A long-range correction scheme for generalized-gradient-approximation exchange functionals

DOI: 10.1063/1.1383587
Journal of Chemical Physics, 2001, 115, 3540-3544.

#	Paper	IF	Citations
1989	Elucidating Batch-to-Batch Variation Caused by Homocoupled Side Products in Solution-Processable Organic Solar Cells.		
1988	Shedding Light on the Basis Set Dependence of the Minnesota Functionals: Differences Between Plane Waves, Slater Functions, and Gaussians.		
1987	Cross-Comparisons between Experiment, TD-DFT, CC and ADC for Transition Energies.		
1986	Selenium Substitution Enhances Reverse Intersystem Crossing in a Delayed Fluorescence Emitter.		
1985	Mapping Long-Lived Dark States in Copper Porphyrin Nanostructures.		
1984	Manganese(II) Molecular Sources for Plasma-Assisted CVD of Mn Oxides and Fluorides: From Precursors to Growth Process.		
1983	Band Alignment in Two-Dimensional Halide Perovskite Heterostructures: Type I or Type II?.		
1982	Electronic Levels of Excess Electrons in Liquid Water.		
1981	Self-Interaction Error in Density Functional Theory: An Appraisal.		
1980	The Sodium Anion Is Strongly Perturbed in the Condensed Phase Even Though It Appears Like a Free Ion in Nuclear Magnetic Resonance Experiments.		
1979	Doubly NMethylated Porphyrinoids.		
1978	On-Surface Synthesis of Antiaromatic and Open-Shell Indeno[2,1b]fluorene Polymers and Their Lateral Fusion into Porous Ribbons.		
1977	.		
1976	Computational Protocol for Precise Prediction of Dye-Sensitized Solar Cell Performance.		
1975	Coupling to Charge Transfer States is the Key to Modulate the Optical Bands for Efficient Light Harvesting in Purple Bacteria.		
1974	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules.		
1973	Charge Transfer Excitations with Range Separated Functionals Using Improved Virtual Orbitals.		

1972	RECENT ADVANCES IN ELECTRONIC STRUCTURE THEORY. **2002**, 01, 109-136		6
1971	A density functional study of van der Waals interactions. *Journal of Chemical Physics*, **2002**, 117, 6010-6015	3.9	245
1970	Hybrid functionals based on a screened Coulomb potential. *Journal of Chemical Physics*, **2003**, 118, 8207-8215	3.9	10573
1969	Local hybrid functionals. *Journal of Chemical Physics*, **2003**, 118, 1068-1073	3.9	255
1968	UTChem A Program for ab initio Quantum Chemistry. **2003**, 84-95		22
1967	Theoretical studies on effective exchange integrals using spin correlation function analysis and magnetic effective density functional (MEDF) method. *International Journal of Quantum Chemistry*, **2004**, 100, 927-936	2.1	3
1966	A new hybrid exchange correlation functional using the Coulomb-attenuating method (CAM-B3LYP). **2004**, 393, 51-57		9128
1965	The molecular physics lecture 2004: (i) Density functional theory, (ii) Quantum Monte Carlo. **2004**, 102, 2399-2409		31
1964	Electrical response of molecular chains from density functional theory. **2004**, 93, 213002		133
1963	Long-range short-range separation of the electron-electron interaction in density-functional theory. **2004**, 70,		344
1962	Assessment and validation of a screened Coulomb hybrid density functional. *Journal of Chemical Physics*, **2004**, 120, 7274-80	3.9	569
1961	A long-range-corrected time-dependent density functional theory. *Journal of Chemical Physics*, **2004**, 120, 8425-33	3.9	1512
1960	Efficient hybrid density functional calculations in solids: assessment of the Heyd-Scuseria-Ernzerhof screened Coulomb hybrid functional. *Journal of Chemical Physics*, **2004**, 121, 1187-92	3.9	1520
1959	Theoretical methods that help understanding the structure and reactivity of gas phase ions. **2005**, 240, 37-99		95
1958	Theoretical investigation of adsorption of organic molecules onto Fe(110) surface. **2005**, 716, 45-60		20
1957	Hybrid functional with separated range. **2005**, 415, 100-105		227
1956	Single-reference ab initio methods for the calculation of excited states of large molecules. **2005**, 105, 4009-37		2042
1955	A CSOV study of the difference between HF and DFT intermolecular interaction energy values: the importance of the charge transfer contribution. *Journal of Computational Chemistry*, **2005**, 26, 1052-62	3.5	95

