

# Fabio Della Sala

## List of Publications by Year in descending order

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204  
papers

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209  
docs citations

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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. <i>Computation</i> , 2022, 10, 30.	1.0	7
2	Boosting the OEP2-sc method with spin-component scaling. <i>Molecular Physics</i> , 2022, 120, .	0.8	2
3	Laplacian-Level Quantum Hydrodynamic Theory for Plasmonics. <i>Physical Review X</i> , 2021, 11, .	2.8	29
4	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, .	1.1	13
5	Noncovalent Interactions from Models for the MÃ¶ller-Plesset Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4867-4875.	2.1	15
6	Plasmon Couplings from Subsystem Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7246-7259.	1.1	9
7	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, .	1.1	0
8	Minimal auxiliary basis set for time-dependent density functional theory and comparison with tight-binding approximations: Application to silver nanoparticles. <i>Journal of Chemical Physics</i> , 2020, 153, 084110.	1.2	14
9	Atomistic investigation of hybrid plasmonic systems. <i>Nanomaterials and Nanotechnology</i> , 2019, 9, 184798041985653.	1.2	6
10	Plasmonic quantum effects on single-emitter strong coupling. <i>Nanophotonics</i> , 2019, 8, 1821-1833.	2.9	24
11	Ab Initio Plasmonics of Externally Doped Silicon Nanocrystals. <i>ACS Photonics</i> , 2019, 6, 1474-1484.	3.2	10
12	Performance of Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3044-3055.	2.3	37
13	The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development. <i>Computation</i> , 2019, 7, 65.	1.0	13
14	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.	2.3	26
15	Nanowire-Enhanced Metal-Enhanced Fluorescence in Hybrid Polymer-Plasmonic Electrospun Filaments. <i>Small</i> , 2018, 14, e1800187.	5.2	13
16	Assessment of interaction-strength interpolation formulas for gold and silver clusters. <i>Journal of Chemical Physics</i> , 2018, 148, 134106.	1.2	28
17	Restoring Size Consistency of Approximate Functionals Constructed from the Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3137-3142.	2.1	26
18	Nonlocal kinetic energy functional from the jellium-with-gap model: Applications to orbital-free density functional theory. <i>Physical Review B</i> , 2018, 97, .	1.1	31

