Fabio Della Sala

List of Publications by Year
in descending order

204 papers	10,005 citations	41344 49 h-index	40979 93 g-index
209 all docs	209 docs citations	209 times ranked	9940 citing authors

#	Article	IF	Citations
1	Kinetic Energy Density Functionals Based on a Generalized Screened Coulomb Potential: Linear Response and Future Perspectives. Computation, 2022, 10, 30.	2.0	7
2	Boosting the OEP2-sc method with spin-component scaling. Molecular Physics, 2022, 120, .	1.7	2
3	Laplacian-Level Quantum Hydrodynamic Theory for Plasmonics. Physical Review X, 2021, 11, .	8.9	29
4	Nonlocal kinetic energy functionals in real space using a Yukawa-potential kernel: Properties, linear response, and model functionals. Physical Review B, 2021, 103, .	3.2	13
5	Noncovalent Interactions from Models for the MÃ¸llerâ€“Plesset Adiabatic Connection. Journal of Physical Chemistry Letters, 2021, 12, 4867-4875.	4.6	15
6	Plasmon Couplings from Subsystem Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2021, 125, 7246-7259.	2.5	9
7	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, .	3.2	0
8	Minimal auxiliary basis set for time-dependent density functional theory and comparison with tight-binding approximations: Application to silver nanoparticles. Journal of Chemical Physics, 2020, 153, 084110.	3.0	14
9	Atomistic investigation of hybrid plasmonic systems. Nanomaterials and Nanotechnology, 2019, 9, 184798041985653.	3.0	6
10	Plasmonic quantum effects on single-emitter strong coupling. Nanophotonics, 2019, 8, 1821-1833.	6.0	24
11	Ab Initio Plasmonics of Externally Doped Silicon Nanocrystals. ACS Photonics, 2019, 6, 1474-1484.	6.6	10
12	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
13	The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development. Computation, 2019, 7, 65.	2.0	13
14	Investigation of the Exchange-Correlation Potentials of Functionals Based on the Adiabatic Connection Interpolation. Journal of Chemical Theory and Computation, 2019, 15, 1006-1015.	5.3	26
15	Nanowireâ€Intensified Metalâ€Enhanced Fluorescence in Hybrid Polymerâ€Plasmonic Electrospun Filaments. Small, 2018, 14, e1800187.	10.0	13
16	Assessment of interaction-strength interpolation formulas for gold and silver clusters. Journal of Chemical Physics, 2018, 148, 134106.	3.0	28
17	Restoring Size Consistency of Approximate Functionals Constructed from the Adiabatic Connection. Journal of Physical Chemistry Letters, 2018, 9, 3137-3142.	4.6	26
18	Nonlocal kinetic energy functional from the jellium-with-gap model: Applications to orbital-free density functional theory. Physical Review B, 2018, 97, .	3.2	31

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19	Optical properties of plasmonic core-shell nanomatryoshkas: a quantum hydrodynamic analysis. Optics Express, 2018, 26, 17322.	3.4	15
20	Semilocal Pauliâ€“Gaussian Kinetic Functionals for Orbital-Free Density Functional Theory Calculations of Solids. Journal of Physical Chemistry Letters, 2018, 9, 4385-4390.	4.6	65
21	Density Functional Tight Binding for Quantum Plasmonics. Journal of Physical Chemistry C, 2018, 122, 19756-19766.	3.1	21
22	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. Computation, 2018, 6, 7.	2.0	17
23	Electrostatic Mechanophores in Tuneable Lightâ€Emitting Piezopolymer Nanowires. Advanced Materials, 2017, 29, 1701031.	21.0	12
24	Jellium-with-gap model applied to semilocal kinetic functionals. Physical Review B, 2017, 95, .	3.2	26
25	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
26	Modified Fourth-Order Kinetic Energy Gradient Expansion with Hartree Potential-Dependent Coefficients. Journal of Chemical Theory and Computation, 2017, 13, 4228-4239.	5.3	33
27	Plasmonic Nonlocal Response Effects on Dipole Decay Dynamics in the Weak- and Strong-Coupling Regimes. Journal of Physical Chemistry C, 2017, 121, 22361-22368.	3.1	24
28	Nonlocal plasmonic effects on dipole decay dynamics in the weak and strong coupling regimes. , 2017, , .		0
29	Kinetic and Exchange Energy Densities near the Nucleus. Computation, 2016, 4, 19.	2.0	20
30	Hartree potential dependent exchange functional. Journal of Chemical Physics, 2016, 145, 084110.	3.0	15
31	Enhancement of radiative processes in nanofibers with embedded plasmonic nanoparticles. Optics Letters, 2016, 41, 1632.	3.3	2
32	Interaction-Strength Interpolation Method for Main-Group Chemistry: Benchmarking, Limitations, and Perspectives. Journal of Chemical Theory and Computation, 2016, 12, 4885-4896.	5.3	34
33	Accurate Kohnâ€“Sham ionization potentials from scaledâ€oppositeâ€spin secondâ€order optimized effective potential methods. Journal of Computational Chemistry, 2016, 37, 2081-2090.	3.3	24
34	Kineticâ€energyâ€dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	2.0	78
35	Semiclassical atom theory applied to solid-state physics. Physical Review B, 2016, 93, .	3.2	51
36	Semilocal density functional theory with correct surface asymptotics. Physical Review B, 2016, 93, .	3.2	41