1954	Recent advances in ab initio, density functional theory, and relativistic electronic structure theory. **2005**, 507-557		13
1953	Density functional theory with correct long-range asymptotic behavior. **2005**, 94, 043002		338
1952	Influence of the long-range exchange effect on dynamic polarizability. **2005**, 103, 2183-2189		42
1951	A density-functional study on pi-aromatic interaction: benzene dimer and naphthalene dimer. *Journal of Chemical Physics*, **2005**, 123, 104307	3.9	167
1950	Progress in the development of exchange-correlation functionals. **2005**, 669-724		96
1949	Multiresolution quantum chemistry in multiwavelet bases: time-dependent density functional theory with asymptotically corrected potentials in local density and generalized gradient approximations. **2005**, 103, 413-424		105
1948	Van der Waals interactions studied by density functional theory. **2005**, 103, 1151-1164		105
1947	Time-dependent density functional theory investigation of electric field effects on absorption spectra of meso-meso-linked zinc porphyrin arrays: Role of charge-transfer States. **2005**, 109, 13921-7		6
1946	van der Waals forces in density functional theory: Perturbational long-range electron-interaction corrections. **2005**, 72,		265
1945	Nonlinear optical property calculations by the long-range-corrected coupled-perturbed Kohn-Sham method. *Journal of Chemical Physics*, **2005**, 122, 234111	3.9	261
1944	Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. *Journal of Chemical Physics*, **2005**, 123, 174101	3.9	1306
1943	Simple model of the static exchange-correlation kernel of a uniform electron gas with long-range electron-electron interaction. **2005**, 72,		15
1942	Semiempirical hybrid functional with improved performance in an extensive chemical assessment. *Journal of Chemical Physics*, **2005**, 123, 121103	3.9	126
1941	Efficient evaluation of short-range Hartree-Fock exchange in large molecules and periodic systems. *Journal of Chemical Physics*, **2006**, 125, 104103	3.9	174
1940	Importance of short-range versus long-range Hartree-Fock exchange for the performance of hybrid density functionals. *Journal of Chemical Physics*, **2006**, 125, 074106	3.9	747
1939	Influence of Coulomb-attenuation on exchange-correlation functional quality. **2006**, 8, 4543-9		124
1938	Many-electron self-interaction error in approximate density functionals. *Journal of Chemical Physics* , **2006**, 125, 201102	3.9	547
1937	Computing counterion densities at intermediate coupling. **2006**, 73, 041512		75

1936	Assessment of a long-range corrected hybrid functional. *Journal of Chemical Physics*, **2006**, 125, 234109	3.9	1356
1935	On the accuracy of density functional theory in transition metal chemistry. **2006**, 102, 203		258
1934	Assessment of a Coulomb-attenuated exchange-correlation energy functional. **2006**, 8, 558-62		418
1933	Electronic excited states of Si(100) and organic molecules adsorbed on Si(100). **2006**, 110, 1701-10		24
1932	Characterization of cationic diarylethene by electron spin resonance and absorption spectra-ratio of open/closed-ring isomers. *Journal of Physical Chemistry A*, **2006**, 110, 8137-43	2.8	35
1931	Excited state geometry optimizations by analytical energy gradient of long-range corrected time-dependent density functional theory. *Journal of Chemical Physics*, **2006**, 124, 144106	3.9	188
1930	Scaling relations, virial theorem, and energy densities for long-range and short-range density functionals. *International Journal of Quantum Chemistry*, **2006**, 106, 2026-2034	2.1	21
1929	Local density approximation for long-range or for short-range energy functionals?. **2006**, 762, 147-150		24
1928	The SCC-DFTB method and its application to biological systems. **2006**, 116, 316-325		296
1927	Avoiding self-repulsion in density functional description of biased molecular junctions. **2006**, 329, 266-275		29
1926	Quantum chemical methods for the investigation of photoinitiated processes in biological systems: theory and applications. *ChemPhysChem*, **2006**, 7, 2259-74	3.2	66
1925	Theoretical studies of molecular scale near-field electron dynamics. *Journal of Chemical Physics*, **2006**, 125, 074709	3.9	8
1924	Properties of short-range and long-range correlation energy density functionals from electron-electron coalescence. **2006**, 73,		53
1923	Exact-exchange time-dependent density-functional theory with the frequency-dependent kernel. **2006**, 73,		29
1922	A study of the ground state of manganese dimer using quasidegenerate perturbation theory. *Journal of Chemical Physics*, **2006**, 124, 124302	3.9	46
1921	Local-spin-density functional for multideterminant density functional theory. **2006**, 73,		88
1920	LONG-RANGE-CORRECTED TIME-DEPENDENT DENSITY FUNCTIONAL STUDY ON ELECTRONIC SPECTRA OF FIVE-MEMBERED RING COMPOUNDS AND FREE-BASE PORPHYRIN. **2006**, 05, 925-944		11
1919	The use of atomic intrinsic polarizabilities in the evaluation of the dispersion energy. *Journal of Chemical Physics*, **2007**, 127, 224105	3.9	30