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19	Optical properties of plasmonic core-shell nanomatryoshkas: a quantum hydrodynamic analysis. <i>Optics Express</i> , 2018, 26, 17322.	1.7	15
20	Semilocal Pauliâ€“Gaussian Kinetic Functionals for Orbital-Free Density Functional Theory Calculations of Solids. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4385-4390.	2.1	65
21	Density Functional Tight Binding for Quantum Plasmonics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19756-19766.	1.5	21
22	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. <i>Computation</i> , 2018, 6, 7.	1.0	17
23	Electrostatic Mechanophores in Tuneable Lightâ€“Emitting Piezopolymer Nanowires. <i>Advanced Materials</i> , 2017, 29, 1701031.	11.1	12
24	Jellium-with-gap model applied to semilocal kinetic functionals. <i>Physical Review B</i> , 2017, 95, .	1.1	26
25	Laplacian-dependent models of the kinetic energy density: Applications in subsystem density functional theory with meta-generalized gradient approximation functionals. <i>Journal of Chemical Physics</i> , 2017, 146, 064105.	1.2	44
26	Modified Fourth-Order Kinetic Energy Gradient Expansion with Hartree Potential-Dependent Coefficients. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4228-4239.	2.3	33
27	Plasmonic Nonlocal Response Effects on Dipole Decay Dynamics in the Weak- and Strong-Coupling Regimes. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22361-22368.	1.5	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. <i>Computation</i> , 2016, 4, 19.	1.0	20
30	Hartree potential dependent exchange functional. <i>Journal of Chemical Physics</i> , 2016, 145, 084110.	1.2	15
31	Enhancement of radiative processes in nanofibers with embedded plasmonic nanoparticles. <i>Optics Letters</i> , 2016, 41, 1632.	1.7	2
32	Interaction-Strength Interpolation Method for Main-Group Chemistry: Benchmarking, Limitations, and Perspectives. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4885-4896.	2.3	34
33	Accurate Kohnâ€“Sham ionization potentials from scaledâ€“oppositeâ€“spin secondâ€“order optimized effective potential methods. <i>Journal of Computational Chemistry</i> , 2016, 37, 2081-2090.	1.5	24
34	Kineticâ€“energyâ€“density dependent semilocal exchangeâ€“correlation functionals. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1641-1694.	1.0	78
35	Semiclassical atom theory applied to solid-state physics. <i>Physical Review B</i> , 2016, 93, .	1.1	51
36	Semilocal density functional theory with correct surface asymptotics. <i>Physical Review B</i> , 2016, 93, .	1.1	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, .	1.1	16
38	Quantum hydrodynamic theory for plasmonics: Impact of the electron density tail. Physical Review B, 2016, 93, .	1.1	122
39	Plasmonic luminescence enhancement by metal nanoparticles embedded in nanofibers. , 2016, , .		0
40	Perturbations of Dipole Decay Dynamics Induced by Plasmonic Nano-Antennas " A Study within the Discrete Dipole Approximation. Nanomaterials and Nanotechnology, 2015, 5, 11.	1.2	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.	2.3	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.	1.5	19
43	Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory. Physical Review B, 2015, 91, .	1.1	31
44	Accurate non-covalent interaction energies via an efficient MP2 scaling procedure. Chemical Physics Letters, 2015, 635, 262-267.	1.2	6
45	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, .	1.1	49
46	Exciton"Plasmon Coupling Enhancement <i>via</i> Metal Oxidation. ACS Nano, 2015, 9, 9691-9699.	7.3	39
47	Assessment of the TCA functional in computational chemistry and solid-state physics. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	10
48	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. Journal of Chemical Physics, 2015, 142, 154121.	1.2	23
49	Optical conductivity renormalization of graphene on $\text{SrTiO}_3$ due to resonant excitonic effects mediated by Ti	1.1	20
50	Frozen density embedding with non-integer subsystems' particle numbers. Journal of Chemical Physics, 2014, 140, 114101.	1.2	17
51	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
52	First principles optical spectra of the $\text{SiC}(100)/\text{Al}$ interface. Journal of Physics Condensed Matter, 2014, 26, 265006.	0.7	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.	7.8	21
54	A density difference based analysis of orbital-dependent exchange-correlation functionals. Molecular Physics, 2014, 112, 700-710.	0.8	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. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 164-179.	2.3	62
56	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3151-3162.	2.3	23
57	Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 673-682.	1.0	33
58	Fluorine-thiophene-substituted organic dyes for dye sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2013, 1, 11909.	5.2	25
59	Metallic-like Stoichiometric Copper Sulfide Nanocrystals: Phase- and Shape-Selective Synthesis, Near-Infrared Surface Plasmon Resonance Properties, and Their Modeling. <i>ACS Nano</i> , 2013, 7, 7352-7369.	7.3	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. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15485.	1.3	13
61	Dipole Decay Rates Engineering via Silver Nanocones. <i>Plasmonics</i> , 2013, 8, 1079-1086.	1.8	11
62	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.	0.6	13
63	Radiative coupling of high-order plasmonic modes with far-field. <i>Photonics and Nanostructures - Fundamentals and Applications</i> , 2013, 11, 335-344.	1.0	2
64	Semilocal and hybrid density embedding calculations of ground-state charge-transfer complexes. <i>Journal of Chemical Physics</i> , 2013, 138, 124112.	1.2	18
65	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, .	1.1	26
66	Optical spectra of solids obtained by time-dependent density functional theory with the jellium-with-gap-model exchange-correlation kernel. <i>Physical Review B</i> , 2013, 87, .	1.1	62
67	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2256-2263.	2.3	60
68	Dipole-excited surface plasmons in metallic nanoparticles: Engineering decay dynamics within the discrete-dipole approximation. <i>Physical Review B</i> , 2013, 87, .	1.1	41
69	A periodic charge-dipole electrostatic model. II. A kinetic-exchange-correlation correction. <i>Journal of Chemical Physics</i> , 2013, 139, 144109.	1.2	2
70	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. <i>Physical Review B</i> , 2013, 88, .	1.1	40
71	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
72	Spin-dependent gradient correction for more accurate atomization energies of molecules. <i>Journal of Chemical Physics</i> , 2012, 137, 194105.	1.2	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.	2.9	57
75	Semilocal dynamical correlation with increased localization. Physical Review B, 2012, 86, .	1.1	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.	1.2	20
77	Toward quantum-dot cellular automata units: thiolated-carbazole linked bisferrocenes. Nanoscale, 2012, 4, 813-823.	2.8	58
78	A periodic charge-dipole electrostatic model: Parametrization for silver slabs. Journal of Chemical Physics, 2012, 137, 134702.	1.2	2
79	Accuracy of basis-set extrapolation schemes for DFT-RPA correlation energies in molecular calculations. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	22
80	Range separated functionals in the density functional based tight-binding method: Formalism. Physica Status Solidi (B): Basic Research, 2012, 249, 237-244.	0.7	47
81	Characterization of TiO2 atomic crystals for nanocomposite materials oriented to optoelectronics. Optical and Quantum Electronics, 2012, 44, 291-296.	1.5	2
82	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	1
83	Silver Nanourchins in Plasmonics: Theoretical Investigation on the Optical Properties of the Branches. Journal of Physical Chemistry C, 2011, 115, 11934-11940.	1.5	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.	2.3	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.	1.5	17
86	Interfacial Electronic Structure of the Dipolar Vanadyl Naphthalocyanine on Au(111): "Push-Back" vs Dipolar Effects. Journal of Physical Chemistry C, 2011, 115, 21128-21138.	1.5	40
87	Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdew-Burke-Ernzerhof-Like Enhancement Factor. Journal of Chemical Theory and Computation, 2011, 7, 3548-3559.	2.3	49
88	Frozen density embedding calculations with the orbital-dependent localized Hartree-Fock Kohn-Sham potential. Chemical Physics Letters, 2011, 518, 114-118.	1.2	20
89	Accurate singlet and triplet excitation energies using the Localized Hartree-Fock Kohn-Sham potential. Chemical Physics, 2011, 391, 19-26.	0.9	13
90	Structure, electronic, and optical properties of TiO2 atomic clusters: An <i>ab initio</i> study. Journal of Chemical Physics, 2011, 135, 244704.	1.2	64

