

Eduardo Fabiano

List of Publications by Year in descending order

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119
papers

3,898
citations

109321

35
h-index

155660

55
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123
all docs

123
docs citations

123
times ranked

2935
citing authors

#	ARTICLE	IF	CITATIONS
1	Implementation of surface hopping molecular dynamics using semiempirical methods. <i>Chemical Physics</i> , 2008, 349, 334-347.	1.9	219
2	Photoinduced Nonadiabatic Dynamics of Pyrimidine Nucleobases: On-the-Fly Surface-Hopping Study with Semiempirical Methods. <i>Journal of Physical Chemistry B</i> , 2009, 113, 3548-3555.	2.6	209
3	“Darker-than-Black” PbS Quantum Dots: Enhancing Optical Absorption of Colloidal Semiconductor Nanocrystals via Short Conjugated Ligands. <i>Journal of the American Chemical Society</i> , 2015, 137, 1875-1886.	13.7	149
4	Semiclassical Neutral Atom as a Reference System in Density Functional Theory. <i>Physical Review Letters</i> , 2011, 106, 186406.	7.8	117
5	Nonradiative Deexcitation Dynamics of 9H-Adenine: An OM2 Surface Hopping Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6859-6863.	2.5	111
6	Photoinduced Nonadiabatic Dynamics of 9 <i>H</i> -Guanine. <i>ChemPhysChem</i> , 2009, 10, 1225-1229.	2.1	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. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2439-2451.	5.3	83
8	QM/MM Nonadiabatic Decay Dynamics of 9 <i>H</i> -Adenine in Aqueous Solution. <i>ChemPhysChem</i> , 2011, 12, 1989-1998.	2.1	79
9	Kinetic energy density dependent semilocal exchange correlation functionals. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1641-1694.	2.0	78
10	Theoretical Study of Singlet and Triplet Excitation Energies in Oligothiophenes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3078-3085.	2.5	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. <i>Chemistry of Materials</i> , 2018, 30, 5610-5620.	6.7	68
12	Semilocal Pauli Gaussian Kinetic Functionals for Orbital-Free Density Functional Theory Calculations of Solids. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4385-4390.	4.6	65
13	Live-Cell-Permeant Thiophene Fluorophores and Cell-Mediated Formation of Fluorescent Fibrils. <i>Journal of the American Chemical Society</i> , 2011, 133, 17777-17785.	13.7	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. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 164-179.	5.3	62
15	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2256-2263.	5.3	60
16	Nonuniform Scaling Applied to Surface Energies of Transition Metals. <i>Physical Review Letters</i> , 2012, 108, 126402.	7.8	57
17	Bright Oligothiophene <i>N</i> -Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. <i>Bioconjugate Chemistry</i> , 2006, 17, 58-67.	3.6	55
18	Approximate switching algorithms for trajectory surface hopping. <i>Chemical Physics</i> , 2008, 351, 111-116.	1.9	54

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19	[1]Benzothieno[3,2- <i>b</i>]benzothiophene-Based Organic Dyes for Dye-Sensitized Solar Cells. Journal of Organic Chemistry, 2016, 81, 3235-3245.	3.2	52
20	Semiclassical atom theory applied to solid-state physics. Physical Review B, 2016, 93, .	3.2	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, .	3.2	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.	5.8	50
23	Frozen density embedding with hybrid functionals. Journal of Chemical Physics, 2010, 133, 164111.	3.0	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.	5.3	49
25	Kohn-Sham kinetic energy density in the nuclear and asymptotic regions: Deviations from the von WeizsÄcker behavior and applications to density functionals. Physical Review B, 2015, 91, .	3.2	49
26	Semilocal dynamical correlation with increased localization. Physical Review B, 2012, 86, .	3.2	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.	3.0	44
28	Relevance of coordinate and particle-number scaling in density-functional theory. Physical Review A, 2013, 87, .	2.5	42
29	Semilocal density functional theory with correct surface asymptotics. Physical Review B, 2016, 93, .	3.2	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.	3.1	40
31	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. Physical Review B, 2013, 88, .	3.2	40
32	Correlation energy functional from jellium surface analysis. Physical Review B, 2011, 84, .	3.2	39
33	High-Performance Electrofluorochromic Switching Devices Using a Novel Arylamine-Fluorene Redox-Active Fluorophore. ACS Applied Materials & Interfaces, 2019, 11, 12202-12208.	8.0	38
34	Self-Assembled Monolayers of Cobalt(II)âˆ“(4-tert-Butylphenyl)-Porphyrins:âˆ“The Influence of the Electronic Dipole on Scanning Tunneling Microscopy Images. Journal of the American Chemical Society, 2004, 126, 16951-16958.	18.7	37
35	Performance of Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory. Journal of Chemical Theory and Computation, 2019, 15, 3044-3055.	5.3	37
36	Torsional potential of ï€-conjugated molecules using the localized Hartreeâ€“Fock Kohnâ€“Sham exchange potential. Chemical Physics Letters, 2006, 418, 496-501.	2.6	35