1918	First hyperpolarizability of polymethineimine with long-range corrected functionals. *Journal of Chemical Physics*, **2007**, 126, 191108	3.9	151
1917	Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. *Journal of Chemical Physics*, **2007**, 127, 054101	3.9	86
1916	The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. *Journal of Chemical Physics*, **2007**, 127, 221103	3.9	139
1915	On the performance of local, semilocal, and nonlocal exchange-correlation functionals on transition metal molecules. *Journal of Chemical Physics*, **2007**, 126, 224105	3.9	6
1914	Local hybrid functionals based on density matrix products. *Journal of Chemical Physics*, **2007**, 127, 164117	3.9	53
1913	Assessment of long-range corrected functionals performance for n-->pi* transitions in organic dyes. *Journal of Chemical Physics*, **2007**, 127, 094102	3.9	112
1912	Evaluation of in density functional theory. *Journal of Chemical Physics*, **2007**, 126, 214104	3.9	83
1911	Double-hybrid density functional theory for excited electronic states of molecules. *Journal of Chemical Physics*, **2007**, 127, 154116	3.9	339
1910	Assessment of the exchange-correlation functionals for the physical description of spin transition phenomena by density functional theory methods: all the same?. *Journal of Chemical Physics*, **2007**, 126, 014105	3.9	97
1909	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. *Journal of Chemical Physics*, **2007**, 126, 144105	3.9	264
1908	A well-tempered density functional theory of electrons in molecules. **2007**, 9, 2932-41		321
1907	Long-range corrected density functional calculations of chemical reactions: redetermination of parameter. *Journal of Chemical Physics*, **2007**, 126, 154105	3.9	258
1906	Polarizability and second hyperpolarizability evaluation of long molecules by the density functional theory with long-range correction. *Journal of Chemical Physics*, **2007**, 126, 014107	3.9	176
1905	Predicting noncovalent interactions between aromatic biomolecules with London-dispersion-corrected DFT. **2007**, 111, 14346-54		61
1904	Theoretical study on the second hyperpolarizabilities of phenalenyl radical systems involving acetylene and vinylene linkers: diradical character and spin multiplicity dependences. *Journal of Physical Chemistry A*, **2007**, 111, 3633-41	2.8	80
1903	Structural and electronic properties of polyacetylene and polyyne from hybrid and Coulomb-attenuated density functionals. *Journal of Physical Chemistry A*, **2007**, 111, 11930-5	2.8	124
1902	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. *Journal of Chemical Physics*, **2007**, 126, 074111	3.9	151
1901	Long-range corrected time-dependent density functional study on fluorescence of 4,4'-dimethylaminobenzonitrile. *Journal of Chemical Physics*, **2007**, 126, 034504	3.9	33

