Fabio Della Sala

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7631782/publications.pdf

Version: 2024-02-01

204 papers	10,005 citations	41323 49 h-index	40954 93 g-index
209 all docs	209 docs citations	209 times ranked	9940 citing authors

#	Article	IF	Citations
1	Synthesis and Micrometer-Scale Assembly of Colloidal CdSe/CdS Nanorods Prepared by a Seeded Growth Approach. Nano Letters, 2007, 7, 2942-2950.	4.5	1,098
2	Metal-enhanced fluorescence of colloidal nanocrystals with nanoscale control. Nature Nanotechnology, 2006, 1, 126-130.	15.6	573
3	Effects of macroscopic polarization in III-V nitride multiple quantum wells. Physical Review B, 1999, 60, 8849-8858.	1.1	488
4	Tight-binding approach to time-dependent density-functional response theory. Physical Review B, 2001, 63, .	1.1	341
5	Efficient localized Hartreeâ€“Fock methods as effective exact-exchange Kohnâ€“Sham methods for molecules. Journal of Chemical Physics, 2001, 115, 5718-5732.	1.2	319
6	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.	7.3	306
7	Free-carrier screening of polarization fields in wurtzite GaN/InGaN laser structures. Applied Physics Letters, 1999, 74, 2002-2004.	1.5	268
8	Bright White Organic Light-Emitting Devices from a Single Active Molecular Material. Advanced Materials, 2005, 17, 34-39.	11.1	252
9	Multiexciton Engineering in Seeded Core/Shell Nanorods: Transfer from Type-I to Quasi-type-II Regimes. Nano Letters, 2009, 9, 3470-3476.	4.5	180
10	Determination of Band Offsets in Heterostructured Colloidal Nanorods Using Scanning Tunneling Spectroscopy. Nano Letters, 2008, 8, 2954-2958.	4.5	179
11	Spontaneous polarization and piezoelectric field inGaN/Al0.15Ga0.85Nquantum wells: Impact on the optical spectra. Physical Review B, 2000, 61, 2711-2715.	1.1	169
12	Electrostatic spin crossover effect in polar magnetic molecules. Nature Materials, 2009, 8, 813-817.	13.3	148
13	Ultrafast Electronâ˜Hole Dynamics in Core/Shell CdSe/CdS Dot/Rod Nanocrystals. Nano Letters, 2008, 8, 4582-4587.	4.5	146
14	Absorption and fluorescence properties of oligothiophene biomarkers from long-range-corrected time-dependent density functional theory. Physical Chemistry Chemical Physics, 2009, 11, 4498.	1.3	145
15	Numerically stable optimized effective potential method with balanced Gaussian basis sets. Journal of Chemical Physics, 2007, 127, 054102.	1.2	130
16	Quantum hydrodynamic theory for plasmonics: Impact of the electron density tail. Physical Review B, 2016, 93, .	1.1	122
17	Semiclassical Neutral Atom as a Reference System in Density Functional Theory. Physical Review Letters, 2011, 106, 186406.	2.9	117
18	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.	1.5	112