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37	Emerging giant resonant exciton induced by Ta substitution in anataseTiO2: A tunable correlation effect. Physical Review B, 2016, 93, .	3.2	16
38	Quantum hydrodynamic theory for plasmonics: Impact of the electron density tail. Physical Review B, 2016, 93, .	3.2	122
39	Plasmonic luminescence enhancement by metal nanoparticles embedded in nanofibers. , 2016, , .		0
40	Perturbations of Dipole Decay Dynamics Induced by Plasmonic Nano-Antennas â€" A Study within the Discrete Dipole Approximation. Nanomaterials and Nanotechnology, 2015, 5, 11.	3.0	3
41	Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. Journal of Chemical Theory and Computation, 2015, 11, 122-131.	5.3	22
42	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.	3.1	19
43	Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory. Physical Review B, 2015, 91, .	3.2	31
44	Accurate non-covalent interaction energies via an efficient MP2 scaling procedure. Chemical Physics Letters, 2015, 635, 262-267.	2.6	6
45	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, .	3.2	49
46	Excitonâ€"Plasmon Coupling Enhancement via Metal Oxidation. ACS Nano, 2015, 9, 9691-9699.	14.6	39
47	Assessment of the TCA functional in computational chemistry and solid-state physics. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
48	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. Journal of Chemical Physics, 2015, 142, 154121.	3.0	23
49	Optical conductivity renormalization of graphene on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">SrTiO</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>due to resonant excitonic effects mediated by Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>	3.2	20
50	Frozen density embedding with non-integer subsystemsâ€™ particle numbers. Journal of Chemical Physics, 2014, 140, 114101.	3.0	17
51	Orbital-dependent second-order scaled-opposite-spin correlation functionals in the optimized effective potential method. Journal of Chemical Physics, 2014, 141, 024113.	3.0	35
52	First principles optical spectra of theÎ²-SiC(0â€‰0â€‰1)/Al interface. Journal of Physics Condensed Matter, 2014, 26, 265006.	1.8	3
53	Polymorphism in Crystalline Microfibers of Achiral Octithiophene: The Effect on Charge Transport, Supramolecular Chirality and Optical Properties. Advanced Functional Materials, 2014, 24, 4943-4951.	14.9	21
54	A density difference based analysis of orbital-dependent exchange-correlation functionals. Molecular Physics, 2014, 112, 700-710.	1.7	25