1900	Tests of functionals for systems with fractional electron number. *Journal of Chemical Physics*, **2007**, 126, 154109	3.9	503
1899	An improved long-range corrected hybrid exchange-correlation functional including a short-range Gaussian attenuation (LCgau-BOP). *Journal of Chemical Physics*, **2007**, 127, 154109	3.9	102
1898	A self-contained and portable density functional theory library for use in Ab Initio quantum chemistry programs. *Journal of Computational Chemistry*, **2007**, 28, 2569-75	3.5	17
1897	NLO responses of small polymethineimine oligomers: A CCSD(T) study. **2007**, 821, 160-165		6
1896	Anharmonic vibrational state calculations in the electronic excited states studied by time-dependent density functional theory. **2007**, 436, 30-35		11
1895	Time-dependent density functional theory with the multilayer fragment molecular orbital method. **2007**, 444, 346-350		59
1894	Density functional study of manganese dimer. *International Journal of Quantum Chemistry*, **2007**, 107, 3178-3190	2.1	20
1893	Time-dependent density functional theory based upon the fragment molecular orbital method. *Journal of Chemical Physics*, **2007**, 127, 104108	3.9	85
1892	Ab Initio Study of Compressed 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane (HMX), Cyclotrimethylenetrinitramine (RDX), 2,4,6,8,10,12-Hexanitrohexaazaisowurzitane (CL-20), 2,4,6-Trinitro-1,3,5-benzenetriamine (TATB), and Pentaerythritol Tetranitrate (PETN). **2007**, 111, 2787-2796		136
1891	Long-range corrected density functional study on weakly bound systems: balanced descriptions of various types of molecular interactions. *Journal of Chemical Physics*, **2007**, 126, 234114	3.9	133
1890	Development of exchange-correlation functionals with minimal many-electron self-interaction error. *Journal of Chemical Physics*, **2007**, 126, 191109	3.9	268
1889	The localized Hartree–Fock method for a self-interaction free Kohn–Sham potential: applications to closed and open-shell molecules. **2007**, 117, 981-989		12
1888	A quantum mechanical polarizable continuum model for the calculation of resonance Raman spectra in condensed phase. **2007**, 117, 1029-1039		41
1887	Hybrid exchange correlation functionals and potentials: Concept elaboration. **2007**, 48, S1-S31		33
1886	The use of Coulomb-attenuated methods for the calculation of electronic circular dichroism spectra. **2008**, 349, 234-243		38
1885	An IEF-PCM study of solvent effects on the Faraday ({mathcal{B}}) term of MCD. **2008**, 119, 231-244		28
1884	Theoretical study on the nonlinear optical properties of phenylenes and influencing factors. **2008**, 21, 954-962		17
1883	Static and frequency-dependent dipole-dipole polarizabilities of all closed-shell atoms up to radium: a four-component relativistic DFT study. *ChemPhysChem*, **2008**, 9, 445-53	3.2	26

1882	Revisiting the relationship between the bond length alternation and the first hyperpolarizability with range-separated hybrid functionals. *Journal of Computational Chemistry*, **2008**, 29, 921-5	3.5	27
1881	A dual-level state-specific time-dependent density-functional theory. *Journal of Computational Chemistry*, **2008**, 29, 1187-97	3.5	11
1880	Polarizable continuum model with the fragment molecular orbital-based time-dependent density functional theory. *Journal of Computational Chemistry*, **2008**, 29, 2667-76	3.5	48
1879	Revisiting the nonlinear optical properties of polybutatriene and polydiacetylene with density functional theory. **2008**, 456, 101-104		22
1878	Range-separation by the Yukawa potential in long-range corrected density functional theory with Gaussian-type basis functions. **2008**, 462, 348-351		53
1877	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. **2008**, 465, 226-229		88
1876	Optimal operators for Hartree□Fock exchange from long-range corrected hybrid density functionals. **2008**, 467, 176-178		61
1875	Orbital-dependent density functionals: Theory and applications. **2008**, 80, 3-60		941
1874	Simultaneous benchmarking of ground- and excited-state properties with long-range-corrected density functional theory. *Journal of Chemical Physics*, **2008**, 129, 034107	3.9	249
1873	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. *Journal of Chemical Theory and Computation*, **2008**, 4, 123-35	6.4	681
1872	Excitation energies in density functional theory: an evaluation and a diagnostic test. *Journal of Chemical Physics*, **2008**, 128, 044118	3.9	1066
1871	Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. **2008**, 10, 6615-20		7709
1870	Charge-transfer excited states in a pi-stacked adenine dimer, as predicted using long-range-corrected time-dependent density functional theory. **2008**, 112, 6304-8		150
1869	Equilibrium Molecular Dynamics Simulations. **2009**, 255-290		9
1868	Hartree-Fock and Kohn-Sham time-dependent response theory in a second-quantization atomic-orbital formalism suitable for linear scaling. *Journal of Chemical Physics*, **2008**, 129, 054106	3.9	41
1867	Electrical response of molecular chains in density functional theory: Ultranonlocal response from a semilocal functional. **2008**, 77,		55
1866	Coumarin dyes for dye-sensitized solar cells: A long-range-corrected density functional study. *Journal of Chemical Physics*, **2008**, 129, 214703	3.9	152
1865	Generalized gradient approximation model exchange holes for range-separated hybrids. *Journal of Chemical Physics*, **2008**, 128, 194105	3.9	200