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91	Semiclassical Neutral Atom as a Reference System in Density Functional Theory. <i>Physical Review Letters</i> , 2011, 106, 186406.	2.9	117
92	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, .	1.1	26
93	Electrostatic-Field-Driven Alignment of Organic Oligomers on ZnO Surfaces. <i>Physical Review Letters</i> , 2011, 107, 146401.	2.9	28
94	Correlation energy functional from jellium surface analysis. <i>Physical Review B</i> , 2011, 84, .	1.1	39
95	Exchange-correlation generalized gradient approximation for gold nanostructures. <i>Journal of Chemical Physics</i> , 2011, 134, 194112.	1.2	34
96	Organic Dyes Containing A Triple Bond Spacer for Dye Sensitized Solar Cells: A Combined Experimental and Theoretical Investigation. <i>Current Organic Chemistry</i> , 2011, 15, 3535-3543.	0.9	8
97	Shaping White Light Through Electroluminescent Fully Organic Coupled Microcavities. <i>Advanced Materials</i> , 2010, 22, 4696-4700.	11.1	18
98	Evidence for an internal field in CdSe/CdS nanorods by time resolved and single rod experiments. <i>Superlattices and Microstructures</i> , 2010, 47, 174-177.	1.4	5
99	Electromagnetic modelling of the optical behaviour of silver nanospheres on dielectric substrates: The role of a silver buffer layer. <i>Superlattices and Microstructures</i> , 2010, 47, 55-59.	1.4	2
100	The role of exact exchange in the theoretical description of organic-metal interfaces. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2162-2171.	1.0	16
101	Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces. <i>Physical Review B</i> , 2010, 82, .	1.1	50
102	Frozen density embedding with hybrid functionals. <i>Journal of Chemical Physics</i> , 2010, 133, 164111.	1.2	49
103	Active Role of Oxide Layers on the Polarization of Plasmonic Nanostructures. <i>ACS Nano</i> , 2010, 4, 4117-4125.	7.3	12
104	Pure white hybrid light-emitting device with color rendering index higher than 90. <i>Optics Letters</i> , 2010, 35, 616.	1.7	19
105	Monodispersed molecular donors for bulk hetero-junction solar cells: from molecular properties to device performances. <i>Chemical Communications</i> , 2010, 46, 6273.	2.2	13
106	Observation and control of coherent torsional dynamics in a quinquethiophene molecule. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7917.	1.3	12
107	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
108	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.	1.2	23