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55	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.	5.3	62
56	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. Journal of Chemical Theory and Computation, 2014, 10, 3151-3162.	5.3	23
57	Testing the broad applicability of the PBEint GGA functional and its oneâ€parameter hybrid form. International Journal of Quantum Chemistry, 2013, 113, 673-682.	2.0	33
58	Fluorineâ€“thiophene-substituted organic dyes for dye sensitized solar cells. Journal of Materials Chemistry A, 2013, 1, 11909.	10.3	25
59	Metallic-like Stoichiometric Copper Sulfide Nanocrystals: Phase- and Shape-Selective Synthesis, Near-Infrared Surface Plasmon Resonance Properties, and Their Modeling. ACS Nano, 2013, 7, 7352-7369.	14.6	306
60	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.	2.8	13
61	Dipole Decay Rates Engineering via Silver Nanocones. Plasmonics, 2013, 8, 1079-1086.	3.4	11
62	Accurate ionization potential of gold anionic clusters from density functional theory and many-body perturbation theory. European Physical Journal B, 2013, 86, 1.	1.5	13
63	Radiative coupling of high-order plasmonic modes with far-field. Photonics and Nanostructures - Fundamentals and Applications, 2013, 11, 335-344.	2.0	2
64	Semilocal and hybrid density embedding calculations of ground-state charge-transfer complexes. Journal of Chemical Physics, 2013, 138, 124112.	3.0	18
65	Optimized effective potential method based on spin-resolved components of the second-order correlation energy in density functional theory. Physical Review B, 2013, 87, .	3.2	26
66	Optical spectra of solids obtained by time-dependent density functional theory with the jellium-with-gap-model exchange-correlation kernel. Physical Review B, 2013, 87, .	3.2	62
67	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. Journal of Chemical Theory and Computation, 2013, 9, 2256-2263.	5.3	60
68	Dipole-excited surface plasmons in metallic nanoparticles: Engineering decay dynamics within the discrete-dipole approximation. Physical Review B, 2013, 87, .	3.2	41
69	A periodic charge-dipole electrostatic model. II. A kinetic-exchange-correlation correction. Journal of Chemical Physics, 2013, 139, 144109.	3.0	2
70	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. Physical Review B, 2013, 88, .	3.2	40
71	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
72	Spin-dependent gradient correction for more accurate atomization energies of molecules. Journal of Chemical Physics, 2012, 137, 194105.	3.0	23

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73	Dipole decay rates engineering via metallic nanosystems. , 2012, , .		1
74	Nonuniform Scaling Applied to Surface Energies of Transition Metals. Physical Review Letters, 2012, 108, 126402.	7.8	57
75	Semilocal dynamical correlation with increased localization. Physical Review B, 2012, 86, .	3.2	45
76	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.	3.0	20
77	Toward quantum-dot cellular automata units: thiolated-carbazole linked bisferrocenes. Nanoscale, 2012, 4, 813-823.	5.6	58
78	A periodic charge-dipole electrostatic model: Parametrization for silver slabs. Journal of Chemical Physics, 2012, 137, 134702.	3.0	2
79	Accuracy of basis-set extrapolation schemes for DFT-RPA correlation energies in molecular calculations. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	22
80	Range separated functionals in the density functional based tightâ€binding method: Formalism. Physica Status Solidi (B): Basic Research, 2012, 249, 237-244.	1.5	47
81	Characterization of TiO2 atomic crystals for nanocomposite materials oriented to optoelectronics. Optical and Quantum Electronics, 2012, 44, 291-296.	3.3	2
82	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	1
83	Silver Nanourchins in Plasmonics: Theoretical Investigation on the Optical Properties of the Branches. Journal of Physical Chemistry C, 2011, 115, 11934-11940.	3.1	17
84	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.	5.3	83
85	Temperature and Size Dependence of the Optical Properties of Tetrapod-Shaped Colloidal Nanocrystals Exhibiting Type-II Transitions. Journal of Physical Chemistry C, 2011, 115, 18094-18104.	3.1	17
86	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
87	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
88	Frozen density embedding calculations with the orbital-dependent localized Hartreeâ€“Fock Kohnâ€“Sham potential. Chemical Physics Letters, 2011, 518, 114-118.	2.6	20
89	Accurate singlet and triplet excitation energies using the Localized Hartreeâ€“Fock Kohnâ€“Sham potential. Chemical Physics, 2011, 391, 19-26.	1.9	13
90	Structure, electronic, and optical properties of TiO2 atomic clusters: An ab initio study. Journal of Chemical Physics, 2011, 135, 244704.	3.0	64