1864	Calculation of electric dipole (hyper)polarizabilities by long-range-correction scheme in density functional theory: a systematic assessment for polydiacetylene and polybutatriene oligomers. *Journal of Chemical Physics*, **2008**, 128, 114108	3.9	107
1863	Interactions in large, polyaromatic hydrocarbon dimers: application of density functional theory with dispersion corrections. *Journal of Physical Chemistry A*, **2008**, 112, 10968-76	2.8	131
1862	Core-excitation energy calculations with a long-range corrected hybrid exchange-correlation functional including a short-range Gaussian attenuation (LCgau-BOP). *Journal of Chemical Physics*, **2008**, 129, 184113	3.9	62
1861	Evaluation of range-separated hybrid density functionals for the prediction of vibrational frequencies, infrared intensities, and Raman activities. **2008**, 10, 6621-9		79
1860	Systematic optimization of long-range corrected hybrid density functionals. *Journal of Chemical Physics*, **2008**, 128, 084106	3.9	2290
1859	Nonlinear optical property calculations of polyynes with long-range corrected hybrid exchange-correlation functionals. *Journal of Chemical Physics*, **2008**, 129, 024117	3.9	59
1858	Intracule densities in the strong-interaction limit of density functional theory. **2008**, 10, 3440-6		14
1857	Polarizability of molecular chains: A self-interaction correction approach. **2008**, 77,		53
1856	Range separation and local hybridization in density functional theory. *Journal of Physical Chemistry A*, **2008**, 112, 12530-42	2.8	81
1855	Development of a finite-temperature density functional approach to electrochemical reactions. *Journal of Physical Chemistry A*, **2008**, 112, 10681-8	2.8	12
1854	A study of the effect of attenuation curvature on molecular correlation energies by introducing an explicit cutoff radius into two-electron integrals. *Journal of Physical Chemistry A*, **2008**, 112, 2110-9	2.8	19
1853	Structural origin of copper ion containing artificial DNA: a density functional study. **2008**, 112, 16960-5		12
1852	A density functional theory for symmetric radical cations from bonding to dissociation. *Journal of Physical Chemistry A*, **2008**, 112, 12789-91	2.8	45
1851	Relativistic model core potential study of the Au+ Xe system. *Journal of Physical Chemistry A*, **2008**, 112, 5236-42	2.8	21
1850	Charge-Transfer Properties of Dye-Sensitized Solar Cells via Long-Range-Corrected Density Functional Theory. **2008**, 1120, 103		2
1849	Assessment of a Middle-Range Hybrid Functional. *Journal of Chemical Theory and Computation*, **2008**, 4, 1254-62	6.4	135
1848	Performance of DFT Methods in the Calculation of Optical Spectra of Chromophores. **2008**,		1
1847	Water cluster anions studied by the long-range corrected density functional theory. *Journal of Physical Chemistry A*, **2008**, 112, 9845-53	2.8	34

1846	Single-Reference Methods for Excited States in Molecules and Polymers. **2008**, 15-64		7
1845	Reliability of range-separated hybrid functionals for describing magnetic coupling in molecular systems. *Journal of Chemical Physics*, **2008**, 129, 184110	3.9	73
1844	Spectroscopic tracking of structural evolution in ultrafast stilbene photoisomerization. **2008**, 322, 1073-7		173
1843	What can we learn from the adiabatic connection formalism about local hybrid functionals?. *Journal of Chemical Physics*, **2008**, 128, 214107	3.9	43
1842	A generalized Poisson equation and short-range self-interaction energies. *Journal of Chemical Physics*, **2008**, 128, 241101	3.9	3
1841	Hybrid functionals with local range separation. *Journal of Chemical Physics*, **2008**, 129, 124103	3.9	113
1840	Self-consistent generalized Kohn-Sham local hybrid functionals of screened exchange: Combining local and range-separated hybridization. *Journal of Chemical Physics*, **2008**, 129, 124110	3.9	59
1839	Hartree-Fock orbitals significantly improve the reaction barrier heights predicted by semilocal density functionals. *Journal of Chemical Physics*, **2008**, 128, 244112	3.9	69
1838	Adsorption and bonding mechanism of a N,N?-di(n-butyl)quinacridone monolayer studied by density functional theory including semiempirical dispersion corrections. **2008**, 78,		3
1837	Accurate density functional calculations of near-edge x-ray and optical absorption spectra of liquid water using nonperiodic boundary conditions: the role of self-interaction and long-range effects. **2008**, 100, 107401		42
1836	Parameterized local hybrid functionals from density-matrix similarity metrics. *Journal of Chemical Physics*, **2008**, 128, 084111	3.9	41
1835	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. II. Investigating f0 actinide species. *Journal of Chemical Physics*, **2009**, 131, 054107	3.9	43
1834	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	3.9	23
1833	Assessment of double-hybrid energy functionals for pi-conjugated systems. *Journal of Chemical Physics*, **2009**, 131, 084108	3.9	70
1832	On the self-consistent implementation of general occupied-orbital dependent exchange-correlation functionals with application to the B05 functional. *Journal of Chemical Physics* , **2009**, 131, 084103	3.9	24
1831	Density functional method including weak interactions: Dispersion coefficients based on the local response approximation. *Journal of Chemical Physics*, **2009**, 131, 224104	3.9	188
1830	Long-range-corrected hybrid density functionals including random phase approximation correlation: application to noncovalent interactions. *Journal of Chemical Physics*, **2009**, 131, 034110	3.9	78
1829	Adiabatic-connection fluctuation-dissipation density-functional theory based on range separation. **2009**, 102, 096404		222