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37	Orbital-dependent second-order scaled-opposite-spin correlation functionals in the optimized effective potential method. <i>Journal of Chemical Physics</i> , 2014, 141, 024113.	3.0	35
38	Exchange-correlation generalized gradient approximation for gold nanostructures. <i>Journal of Chemical Physics</i> , 2011, 134, 194112.	3.0	34
39	Interaction-Strength Interpolation Method for Main-Group Chemistry: Benchmarking, Limitations, and Perspectives. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4885-4896.	5.3	34
40	Testing the broad applicability of the PBEint GGA functional and its one- ϵ -parameter hybrid form. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 673-682.	2.0	33
41	Modified Fourth-Order Kinetic Energy Gradient Expansion with Hartree Potential-Dependent Coefficients. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4228-4239.	5.3	33
42	Localized exchange-correlation potential from second-order self-energy for accurate Kohn-Sham energy gap. <i>Journal of Chemical Physics</i> , 2007, 126, 214102.	3.0	31
43	New organic dyes based on a dibenzofulvene bridge for highly efficient dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2014, 2, 14181-14188.	10.3	31
44	Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory. <i>Physical Review B</i> , 2015, 91, .	3.2	31
45	Nonlocal kinetic energy functional from the jellium-with-gap model: Applications to orbital-free density functional theory. <i>Physical Review B</i> , 2018, 97, .	3.2	31
46	First disubstituted dibenzothiophene-5,5-dioxide monodispersed molecular materials for efficient blue-electroluminescence. <i>Journal of Materials Chemistry</i> , 2010, 20, 1012-1018.	6.7	29
47	Assessment of interaction-strength interpolation formulas for gold and silver clusters. <i>Journal of Chemical Physics</i> , 2018, 148, 134106.	3.0	28
48	Optical Properties of N-Succinimidyl Bithiophene and the Effects of the Binding to Biomolecules: A Comparison between Coupled-Cluster and Time-Dependent Density Functional Theory Calculations and Experiments. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18651-18660.	2.6	26
49	Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis. <i>Physical Review B</i> , 2011, 84, .	3.2	26
50	Optimized effective potential method based on spin-resolved components of the second-order correlation energy in density functional theory. <i>Physical Review B</i> , 2013, 87, .	3.2	26
51	Synthesis and characterization of a new series of dibenzofulvene based organic dyes for DSSCs. <i>Dyes and Pigments</i> , 2016, 130, 79-89.	3.7	26
52	Jellium-with-gap model applied to semilocal kinetic functionals. <i>Physical Review B</i> , 2017, 95, .	3.2	26
53	Restoring Size Consistency of Approximate Functionals Constructed from the Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3137-3142.	4.6	26
54	Investigation of the Exchange-Correlation Potentials of Functionals Based on the Adiabatic Connection Interpolation. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1006-1015.	5.3	26