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91	Semiclassical Neutral Atom as a Reference System in Density Functional Theory. Physical Review Letters, 2011, 106, 186406.	7.8	117
92	Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis. Physical Review B, 2011, 84, .	3.2	26
93	Electrostatic-Field-Driven Alignment of Organic Oligomers on ZnO Surfaces. Physical Review Letters, 2011, 107, 146401.	7.8	28
94	Correlation energy functional from jellium surface analysis. Physical Review B, 2011, 84, .	3.2	39
95	Exchange-correlation generalized gradient approximation for gold nanostructures. Journal of Chemical Physics, 2011, 134, 194112.	3.0	34
96	Organic Dyes Containing A Triple Bond Spacer for Dye Sensitized Solar Cells: A Combined Experimental and Theoretical Investigation. Current Organic Chemistry, 2011, 15, 3535-3543.	1.6	8
97	Shaping White Light Through Electroluminescent Fully Organic Coupled Microcavities. Advanced Materials, 2010, 22, 4696-4700.	21.0	18
98	Evidence for an internal field in CdSe/CdS nanorods by time resolved and single rod experiments. Superlattices and Microstructures, 2010, 47, 174-177.	3.1	5
99	Electromagnetic modelling of the optical behaviour of silver nanospheres on dielectric substrates: The role of a silver buffer layer. Superlattices and Microstructures, 2010, 47, 55-59.	3.1	2
100	The role of exactâ€exchange in the theoretical description of organicâ€metal interfaces. International Journal of Quantum Chemistry, 2010, 110, 2162-2171.	2.0	16
101	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
102	Frozen density embedding with hybrid functionals. Journal of Chemical Physics, 2010, 133, 164111.	3.0	49
103	Active Role of Oxide Layers on the Polarization of Plasmonic Nanostructures. ACS Nano, 2010, 4, 4117-4125.	14.6	12
104	Pure white hybrid light-emitting device with color rendering index higher than 90. Optics Letters, 2010, 35, 616.	3.3	19
105	Monodispersed molecular donors for bulk hetero-junction solar cells: from molecular properties to device performances. Chemical Communications, 2010, 46, 6273.	4.1	13
106	Observation and control of coherent torsional dynamics in a quinquethiophene molecule. Physical Chemistry Chemical Physics, 2010, 12, 7917.	2.8	12
107	First disubstituted dibenzothiophene-5,5-dioxide monodispersed molecular materials for efficient blue-electroluminescence. Journal of Materials Chemistry, 2010, 20, 1012-1018.	6.7	29
108	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.	3.0	23

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109	Anab initiostudy of the magneticâ€“metallic CoPt₃â€“Au interfaces. Journal of Physics Condensed Matter, 2009, 21, 015001.	1.8	1
110	Raman Spectra of Poly(pâ€phenylenevinylene)s with Fluorinated Vinylene Units: Evidence of Interâ€ring Distortion. ChemPhysChem, 2009, 10, 1284-1290.	2.1	23
111	Rectification in Supramolecular Zinc Porphyrin/Fulleropyrrolidine Dyads Selfâ€Organized on Gold(111). ChemPhysChem, 2009, 10, 2633-2641.	2.1	12
112	Electrostatic spin crossover effect in polar magnetic molecules. Nature Materials, 2009, 8, 813-817.	27.5	148
113	Ab initiodepolarization in self-assembled molecular monolayers: Beyond conventional density-functional theory. Physical Review B, 2009, 80, .	3.2	24
114	Ultrafast electron-hole dynamics and optical gain in CdSe/CdS nanorods. , 2009, , .		0
115	Multiexciton Engineering in Seeded Core/Shell Nanorods: Transfer from Type-I to Quasi-type-II Regimes. Nano Letters, 2009, 9, 3470-3476.	9.1	180
116	Enhanced fluorescence by metal nanospheres on metal substrates. Optics Letters, 2009, 34, 2381.	3.3	39
117	Absorption and fluorescence properties of oligothiophene biomarkers from long-range-corrected time-dependent density functional theory. Physical Chemistry Chemical Physics, 2009, 11, 4498.	2.8	145
118	Experimental and Computational Studies on Non-Covalent Imprinted Microspheres as Recognition System for Nicotinamide Molecules. Molecules, 2009, 14, 2632-2649.	3.8	39
119	Microwave-Assisted Synthesis of Thiophene Fluorophores, Labeling and Multilabeling of Monoclonal Antibodies, and Long Lasting Staining of Fixed Cells. Journal of the American Chemical Society, 2009, 131, 10892-10900.	13.7	64
120	Structural and electronic properties of gold microclusters: assessment of the localized Hartreeâ€“Fock method. Physical Chemistry Chemical Physics, 2009, 11, 9160.	2.8	10
121	Ultrafast electron-hole dynamics in core/shell CdSe/CdS dot/rod nanocrystals. , 2009, , .		0
122	Zinc Porphyrinâ€Driven Assembly of Gold Nanofingers. Small, 2008, 4, 497-506.	10.0	8
123	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.	3.3	11
124	Ultrafast Electronâ^'Hole Dynamics in Core/Shell CdSe/CdS Dot/Rod Nanocrystals. Nano Letters, 2008, 8, 4582-4587.	9.1	146
125	Determination of Band Offsets in Heterostructured Colloidal Nanorods Using Scanning Tunneling Spectroscopy. Nano Letters, 2008, 8, 2954-2958.	9.1	179
126	Theoretical study on oligothiophene N-succinimidyl esters: size and pushâ€“pull effects. Physical Chemistry Chemical Physics, 2008, 10, 5363.	2.8	10