#	Article	IF	Citations
19	Asymptotic Behavior of the Kohn-Sham Exchange Potential. Physical Review Letters, 2002, 89, 033003.	2.9	105
20	Intrinsic optical nonlinearity in colloidal seeded grown CdSe/CdS nanostructures: Photoinduced screening of the internal electric field. Physical Review B, 2008, 78, .	1.1	91
21	The asymptotic region of the Kohnâ€“Sham exchange potential in molecules. Journal of Chemical Physics, 2002, 116, 5374-5388.	1.2	89
22	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
23	Blue light emitting diodes based on fluorescent CdSeâ•ZnS nanocrystals. Applied Physics Letters, 2007, 90, 051106.	1.5	82
24	Kineticâ€energyâ€dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	1.0	78
25	Theoretical Study of Singlet and Triplet Excitation Energies in Oligothiophenes. Journal of Physical Chemistry A, 2005, 109, 3078-3085.	1.1	73
26	Ultrafast carrier dynamics in core and core/shell CdSe quantum rods: Role of the surface and interface defects. Physical Review B, 2005, 72, .	1.1	72
27	Electronic and optical properties of functionalized carbon chains with the localized Hartreeâ€“Fock and conventional Kohnâ€“Sham methods. Chemical Physics, 2005, 309, 77-87.	0.9	68
28	Quantum and Thermal Fluctuation Effects on the Photoabsorption Spectra of Clusters. Physical Review Letters, 2004, 92, 183401.	2.9	67
29	Transferable tight-binding parametrization for the group-III nitrides. Applied Physics Letters, 2002, 81, 4838-4840.	1.5	65
30	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
31	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.	6.6	64
32	Structure, electronic, and optical properties of TiO2 atomic clusters: An ab initio study. Journal of Chemical Physics, 2011, 135, 244704.	1.2	64
33	Solid-State Supramolecular Organization, Established Directly from Powder Diffraction Data, and Photoluminescence Efficiency of Rigid-Core Oligothiophene-S,S-dioxides. Journal of the American Chemical Society, 2003, 125, 12277-12283.	6.6	62
34	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, .	1.1	62
35	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
36	Î²-Fused Oligoporphyrins:Â A Novel Approach to a New Type of Extended Aromatic System. Journal of the American Chemical Society, 2000, 122, 11295-11302.	6.6	61

#	Article	IF	Citations
37	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. Journal of Chemical Theory and Computation, 2013, 9, 2256-2263.	2.3	60
38	Toward quantum-dot cellular automata units: thiolated-carbazole linked bisferrocenes. Nanoscale, 2012, 4, 813-823.	2.8	58
39	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.	1.0	57
40	Nonuniform Scaling Applied to Surface Energies of Transition Metals. Physical Review Letters, 2012, 108, 126402.	2.9	57
41	Doping screening of polarization fields in nitride heterostructures. Applied Physics Letters, 2000, 76, 3950-3952.	1.5	56
42	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. Bioconjugate Chemistry, 2006, 17, 58-67.	1.8	55
43	New Branched Thiophene-Based Oligomers for Bright Organic Light-Emitting Devices. Advanced Materials, 2003, 15, 2060-2063.	11.1	54
44	Quasiparticle energies for large molecules: A tight-binding-based Greenâ€™s-function approach. Physical Review A, 2005, 71, .	1.0	51
45	Semiclassical atom theory applied to solid-state physics. Physical Review B, 2016, 93, .	1.1	51
46	Excitation energies of terthiophene and its dioxide derivative: a first-principles study. Chemical Physics Letters, 2001, 339, 343-350.	1.2	50
47	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
48	Frozen density embedding with hybrid functionals. Journal of Chemical Physics, 2010, 133, 164111.	1.2	49
49	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
50	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
51	AlN and GaN epitaxial heterojunctions on 6Hâ€“SiC(0001): Valence band offsets and polarization fields. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1999, 17, 1674.	1.6	48
52	Absorption and luminescence spectra of electroluminescent liquid crystals with triphenylene, pyrene and perylene units. Liquid Crystals, 2001, 28, 1105-1113.	0.9	48
53	Photoluminescence Efficiency of Substituted Quaterthiophene Crystals. Physical Review Letters, 2001, 86, 167-170.	2.9	47
54	Density-functional calculations of NMR shielding constants using the localized Hartreeâ€“Fock method. Chemical Physics Letters, 2004, 383, 115-121.	1.2	47