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109	An <i>ab initio</i> study of the magnetic “metallic CoPt <sub>3</sub> ”Au interfaces. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 015001.	0.7	1
110	Raman Spectra of Poly( <i>p</i> -phenylenevinylene)s with Fluorinated Vinylene Units: Evidence of Inter-ring Distortion. <i>ChemPhysChem</i> , 2009, 10, 1284-1290.	1.0	23
111	Rectification in Supramolecular Zinc Porphyrin/Fulleropyrrolidine Dyads Self-Organized on Gold(111). <i>ChemPhysChem</i> , 2009, 10, 2633-2641.	1.0	12
112	Electrostatic spin crossover effect in polar magnetic molecules. <i>Nature Materials</i> , 2009, 8, 813-817.	13.3	148
113	<i>Ab initio</i> depolarization in self-assembled molecular monolayers: Beyond conventional density-functional theory. <i>Physical Review B</i> , 2009, 80, .	1.1	24
114	Ultrafast electron-hole dynamics and optical gain in CdSe/CdS nanorods. , 2009, , .		0
115	Multixciton Engineering in Seeded Core/Shell Nanorods: Transfer from Type-I to Quasi-type-II Regimes. <i>Nano Letters</i> , 2009, 9, 3470-3476.	4.5	180
116	Enhanced fluorescence by metal nanospheres on metal substrates. <i>Optics Letters</i> , 2009, 34, 2381.	1.7	39
117	Absorption and fluorescence properties of oligothiophene biomarkers from long-range-corrected time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4498.	1.3	145
118	Experimental and Computational Studies on Non-Covalent Imprinted Microspheres as Recognition System for Nicotinamide Molecules. <i>Molecules</i> , 2009, 14, 2632-2649.	1.7	39
119	Microwave-Assisted Synthesis of Thiophene Fluorophores, Labeling and Multilabeling of Monoclonal Antibodies, and Long Lasting Staining of Fixed Cells. <i>Journal of the American Chemical Society</i> , 2009, 131, 10892-10900.	6.6	64
120	Structural and electronic properties of gold microclusters: assessment of the localized Hartree-Fock method. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9160.	1.3	10
121	Ultrafast electron-hole dynamics in core/shell CdSe/CdS dot/rod nanocrystals. , 2009, , .		0
122	Zinc Porphyrin-Driven Assembly of Gold Nanofingers. <i>Small</i> , 2008, 4, 497-506.	5.2	8
123	Torsional effects on excitation energies of thiophene derivatives induced by $\text{I}^2$ substituents: Comparison between time-dependent density functional theory and approximated coupled cluster approaches. <i>Journal of Computational Chemistry</i> , 2008, 29, 451-457.	1.5	11
124	Ultrafast Electron-Hole Dynamics in Core/Shell CdSe/CdS Dot/Rod Nanocrystals. <i>Nano Letters</i> , 2008, 8, 4582-4587.	4.5	146
125	Determination of Band Offsets in Heterostructured Colloidal Nanorods Using Scanning Tunneling Spectroscopy. <i>Nano Letters</i> , 2008, 8, 2954-2958.	4.5	179
126	Theoretical study on oligothiophene N-succinimidyl esters: size and push-pull effects. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5363.	1.3	10