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55	Fluorine- <i>thiophene</i> -substituted organic dyes for dye sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2013, 1, 11909.	10.3	25
56	A density difference based analysis of orbital-dependent exchange-correlation functionals. <i>Molecular Physics</i> , 2014, 112, 700-710.	1.7	25
57	Improving the Property-Function Tuning Range of Thiophene Materials via Facile Synthesis of Oligo/Polythiophene-S ₂ Oxides and Mixed Oligo/Polythiophene-S ₂ Oxides/Oligo/Polythiophene-S ₂ Oxides. <i>Advanced Functional Materials</i> , 2016, 26, 6970-6984.	1.9	25
58	Communication: Strong-interaction limit of an adiabatic connection in Hartree-Fock theory. <i>Journal of Chemical Physics</i> , 2018, 149, 241101.	3.0	25
59	<i>Ab initio</i> depolarization in self-assembled molecular monolayers: Beyond conventional density-functional theory. <i>Physical Review B</i> , 2009, 80, .	3.2	24
60	Accurate Kohn-Sham ionization potentials from scaled-opposite-spin second-order optimized effective potential methods. <i>Journal of Computational Chemistry</i> , 2016, 37, 2081-2090.	3.3	24
61	Towards an accurate description of the electronic properties of the biphenylthiol/gold interface: The role of exact exchange. <i>Journal of Chemical Physics</i> , 2009, 131, 234101.	3.0	23
62	Spin-dependent gradient correction for more accurate atomization energies of molecules. <i>Journal of Chemical Physics</i> , 2012, 137, 194105.	3.0	23
63	Generalized Gradient Approximation Correlation Energy Functionals Based on the Uniform Electron Gas with Gap Model. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2016-2026.	5.3	23
64	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3151-3162.	5.3	23
65	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. <i>Journal of Chemical Physics</i> , 2015, 142, 154121.	3.0	23
66	Accuracy of basis-set extrapolation schemes for DFT-RPA correlation energies in molecular calculations. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	22
67	Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 122-131.	5.3	22
68	Nonradiative Relaxation in Thiophene-S,S-dioxide Derivatives: The Role of the Environment. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6004-6011.	2.6	21
69	Polymorphism in Crystalline Microfibers of Achiral Octithiophene: The Effect on Charge Transport, Supramolecular Chirality and Optical Properties. <i>Advanced Functional Materials</i> , 2014, 24, 4943-4951.	14.9	21
70	Controlling the Functional Properties of Oligothiophene Crystalline Nano/Microfibers via Tailoring of the Self-Assembling Molecular Precursors. <i>Advanced Functional Materials</i> , 2018, 28, 1801946.	14.9	21
71	Frozen density embedding calculations with the orbital-dependent localized Hartree-Fock Kohn-Sham potential. <i>Chemical Physics Letters</i> , 2011, 518, 114-118.	2.6	20
72	On the accuracy of frozen density embedding calculations with hybrid and orbital-dependent functionals for non-bonded interaction energies. <i>Journal of Chemical Physics</i> , 2012, 137, 014102.	3.0	20

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73	Kinetic and Exchange Energy Densities near the Nucleus. <i>Computation</i> , 2016, 4, 19.	2.0	20
74	Nanoscale Characterization and Unexpected Photovoltaic Behavior of Low Band Gap Sulfur-Overrich-Thiophene/Benzothiadiazole Decamers and Polymers. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27200-27211.	3.1	19
75	Orthogonal electronic coupling in multicentre arylamine mixed-valence compounds based on a dibenzofulvene-thiophene conjugated bridge. <i>Chemical Communications</i> , 2017, 53, 8960-8963.	4.1	19
76	The <i>ab initio</i> density functional theory applied for spin-polarized calculations. <i>Journal of Chemical Physics</i> , 2020, 152, 054109.	3.0	19
77	Semilocal and hybrid density embedding calculations of ground-state charge-transfer complexes. <i>Journal of Chemical Physics</i> , 2013, 138, 124112.	3.0	18
78	Frozen density embedding with non-integer subsystems' particle numbers. <i>Journal of Chemical Physics</i> , 2014, 140, 114101.	3.0	17
79	A series of diphenylamine-fluorenone derivatives as potential fluorescent probes for neuroblastoma cell staining. <i>Tetrahedron</i> , 2016, 72, 2920-2928.	1.9	17
80	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. <i>Computation</i> , 2018, 6, 7.	2.0	17
81	Arylamino-fluorene derivatives: Optically induced electron transfer investigation, redox-controlled modulation of absorption and fluorescence. <i>Dyes and Pigments</i> , 2020, 177, 108325.	3.7	17
82	The role of exact exchange in the theoretical description of organic-metal interfaces. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2162-2171.	2.0	16
83	Hartree potential dependent exchange functional. <i>Journal of Chemical Physics</i> , 2016, 145, 084110.	3.0	15
84	Noncovalent Interactions from Models for the Møller-Plesset Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4867-4875.	4.6	15
85	Methods to generate reference total and Pauli kinetic potentials. <i>Physical Review B</i> , 2020, 101, .	3.2	14
86	Monodispersed molecular donors for bulk hetero-junction solar cells: from molecular properties to device performances. <i>Chemical Communications</i> , 2010, 46, 6273.	4.1	13
87	Accurate singlet and triplet excitation energies using the Localized Hartree-Fock Kohn-Sham potential. <i>Chemical Physics</i> , 2011, 391, 19-26.	1.9	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. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15485.	2.8	13
89	Accurate ionization potential of gold anionic clusters from density functional theory and many-body perturbation theory. <i>European Physical Journal B</i> , 2013, 86, 1.	1.5	13
90	The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development. <i>Computation</i> , 2019, 7, 65.	2.0	13