#	Article	IF	Citations
55	Range separated functionals in the density functional based tightâ€binding method: Formalism. Physica Status Solidi (B): Basic Research, 2012, 249, 237-244.	0.7	47
56	Semilocal dynamical correlation with increased localization. Physical Review B, 2012, 86, .	1.1	45
57	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.	1.2	44
58	Optical properties of tetrapod-shaped CdTe nanocrystals. Applied Physics Letters, 2005, 87, 224101.	1.5	44
59	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
60	Well-width dependence of the ground level emission of GaN/AlGaN quantum wells. Journal of Applied Physics, 2000, 87, 2289-2292.	1.1	41
61	Dipole-excited surface plasmons in metallic nanoparticles: Engineering decay dynamics within the discrete-dipole approximation. Physical Review B, 2013, 87, .	1.1	41
62	Semilocal density functional theory with correct surface asymptotics. Physical Review B, 2016, 93, .	1.1	41
63	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
64	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. Physical Review B, 2013, 88, .	1.1	40
65	Enhanced fluorescence by metal nanospheres on metal substrates. Optics Letters, 2009, 34, 2381.	1.7	39
66	Experimental and Computational Studies on Non-Covalent Imprinted Microspheres as Recognition System for Nicotinamide Molecules. Molecules, 2009, 14, 2632-2649.	1.7	39
67	Correlation energy functional from jellium surface analysis. Physical Review B, 2011, 84, .	1.1	39
68	Excitonâ€“Plasmon Coupling Enhancement via Metal Oxidation. ACS Nano, 2015, 9, 9691-9699.	7.3	39
69	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.	1.2	38
70	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
71	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
72	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

#	Article	IF	Citations
73	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
74	Exchange-correlation generalized gradient approximation for gold nanostructures. Journal of Chemical Physics, 2011, 134, 194112.	1.2	34
75	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
76	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
77	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
78	The Kohnâ€“Sham treatment of anions via the localized Hartreeâ€“Fock method. Chemical Physics Letters, 2003, 372, 538-547.	1.2	31
79	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
80	Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory. Physical Review B, 2015, 91, .	1.1	31
81	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
82	First disubstituted dibenzothiophene-5,5-dioxide monodispersed molecular materials for efficient blue-electroluminescence. Journal of Materials Chemistry, 2010, 20, 1012-1018.	6.7	29
83	Laplacian-Level Quantum Hydrodynamic Theory for Plasmonics. Physical Review X, 2021, 11, .	2.8	29
84	Optical anisotropy of Langmuirâ€“Blodgett sapphyrin films. Applied Physics Letters, 2000, 77, 3164-3166.	1.5	28
85	Electrostatic-Field-Driven Alignment of Organic Oligomers on ZnO Surfaces. Physical Review Letters, 2011, 107, 146401.	2.9	28
86	Assessment of interaction-strength interpolation formulas for gold and silver clusters. Journal of Chemical Physics, 2018, 148, 134106.	1.2	28
87	Many-body effects on excitons properties in GaN/AlGaN quantum wells. Applied Physics Letters, 2000, 76, 1042-1044.	1.5	27
88	Multiconfiguration optimized effective potential method for a density-functional treatment of static correlation. Journal of Chemical Physics, 2008, 128, 144109.	1.2	27
89	Relationship between optical and structural properties in substituted quaterthiophene crystals. Applied Physics Letters, 1998, 73, 2414-2416.	1.5	26
90	Efficient methods to calculate dynamic hyperpolarizability tensors by time-dependent density-functional theory. Journal of Chemical Physics, 2002, 116, 9624-9640.	1.2	26

#	Article	IF	Citations
91	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
92	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
93	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
94	Jellium-with-gap model applied to semilocal kinetic functionals. Physical Review B, 2017, 95, .	1.1	26
95	Restoring Size Consistency of Approximate Functionals Constructed from the Adiabatic Connection. Journal of Physical Chemistry Letters, 2018, 9, 3137-3142.	2.1	26
96	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
97	Fluorineâ€“thiophene-substituted organic dyes for dye sensitized solar cells. Journal of Materials Chemistry A, 2013, 1, 11909.	5.2	25
98	A density difference based analysis of orbital-dependent exchange-correlation functionals. Molecular Physics, 2014, 112, 700-710.	0.8	25
99	Scanning tunneling current-voltage spectroscopy on poly(p-phenylene vinylene) films: A nanoscale probe for the electronic conduction. Physical Review B, 2001, 63, .	1.1	24
100	Ab initiodepolarization in self-assembled molecular monolayers: Beyond conventional density-functional theory. Physical Review B, 2009, 80, .	1.1	24
101	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
102	Plasmonic Nonlocal Response Effects on Dipole Decay Dynamics in the Weak- and Strong-Coupling Regimes. Journal of Physical Chemistry C, 2017, 121, 22361-22368.	1.5	24
103	Plasmonic quantum effects on single-emitter strong coupling. Nanophotonics, 2019, 8, 1821-1833.	2.9	24
104	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
105	Raman Spectra of Poly(pâ€phenylenevinylene)s with Fluorinated Vinylene Units: Evidence of Interâ€ring Distortion. ChemPhysChem, 2009, 10, 1284-1290.	1.0	23
106	Spin-dependent gradient correction for more accurate atomization energies of molecules. Journal of Chemical Physics, 2012, 137, 194105.	1.2	23
107	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. Journal of Chemical Theory and Computation, 2014, 10, 3151-3162.	2.3	23
108	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. Journal of Chemical Physics, 2015, 142, 154121.	1.2	23