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127	Large Blue-Shift in the Optical Spectra of Fluorinated Polyphenylenevinylenes. A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2996-3004.	1.2	38
128	Multiconfiguration optimized effective potential method for a density-functional treatment of static correlation. <i>Journal of Chemical Physics</i> , 2008, 128, 144109.	1.2	27
129	Intrinsic optical nonlinearity in colloidal seeded grown CdSe/CdS nanostructures: Photoinduced screening of the internal electric field. <i>Physical Review B</i> , 2008, 78, .	1.1	91
130	Type II transition in InSb-based nanostructures for midinfrared applications. <i>Journal of Applied Physics</i> , 2008, 103, 114516.	1.1	9
131	Localized exchange-correlation potential from second-order self-energy for accurate Kohn-Sham energy gap. <i>Journal of Chemical Physics</i> , 2007, 126, 214102.	1.2	31
132	Numerically stable optimized effective potential method with balanced Gaussian basis sets. <i>Journal of Chemical Physics</i> , 2007, 127, 054102.	1.2	130
133	Fabrication of Molecular Micro-NanoStructures by Surface-Tension-Driven Technique. <i>Materials Research Society Symposia Proceedings</i> , 2007, 1002, 1.	0.1	0
134	Synthesis and Micrometer-Scale Assembly of Colloidal CdSe/CdS Nanorods Prepared by a Seeded Growth Approach. <i>Nano Letters</i> , 2007, 7, 2942-2950.	4.5	1,098
135	Imaging Photoelectron Transmission through Self-Assembled Monolayers: The Work-Function of Alkanethiols Coated Gold. <i>Langmuir</i> , 2007, 23, 6156-6162.	1.6	17
136	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. <i>Bioconjugate Chemistry</i> , 2007, 18, 1015-1015.	1.8	0
137	Ab initio structural and electronic analysis of CH <sub>3</sub> SH self-assembled on a Cu(110) substrate. <i>Physical Review B</i> , 2007, 75, .	1.1	11
138	Blue light emitting diodes based on fluorescent CdSe/ZnS nanocrystals. <i>Applied Physics Letters</i> , 2007, 90, 051106.	1.5	82
139	Bicolor Pixels from a Single Active Molecular Material by Surface-Tension-Driven Deposition. <i>Advanced Materials</i> , 2007, 19, 1597-1602.	11.1	19
140	The localized Hartree-Fock method for a self-interaction free Kohn-Sham potential: applications to closed and open-shell molecules. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 981-989.	0.5	13
141	Entanglement of electrons in interacting molecules. <i>Theoretical and Mathematical Physics (Russian)</i> Tj ETQq1 1 0.784314 rgBT / Overl	0.3	6
142	Rydberg states with quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2006, 124, 114114.	1.2	15
143	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.	1.2	26
144	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. <i>Bioconjugate Chemistry</i> , 2006, 17, 58-67.	1.8	55

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145	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.	1.5	0
146	The effects of oxygen and boron functionalization on the optical properties of dithienothiophenes. <i>Journal of Non-Crystalline Solids</i> , 2006, 352, 2461-2464.	1.5	3
147	Metal-enhanced fluorescence of colloidal nanocrystals with nanoscale control. <i>Nature Nanotechnology</i> , 2006, 1, 126-130.	15.6	573
148	Torsional potential of $\pi$ -conjugated molecules using the localized Hartree-Fock Kohn-Sham exchange potential. <i>Chemical Physics Letters</i> , 2006, 418, 496-501.	1.2	35
149	Electronic and optical properties of functionalized carbon chains with the localized Hartree-Fock and conventional Kohn-Sham methods. <i>Chemical Physics</i> , 2005, 309, 77-87.	0.9	68
150	Bright White Organic Light-Emitting Devices from a Single Active Molecular Material. <i>Advanced Materials</i> , 2005, 17, 34-39.	11.1	252
151	Ultrafast carrier dynamics in core and core/shell CdSe quantum rods: Role of the surface and interface defects. <i>Physical Review B</i> , 2005, 72, .	1.1	72
152	Quasiparticle energies for large molecules: A tight-binding-based Green's-function approach. <i>Physical Review A</i> , 2005, 71, .	1.0	51
153	Electronic structure of organic films in the first excited states determined using scanning tunneling spectroscopy: An experimental and theoretical study. <i>Physical Review B</i> , 2005, 72, .	1.1	2
154	Optical properties of tetrapod-shaped CdTe nanocrystals. <i>Applied Physics Letters</i> , 2005, 87, 224101.	1.5	44
155	Nonradiative Relaxation in Thiophene-S,S-dioxide Derivatives: The Role of the Environment. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6004-6011.	1.2	21
156	Open-shell localized Hartree-Fock method based on the generalized adiabatic connection Kohn-Sham formalism for a self-consistent treatment of excited states. <i>Journal of Chemical Physics</i> , 2005, 122, 244102.	1.2	17
157	Theoretical Study of Singlet and Triplet Excitation Energies in Oligothiophenes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3078-3085.	1.1	73
158	The effects of oxygenation on the optical properties of dimethyl-dithienothiophenes: Comparison between experiments and first-principles calculations. <i>Journal of Chemical Physics</i> , 2004, 121, 3784-3791.	1.2	16
159	Quantum and Thermal Fluctuation Effects on the Photoabsorption Spectra of Clusters. <i>Physical Review Letters</i> , 2004, 92, 183401.	2.9	67
160	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
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