: Properties, linear response, and model functionals. Physical Review B, 2021, 103, .	1.1	13
92	Electrostatic Mechanophores in Tuneable Lightâ€Emitting Piezopolymer Nanowires. Advanced Materials, 2017, 29, 1701031.	11.1	12
93	Torsional effects on excitation energies of thiophene derivatives induced by Î²â€substituents: Comparison between timeâ€dependent density functional theory and approximated coupled cluster approaches. Journal of Computational Chemistry, 2008, 29, 451-457.	1.5	11
94	Structural and electronic properties of gold microclusters: assessment of the localized Hartreeâ€“Fock method. Physical Chemistry Chemical Physics, 2009, 11, 9160.	1.3	10
95	Assessment of the TCA functional in computational chemistry and solid-state physics. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	10
96	Ab Initio Plasmonics of Externally Doped Silicon Nanocrystals. ACS Photonics, 2019, 6, 1474-1484.	3.2	10
97	MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory. Journal of Chemical Theory and Computation, 2020, 16, 4141-4149.	2.3	10
98	Approximate solution of coupled cluster equations: application to the coupled cluster doubles method and non-covalent interacting systems. Physical Chemistry Chemical Physics, 2017, 19, 30249-30260.	1.3	9
99	Processable Thiopheneâ€Based Polymers with Tailored Electronic Properties and their Application in Solidâ€State Electrochromic Devices Using Nanoparticle Films. Advanced Electronic Materials, 2021, 7, 2100166.	2.6	9
100	Plasmon Couplings from Subsystem Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2021, 125, 7246-7259.	1.1	9
101	Effects of donor position on dibenzofulvene-based organic dyes for photovoltaics. Journal of Materials Science: Materials in Electronics, 2017, 28, 8694-8707.	1.1	8
102	Control of Electron Transfer Processes in Multidimensional Arylamine-Based Mixed-Valence Compounds by Molecular Backbone Design. Journal of Physical Chemistry A, 2021, 125, 7840-7851.	1.1	7
103	Kinetic Energy Density Functionals Based on a Generalized Screened Coulomb Potential: Linear Response and Future Perspectives. Computation, 2022, 10, 30.	1.0	7
104	Ab-initio study of singlet and triplet excitation energies in oligothiophenes. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 539-542.	0.8	6
105	Accurate non-covalent interaction energies via an efficient MP2 scaling procedure. Chemical Physics Letters, 2015, 635, 262-267.	1.2	6
106	Synthesis and photovoltaic performance of dibenzofulvene-based organic sensitizers for DSSC. Tetrahedron, 2016, 72, 5788-5797.	1.0	5
107	Exploiting Photo- and Electroluminescence Properties of FIrpic Organic Crystals. Inorganic Chemistry, 2016, 55, 6532-6538.	1.9	5
108	Dispersion corrections applied to the TCA family of exchange-correlation functionals. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	4

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109	Correlating the chemical structure and charge transport ability of dibenzofulvene-based hole transporting materials for stable perovskite solar cells. Journal of Materials Chemistry C, 2022, 10, 5981-5993.	2.7	4
110	Synthesis and Investigation of Electro-Optical Properties of H-Shape Dibenzofulvene Derivatives. Molecules, 2022, 27, 1091.	1.7	3
111	A periodic charge-dipole electrostatic model: Parametrization for silver slabs. Journal of Chemical Physics, 2012, 137, 134702.	1.2	2
112	Tailoring of the self-assembled structures and optical waveguide behaviour of arylaminofluorenone derivatives. Dyes and Pigments, 2019, 171, 107780.	2.0	2
113	Boosting the OEP2-sc method with spin-component scaling. Molecular Physics, 2022, 120, .	0.8	2
114	Spontaneous Coassembly of the Protein Terthiophene into Fluorescent Electroactive Microfibers in 2D and 3D Cell Cultures. ACS Omega, 2022, 7, 12624-12636.	1.6	2
115	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	1
116	Theoretical study on N-succinimidyl oligothiophenes: A novel class of materials for biological applications. Journal of Non-Crystalline Solids, 2006, 352, 2452-2456.	1.5	0
117	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. Bioconjugate Chemistry, 2007, 18, 1015-1015.	1.8	0
118	Nonlocal exchange and correlation energy functionals using the Yukawa potential as ingredient: Application to the linear response of the uniform electron gas. Physical Review B, 2021, 104, .	1.1	0
119	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. Highlights in Theoretical Chemistry, 2013, , 121-128.	0.0	0