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127	Large Blue-Shift in the Optical Spectra of Fluorinated Polyphenylenevinylenes. A Combined Theoretical and Experimental Study. Journal of Physical Chemistry B, 2008, 112, 2996-3004.	2.6	38
128	Multiconfiguration optimized effective potential method for a density-functional treatment of static correlation. Journal of Chemical Physics, 2008, 128, 144109.	3.0	27
129	Intrinsic optical nonlinearity in colloidal seeded grown CdSe/CdS nanostructures: Photoinduced screening of the internal electric field. Physical Review B, 2008, 78, .	3.2	91
130	Type II transition in InSb-based nanostructures for midinfrared applications. Journal of Applied Physics, 2008, 103, 114516.	2.5	9
131	Localized exchange-correlation potential from second-order self-energy for accurate Kohn-Sham energy gap. Journal of Chemical Physics, 2007, 126, 214102.	3.0	31
132	Numerically stable optimized effective potential method with balanced Gaussian basis sets. Journal of Chemical Physics, 2007, 127, 054102.	3.0	130
133	Fabrication of Molecular Micro-NanoStructures by Surface-Tension-Driven Technique. Materials Research Society Symposia Proceedings, 2007, 1002, 1.	0.1	0
134	Synthesis and Micrometer-Scale Assembly of Colloidal CdSe/CdS Nanorods Prepared by a Seeded Growth Approach. Nano Letters, 2007, 7, 2942-2950.	9.1	1,098
135	Imaging Photoelectron Transmission through Self-Assembled Monolayers:Â The Work-Function of Alkanethiols Coated Gold. Langmuir, 2007, 23, 6156-6162.	3.5	17
136	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. Bioconjugate Chemistry, 2007, 18, 1015-1015.	3.6	0
137	Ab initiostructural and electronic analysis ofCH3SHself-assembled on a Cu(110) substrate. Physical Review B, 2007, 75, .	3.2	11
138	Blue light emitting diodes based on fluorescent CdSeâˆ•ZnS nanocrystals. Applied Physics Letters, 2007, 90, 051106.	3.3	82
139	Bicolor Pixels from a Single Active Molecular Material by Surface-Tension-Driven Deposition. Advanced Materials, 2007, 19, 1597-1602.	21.0	19
140	The localized Hartreeâ€“Fock method for a self-interaction free Kohnâ€“Sham potential: applications to closed and open-shell molecules. Theoretical Chemistry Accounts, 2007, 117, 981-989.	1.4	13
141	Entanglement of electrons in interacting molecules. Theoretical and Mathematical Physics(Russian) Tj ETQq1 1 0.784314 rgBT /Overlo	0.9	6
142	Rydberg states with quantum Monte Carlo. Journal of Chemical Physics, 2006, 124, 114114.	3.0	15
143	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.	2.6	26
144	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. Bioconjugate Chemistry, 2006, 17, 58-67.	3.6	55