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91	Nonlocal kinetic energy functionals in real space using a Yukawa-potential kernel: Properties, linear response, and model functionals. <i>Physical Review B</i> , 2021, 103, .	3.2	13
92	Electrostatic Mechanophores in Tuneable Light-Emitting Piezopolymer Nanowires. <i>Advanced Materials</i> , 2017, 29, 1701031.	21.0	12
93	Torsional effects on excitation energies of thiophene derivatives induced by I^2A -substituents: Comparison between time-dependent density functional theory and approximated coupled cluster approaches. <i>Journal of Computational Chemistry</i> , 2008, 29, 451-457.	3.3	11
94	Structural and electronic properties of gold microclusters: assessment of the localized Hartree-Fock method. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9160.	2.8	10
95	Assessment of the TCA functional in computational chemistry and solid-state physics. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	10
96	Ab Initio Plasmonics of Externally Doped Silicon Nanocrystals. <i>ACS Photonics</i> , 2019, 6, 1474-1484.	6.6	10
97	MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4141-4149.	5.3	10
98	Approximate solution of coupled cluster equations: application to the coupled cluster doubles method and non-covalent interacting systems. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30249-30260.	2.8	9
99	Processable Thiophene-Based Polymers with Tailored Electronic Properties and their Application in Solid-State Electrochromic Devices Using Nanoparticle Films. <i>Advanced Electronic Materials</i> , 2021, 7, 2100166.	5.1	9
100	Plasmon Couplings from Subsystem Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7246-7259.	2.5	9
101	Effects of donor position on dibenzofulvene-based organic dyes for photovoltaics. <i>Journal of Materials Science: Materials in Electronics</i> , 2017, 28, 8694-8707.	2.2	8
102	Control of Electron Transfer Processes in Multidimensional Arylamine-Based Mixed-Valence Compounds by Molecular Backbone Design. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7840-7851.	2.5	7
103	Kinetic Energy Density Functionals Based on a Generalized Screened Coulomb Potential: Linear Response and Future Perspectives. <i>Computation</i> , 2022, 10, 30.	2.0	7
104	Ab-initio study of singlet and triplet excitation energies in oligothiophenes. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2004, 1, 539-542.	0.8	6
105	Accurate non-covalent interaction energies via an efficient MP2 scaling procedure. <i>Chemical Physics Letters</i> , 2015, 635, 262-267.	2.6	6
106	Synthesis and photovoltaic performance of dibenzofulvene-based organic sensitizers for DSSC. <i>Tetrahedron</i> , 2016, 72, 5788-5797.	1.9	5
107	Exploiting Photo- and Electroluminescence Properties of FIrpic Organic Crystals. <i>Inorganic Chemistry</i> , 2016, 55, 6532-6538.	4.0	5
108	Dispersion corrections applied to the TCA family of exchange-correlation functionals. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	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. <i>Journal of Materials Chemistry C</i> , 2022, 10, 5981-5993.	5.5	4
110	Synthesis and Investigation of Electro-Optical Properties of H-Shape Dibenzofulvene Derivatives. <i>Molecules</i> , 2022, 27, 1091.	3.8	3
111	A periodic charge-dipole electrostatic model: Parametrization for silver slabs. <i>Journal of Chemical Physics</i> , 2012, 137, 134702.	3.0	2
112	Tailoring of the self-assembled structures and optical waveguide behaviour of arylaminofluorenone derivatives. <i>Dyes and Pigments</i> , 2019, 171, 107780.	3.7	2
113	Boosting the OEP2-sc method with spin-component scaling. <i>Molecular Physics</i> , 2022, 120, .	1.7	2
114	Spontaneous Coassembly of the Protein Terthiophene into Fluorescent Electroactive Microfibers in 2D and 3D Cell Cultures. <i>ACS Omega</i> , 2022, 7, 12624-12636.	3.5	2
115	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	1
116	Theoretical study on N-succinimidyl oligothiophenes: A novel class of materials for biological applications. <i>Journal of Non-Crystalline Solids</i> , 2006, 352, 2452-2456.	3.1	0
117	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. <i>Bioconjugate Chemistry</i> , 2007, 18, 1015-1015.	3.6	0
118	Nonlocal exchange and correlation energy functionals using the Yukawa potential as ingredient: Application to the linear response of the uniform electron gas. <i>Physical Review B</i> , 2021, 104, .	3.2	0
119	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. <i>Highlights in Theoretical Chemistry</i> , 2013, , 121-128.	0.0	0