#	Article	IF	Citations
109	Accuracy of basis-set extrapolation schemes for DFT-RPA correlation energies in molecular calculations. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	22
110	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
111	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
112	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
113	Density Functional Tight Binding for Quantum Plasmonics. Journal of Physical Chemistry C, 2018, 122, 19756-19766.	1.5	21
114	Orbitals from a self-interaction free Kohnâ€“Sham potential as a single electron basis for ab initio methods. Chemical Physics Letters, 2002, 360, 175-181.	1.2	20
115	Frozen density embedding calculations with the orbital-dependent localized Hartreeâ€“Fock Kohnâ€“Sham potential. Chemical Physics Letters, 2011, 518, 114-118.	1.2	20
116	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
117	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:r	1.1	20
118	Kinetic and Exchange Energy Densities near the Nucleus. Computation, 2016, 4, 19.	1.0	20
119	Bicolor Pixels from a Single Active Molecular Material by Surface-Tension-Driven Deposition. Advanced Materials, 2007, 19, 1597-1602.	11.1	19
120	Pure white hybrid light-emitting device with color rendering index higher than 90. Optics Letters, 2010, 35, 616.	1.7	19
121	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
122	Shaping White Light Through Electroluminescent Fully Organic Coupled Microcavities. Advanced Materials, 2010, 22, 4696-4700.	11.1	18
123	Semilocal and hybrid density embedding calculations of ground-state charge-transfer complexes. Journal of Chemical Physics, 2013, 138, 124112.	1.2	18
124	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.	1.2	17
125	Imaging Photoelectron Transmission through Self-Assembled Monolayers:Â The Work-Function of Alkanethiols Coated Gold. Langmuir, 2007, 23, 6156-6162.	1.6	17
126	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

#	Article	IF	Citations
127	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
128	Frozen density embedding with non-integer subsystemsâ€™ particle numbers. Journal of Chemical Physics, 2014, 140, 114101.	1.2	17
129	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
130	Bis-vinylogous Corrole: The First Expanded Corrole. Angewandte Chemie - International Edition, 1999, 38, 2577-2579.	7.2	16
131	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.	1.2	16
132	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
133	Emerging giant resonant exciton induced by Ta substitution in anataseTiO2: A tunable correlation effect. Physical Review B, 2016, 93, .	1.1	16
134	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.	3.8	15
135	Rydberg states with quantum Monte Carlo. Journal of Chemical Physics, 2006, 124, 114114.	1.2	15
136	Hartree potential dependent exchange functional. Journal of Chemical Physics, 2016, 145, 084110.	1.2	15
137	Optical properties of plasmonic core-shell nanomatryoshkas: a quantum hydrodynamic analysis. Optics Express, 2018, 26, 17322.	1.7	15
138	Noncovalent Interactions from Models for the MÃ¸llerâ€“Plesset Adiabatic Connection. Journal of Physical Chemistry Letters, 2021, 12, 4867-4875.	2.1	15
139	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.	1.2	14
140	Comparison of Simulation Methods for Organic Molecular Systems: Porphyrin Stacks. Physica Status Solidi (B): Basic Research, 2000, 217, 565-575.	0.7	13
141	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.	0.5	13
142	Monodispersed molecular donors for bulk hetero-junction solar cells: from molecular properties to device performances. Chemical Communications, 2010, 46, 6273.	2.2	13
143	Accurate singlet and triplet excitation energies using the Localized Hartreeâ€“Fock Kohnâ€“Sham potential. Chemical Physics, 2011, 391, 19-26.	0.9	13
144	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