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145	Theoretical study on N-succinimidyl oligothiophenes: A novel class of materials for biological applications. Journal of Non-Crystalline Solids, 2006, 352, 2452-2456.	3.1	0
146	The effects of oxygen and boron functionalization on the optical properties of dithienothiophenes. Journal of Non-Crystalline Solids, 2006, 352, 2461-2464.	3.1	3
147	Metal-enhanced fluorescence of colloidal nanocrystals with nanoscale control. Nature Nanotechnology, 2006, 1, 126-130.	31.5	573
148	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
149	Electronic and optical properties of functionalized carbon chains with the localized Hartreeâ€“Fock and conventional Kohnâ€“Sham methods. Chemical Physics, 2005, 309, 77-87.	1.9	68
150	Bright White Organic Light-Emitting Devices from a Single Active Molecular Material. Advanced Materials, 2005, 17, 34-39.	21.0	252
151	Ultrafast carrier dynamics in core and core/shell CdSe quantum rods: Role of the surface and interface defects. Physical Review B, 2005, 72, .	3.2	72
152	Quasiparticle energies for large molecules: A tight-binding-based Greenâ€™s-function approach. Physical Review A, 2005, 71, .	2.5	51
153	Electronic structure of organic films in the first excited states determined using scanning tunneling spectroscopy: An experimental and theoretical study. Physical Review B, 2005, 72, .	3.2	2
154	Optical properties of tetrapod-shaped CdTe nanocrystals. Applied Physics Letters, 2005, 87, 224101.	3.3	44
155	Nonradiative Relaxation in Thiophene-S,S-dioxide Derivatives:Â The Role of the Environment. Journal of Physical Chemistry B, 2005, 109, 6004-6011.	2.6	21
156	Open-shell localized Hartreeâ€“Fock method based on the generalized adiabatic connection Kohnâ€“Sham formalism for a self-consistent treatment of excited states. Journal of Chemical Physics, 2005, 122, 244102.	3.0	17
157	Theoretical Study of Singlet and Triplet Excitation Energies in Oligothiophenes. Journal of Physical Chemistry A, 2005, 109, 3078-3085.	2.5	73
158	The effects of oxygenation on the optical properties of dimethyl-dithienothiophenes: Comparison between experiments and first-principles calculations. Journal of Chemical Physics, 2004, 121, 3784-3791.	3.0	16
159	Quantum and Thermal Fluctuation Effects on the Photoabsorption Spectra of Clusters. Physical Review Letters, 2004, 92, 183401.	7.8	67
160	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
161	First-principles time-dependent density-functional theory study of functionalized benzo[b]thiophenes. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 555-559.	0.8	1
162	Long-range order induced by cobalt porphyrin adsorption on aminothiophenol-functionalized Au(111): the influence of the induced dipole. Materials Science and Engineering C, 2004, 24, 569-573.	7.3	15

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163	Effects of intermolecular interactions on photoluminescence efficiency of crystalline thienylene-S,S-dioxide molecular semiconductors. Organic Electronics, 2004, 5, 129-134.	2.6	10
164	Oligomer molecules: first-principles investigation of the optical properties and applications to luminescent devices. Physica A: Statistical Mechanics and Its Applications, 2004, 339, 106-111.	2.6	1
165	Density-functional calculations of NMR shielding constants using the localized Hartreeâ€“Fock method. Chemical Physics Letters, 2004, 383, 115-121.	2.6	47
166	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.	13.7	37
167	New Branched Thiophene-Based Oligomers for Bright Organic Light-Emitting Devices. Advanced Materials, 2003, 15, 2060-2063.	21.0	54
168	The Kohnâ€“Sham treatment of anions via the localized Hartreeâ€“Fock method. Chemical Physics Letters, 2003, 372, 538-547.	2.6	31
169	Excitation energies of molecules by time-dependent density functional theory based on effective exact exchange Kohn-Sham potentials. International Journal of Quantum Chemistry, 2003, 91, 131-138.	2.0	57
170	Organic single-layer white light-emitting diodes by exciplex emission from spin-coated blends of blue-emitting molecules. Applied Physics Letters, 2003, 82, 334-336.	3.3	112
171	Open-shell localized Hartreeâ€“Fock approach for an efficient effective exact-exchange Kohnâ€“Sham treatment of open-shell atoms and molecules. Journal of Chemical Physics, 2003, 118, 10439-10454.	3.0	44
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