1828	Combined experimental and quantum chemical investigation of chiroptical properties of nicotinamide derivatives with and without intramolecular cation-pi interactions. *Journal of Physical Chemistry A*, **2009**, 113, 8754-64	2.8	31
1827	Approximate Density Functionals: Which Should I Choose?. **2009**,		14
1826	A systematic analysis of the structure and (hyper)polarizability of donor-acceptor substituted polyacetylenes using a Coulomb-attenuating density functional. *Journal of Chemical Physics*, **2009**, 131, 124105	3.9	33
1825	Local hybrids as a perturbation to global hybrid functionals. *Journal of Chemical Physics*, **2009**, 131, 154112	3.9	30
1824	The role of the reference state in long-range random phase approximation correlation. *Journal of Chemical Physics*, **2009**, 131, 154106	3.9	28
1823	The static-exchange electron-water pseudopotential, in conjunction with a polarizable water model: a new Hamiltonian for hydrated-electron simulations. *Journal of Chemical Physics*, **2009**, 130, 124115	3.9	44
1822	Structure versus solvent effects on nonlinear optical properties of push-pull systems: a quantum-mechanical study based on a polarizable continuum model. *Journal of Physical Chemistry A* , **2009**, 113, 14774-84	2.8	28
1821	A new hybrid DFT approach to electronic excitation and first hyperpolarizabilities of transition metal complexes. *Journal of Computational Chemistry*, **2009**, 30, 2056-63	3.5	27
1820	Modified regional self-interaction corrected time-dependent density functional theory for core excited-state calculations. *Journal of Computational Chemistry*, **2009**, 30, 2583-93	3.5	5
1819	Linear and nonlinear optical properties of azobenzene derivatives. *Journal of Molecular Modeling*, **2009**, 15, 581-90	2	21
1818	Reinvestigation of electronic structure and electric properties of large betaine molecules: A combined long-range-corrected DFT and coupled-cluster study. **2009**, 480, 37-40		5
1817	Testing the performance of density functionals for the calculation of energetic properties of complex-forming radical-molecule reactions. **2009**, 96, 233-244		4
1816	Intramolecular charge-transfer excitation energies from range-separated hybrid functionals using the Yukawa potential. *International Journal of Quantum Chemistry*, **2009**, 109, 1905-1914	2.1	28
1815	Rydberg states of the helium atom. *International Journal of Quantum Chemistry*, **2009**, 109, 1915-1919	2.1	10
1814	The effect of silyl and phenyl functional group end caps on the nonlinear optical properties of polyynes: A long-range corrected density functional theory study. *International Journal of Quantum Chemistry*, **2009**, 109, 2012-2022	2.1	16
1813	Range separation combined with the Overhauser model: Application to the H2 molecule along the dissociation curve. *International Journal of Quantum Chemistry*, **2009**, 109, 1950-1961	2.1	8
1812	Locally range-separated hybrids as linear combinations of range-separated local hybrids. *International Journal of Quantum Chemistry*, **2009**, 109, 2023-2032	2.1	25
1811	Polarizabilities and second hyperpolarizabilities of hydrogen chains using the spin-component-scaled M□ller□Plesset second-order method. *International Journal of Quantum Chemistry*, **2009**, 109, 3103-3111	2.1	21