#	Article	IF	Citations
145	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
146	Nanowireâ€Intensified Metalâ€Enhanced Fluorescence in Hybrid Polymerâ€Plasmonic Electrospun Filaments. Small, 2018, 14, e1800187.	5.2	13
147	The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development. Computation, 2019, 7, 65.	1.0	13
148	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
149	Rectification in Supramolecular Zinc Porphyrin/Fulleropyrrolidine Dyads Selfâ€Organized on Gold(111). ChemPhysChem, 2009, 10, 2633-2641.	1.0	12
150	Active Role of Oxide Layers on the Polarization of Plasmonic Nanostructures. ACS Nano, 2010, 4, 4117-4125.	7.3	12
151	Observation and control of coherent torsional dynamics in a quinquethiophene molecule. Physical Chemistry Chemical Physics, 2010, 12, 7917.	1.3	12
152	Electrostatic Mechanophores in Tuneable Lightâ€Emitting Piezopolymer Nanowires. Advanced Materials, 2017, 29, 1701031.	11.1	12
153	Ab initiostructural and electronic analysis ofCH3SHself-assembled on a Cu(110) substrate. Physical Review B, 2007, 75, .	1.1	11
154	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
155	Dipole Decay Rates Engineering via Silver Nanocones. Plasmonics, 2013, 8, 1079-1086.	1.8	11
156	Optical properties of functionalized thiophenes: a theoretical and experimental study. Synthetic Metals, 2003, 139, 897-899.	2.1	10
157	Effects of intermolecular interactions on photoluminescence efficiency of crystalline thienylene-S,S-dioxide molecular semiconductors. Organic Electronics, 2004, 5, 129-134.	1.4	10
158	Theoretical study on oligothiophene N-succinimidyl esters: size and pushâ€“pull effects. Physical Chemistry Chemical Physics, 2008, 10, 5363.	1.3	10
159	Structural and electronic properties of gold microclusters: assessment of the localized Hartreeâ€“Fock method. Physical Chemistry Chemical Physics, 2009, 11, 9160.	1.3	10
160	Assessment of the TCA functional in computational chemistry and solid-state physics. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	10
161	Ab Initio Plasmonics of Externally Doped Silicon Nanocrystals. ACS Photonics, 2019, 6, 1474-1484.	3.2	10
162	Type II transition in InSb-based nanostructures for midinfrared applications. Journal of Applied Physics, 2008, 103, 114516.	1.1	9