1810	TD-DFT benchmark for indigo□□d dyes. **2009**, 914, 100-105		32
1809	Illustration of a TDDFT spatial overlap diagnostic by basis function exponent scaling. **2009**, 914, 110-114		35
1808	Static electronic and vibrational first hyperpolarizability of meta-dinitrobenzene as studied by quantum chemical calculations. **2009**, 907, 46-50		31
1807	Is size-consistency possible with density functional approximations?. **2009**, 356, 91-97		39
1806	Excited state geometry optimizations by time-dependent density functional theory based on the fragment molecular orbital method. **2009**, 474, 227-232		30
1805	Electron donor solvent effects on the (hyper)polarizabilities of a singlet diradical molecule involving a boron atom. **2009**, 477, 309-314		9
1804	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. **2009** , 478, 283-286		9
1803	Sequence-dependent proton-transfer reaction in stacked GC pair II: The origin of stabilities of proton-transfer products. **2009**, 478, 238-242		20
1802	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. *Journal of Chemical Theory and Computation*, **2009**, 5, 2420-35	6.4	799
1801	A long-range-corrected density functional that performs well for both ground-state properties and time-dependent density functional theory excitation energies, including charge-transfer excited states. *Journal of Chemical Physics*, **2009**, 130, 054112	3.9	478
1800	Performance of DFT Methods in the Calculation of Optical Spectra of TCF-Chromophores. *Journal of Chemical Theory and Computation*, **2009**, 5, 2835-46	6.4	50
1799	Accurate simulation of optical properties in dyes. **2009**, 42, 326-34		404
1798	Theoretical studies on sulfur and metal cation (Cu(II), Ni(II), Pd(II), and Pt(II))-containing artificial DNA. **2009**, 113, 12790-5		8
1797	Electronic Zero-Point Oscillations in the Strong-Interaction Limit of Density Functional Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 743-53	6.4	61
1796	Theoretical Study of Dispersion Binding of Hydrocarbon Molecules to Hydrogen-Terminated Silicon(100)-2□□1. **2009**, 113, 5681-5689		24
1795	Toward a combined DFT/QTAIM description of agostic bonds: the critical case of a Nb(III) complex. *Journal of Physical Chemistry A*, **2009**, 113, 12322-7	2.8	30
1794	Excited states of DNA base pairs using long-range corrected time-dependent density functional theory. *Journal of Physical Chemistry A*, **2009**, 113, 9761-5	2.8	63
1793	Hydrates of copper dichloride in aqueous solution: a density functional theory and polarized continuum model investigation. *Journal of Physical Chemistry A*, **2009**, 113, 14029-38	2.8	19

1792	Local hybrid functionals with an explicit dependence on spin polarization. *Journal of Physical Chemistry A*, **2009**, 113, 11898-906	2.8	41
1791	Both intra- and interstrand charge-transfer excited states in aqueous B-DNA are present at energies comparable to, or just above, the (1)pipi* excitonic bright states. **2009**, 131, 3913-22		168
1790	Optoelectronic Properties of Carbon Nanorings: Excitonic Effects from Time-Dependent Density Functional Theory. **2009**, 113, 21921-21927		122
1789	Electronic hyperpolarizabilities for donor-acceptor molecules with long conjugated bridges: calculations versus experiment. *Journal of Physical Chemistry A*, **2009**, 113, 10994-1001	2.8	119
1788	Nature of low-lying excited states in H-aggregated perylene bisimide dyes: results of TD-LRC-DFT and the mixed exciton model. **2009**, 113, 14581-7		29
1787	Deleterious effects of long-range self-repulsion on the density functional description of O2 sticking on aluminum. *Journal of Physical Chemistry A*, **2009**, 113, 7521-7	2.8	26
1786	Binding in thiophene and benzothiophene dimers investigated by density functional theory with dispersion-correcting potentials. *Journal of Physical Chemistry A*, **2009**, 113, 5476-84	2.8	20
1785	Pentacene Binds Strongly to Hydrogen-Terminated Silicon Surfaces Via Dispersion Interactions. **2009**, 113, 9969-9973		12
1784	Long-Range-Corrected Hybrids Based on a New Model Exchange Hole. *Journal of Chemical Theory and Computation*, **2009**, 5, 754-62	6.4	58
1783	Linear and nonlinear optical properties of [60]fullerene derivatives. *Journal of Physical Chemistry A*, **2009**, 113, 1159-70	2.8	98
1782	Evaluation of range-separated hybrid and other density functional approaches on test sets relevant for transition metal-based homogeneous catalysts. *Journal of Physical Chemistry A*, **2009**, 113, 11742-9	2.8	48
1781	Accurate interaction energies at density functional theory level by means of an efficient dispersion correction. *Journal of Chemical Physics*, **2009**, 130, 174101	3.9	40
1780	Third-order nonlinear optical properties of open-shell singlet molecular aggregates composed of diphenalenyl diradicals. **2009**, 159, 2413-2415		3
1779	Coulomb-only second-order perturbation theory in long-range-corrected hybrid density functionals. **2009**, 11, 9677-86		28
1778	Density functional theory for transition metals and transition metal chemistry. **2009**, 11, 10757-816		1248
1777	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore. 1. Electronically Excited and Ionized States of the Anionic Chromophore in the Gas Phase. *Journal of Chemical Theory and Computation*, **2009**, 5, 1895-906	6.4	104
1776	On the accurate calculation of polarizabilities and second hyperpolarizabilities of polyacetylene oligomer chains using the CAM-B3LYP density functional. *Journal of Chemical Physics*, **2009**, 130, 194114	3.9	234
1775	Long-range corrected double-hybrid density functionals. *Journal of Chemical Physics*, **2009**, 131, 174105	3.9	271