#	Article	IF	Citations
163	Plasmon Couplings from Subsystem Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2021, 125, 7246-7259.	1.1	9
164	Analysis of the Quality of Kohnâ€“Sham Orbitals for Subsequent MRSD-CI Calculations of Excitation Energies. Zeitschrift Fur Physikalische Chemie, 2003, 217, 133-160.	1.4	8
165	Zinc Porphyrinâ€Driven Assembly of Gold Nanofingers. Small, 2008, 4, 497-506.	5.2	8
166	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.	0.9	8
167	Orbital-dependent exact-exchange methods in density functional theory. Chemical Modelling, 0, , 115-161.	0.2	7
168	Kinetic Energy Density Functionals Based on a Generalized Screened Coulomb Potential: Linear Response and Future Perspectives. Computation, 2022, 10, 30.	1.0	7
169	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
170	Entanglement of electrons in interacting molecules. Theoretical and Mathematical Physics(Russian) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.3	6
171	Accurate non-covalent interaction energies via an efficient MP2 scaling procedure. Chemical Physics Letters, 2015, 635, 262-267.	1.2	6
172	Atomistic investigation of hybrid plasmonic systems. Nanomaterials and Nanotechnology, 2019, 9, 184798041985653.	1.2	6
173	Evidence for an internal field in CdSe/CdS nanorods by time resolved and single rod experiments. Superlattices and Microstructures, 2010, 47, 174-177.	1.4	5
174	Carrier screening and polarization fields in nitride-based heterostructure devices. Physica B: Condensed Matter, 1999, 272, 397-401.	1.3	3
175	The effects of oxygen and boron functionalization on the optical properties of dithienothiophenes. Journal of Non-Crystalline Solids, 2006, 352, 2461-2464.	1.5	3
176	First principles optical spectra of theÎ²-SiC(0â€‰0â€‰1)/Al interface. Journal of Physics Condensed Matter, 2014, 26, 265006.	0.7	3
177	Perturbations of Dipole Decay Dynamics Induced by Plasmonic Nano-Antennas â€” A Study within the Discrete Dipole Approximation. Nanomaterials and Nanotechnology, 2015, 5, 11.	1.2	3
178	Optical and Transport Properties of GaN/Al0.15Ga0.85N Quantum Wells. Physica Status Solidi A, 2000, 178, 73-78.	1.7	2
179	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, .	1.1	2
180	Development of an artificial nose integrating NEMS and biological olfactory receptors. , 0, , .		2

#	Article	IF	Citations
181	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.	1.4	2
182	A periodic charge-dipole electrostatic model: Parametrization for silver slabs. Journal of Chemical Physics, 2012, 137, 134702.	1.2	2
183	Characterization of TiO2 atomic crystals for nanocomposite materials oriented to optoelectronics. Optical and Quantum Electronics, 2012, 44, 291-296.	1.5	2
184	Radiative coupling of high-order plasmonic modes with far-field. Photonics and Nanostructures - Fundamentals and Applications, 2013, 11, 335-344.	1.0	2
185	A periodic charge-dipole electrostatic model. II. A kinetic-exchange-correlation correction. Journal of Chemical Physics, 2013, 139, 144109.	1.2	2
186	Enhancement of radiative processes in nanofibers with embedded plasmonic nanoparticles. Optics Letters, 2016, 41, 1632.	1.7	2
187	Boosting the OEP2-sc method with spin-component scaling. Molecular Physics, 2022, 120, .	0.8	2
188	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
189	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.	1.2	1
190	Anab initiostudy of the magneticâ€“metallic CoPt₃â€“Au interfaces. Journal of Physics Condensed Matter, 2009, 21, 015001.	0.7	1
191	Dipole decay rates engineering via metallic nanosystems. , 2012, , .		1
192	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	1
193	Influence of Internal Electric Fields on the Ground Level Emission of GaN/AlGaN Multi-Quantum Wells. Materials Research Society Symposia Proceedings, 1999, 595, 1.	0.1	0
194	Microscopic Modeling of GaN-based Heterostructures. VLSI Design, 2001, 13, 387-391.	0.5	0
195	Role of surface and interface defects in ultrafast carrier dynamics in core and core/shell CdSe quantum rods. , 0, , .		0
196	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
197	Fabrication of Molecular Micro-NanoStructures by Surface-Tension-Driven Technique. Materials Research Society Symposia Proceedings, 2007, 1002, 1.	0.1	0
198	Bright OligothiopheneN-Succinimidyl Esters for Efficient Fluorescent Labeling of Proteins and Oligonucleotides. Bioconjugate Chemistry, 2007, 18, 1015-1015.	1.8	0

#	Article	IF	Citations
199	Ultrafast electron-hole dynamics and optical gain in CdSe/CdS nanorods. , 2009, , .		0
200	Ultrafast electron-hole dynamics in core/shell CdSe/CdS dot/rod nanocrystals. , 2009, , .		0
201	Plasmonic luminescence enhancement by metal nanoparticles embedded in nanofibers. , 2016, , .		0
202	Nonlocal plasmonic effects on dipole decay dynamics in the weak and strong coupling regimes. , 2017, , .		0
203	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
204	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