1774	Theoretische Chemie 2008. **2009**, 57, 305-311		3
1773	Excitation energies of zinc porphyrin in aqueous solution using long-range corrected time-dependent density functional theory. *Journal of Physical Chemistry A*, **2009**, 113, 6041-3	2.8	58
1772	Long-range-corrected hybrids including random phase approximation correlation. *Journal of Chemical Physics*, **2009**, 130, 081105	3.9	152
1771	Polarizabilities of Polyacetylene from a Field-Counteracting Semilocal Functional. *Journal of Chemical Theory and Computation*, **2009**, 5, 712-8	6.4	59
1770	Spectral properties of spirooxazine photochromes: TD-DFT insights. *Journal of Physical Chemistry A*, **2009**, 113, 13004-12	2.8	28
1769	Koopmans' springs to life. *Journal of Chemical Physics*, **2009**, 131, 231101	3.9	164
1768	Understanding the molecule-surface chemical coupling in SERS. **2009**, 131, 4090-8		324
1767	Calculation of electronic circular dichroism spectra with time-dependent double-hybrid density functional theory. *Journal of Physical Chemistry A*, **2009**, 113, 767-76	2.8	120
1766	An improved long-range corrected hybrid functional with vanishing Hartree-Fock exchange at zero interelectronic distance (LC2gau-BOP). *Journal of Chemical Physics*, **2009**, 131, 144108	3.9	40
1765	Absorption and fluorescence properties of oligothiophene biomarkers from long-range-corrected time-dependent density functional theory. **2009**, 11, 4498-508		131
1764	Can short-range hybrids describe long-range-dependent properties?. *Journal of Chemical Physics*, **2009**, 131, 044108	3.9	322
1763	Self-consistent-field calculations of core excited states. *Journal of Chemical Physics*, **2009**, 130, 124308	3.9	198
1762	Screened hybrid density functionals for solid-state chemistry and physics. **2009**, 11, 443-54		331
1761	A new generalized Kohn-Sham method for fundamental band-gaps in solids. **2009**, 11, 4674-80		34
1760	Resolutions of the Coulomb operator. Part III. Reduced-rank Schr□dinger equations. **2009**, 11, 9176-81		14
1759	Theoretical study of intermolecular interactions in meso-tetraphenylporphyrin diacid dimer (H4TPPCl2)2. **2009**, 11, 2543-52		11
1758	In search for an optimal methodology to calculate the valence electron affinities of temporary anions. **2009**, 11, 9013-24		24
1757	Excited state surfaces in density functional theory: a new twist on an old problem. *Journal of Chemical Physics*, **2009**, 131, 091101	3.9	150

1756	A simple nonlocal model for exchange. *Journal of Chemical Physics*, **2009**, 131, 234111	3.9	19
1755	Infrared spectroscopy of phenol-(H2O)(n>10): structural strains in hydrogen bond networks of neutral water clusters. *Journal of Physical Chemistry A*, **2009**, 113, 12134-41	2.8	48
1754	Calculating the fluorescence of 5-hydroxytryptophan in proteins. **2009**, 113, 14521-8		14
1753	Structures and properties of electronically excited chromophores in solution from the polarizable continuum model coupled to the time-dependent density functional theory. *Journal of Physical Chemistry A*, **2009**, 113, 3009-20	2.8	158
1752	Prediction of charge-transfer excitations in coumarin-based dyes using a range-separated functional tuned from first principles. *Journal of Chemical Physics*, **2009**, 131, 244119	3.9	270
1751	Reliable prediction of charge transfer excitations in molecular complexes using time-dependent density functional theory. **2009**, 131, 2818-20		632
1750	Theoretical Investigations on How to Reproduce d Bonds: Transition-Metal Cation Benzene Complex Calculations. **2009**, 82, 1367-1371		1
1749	On Occupied-orbital Dependent Exchange-correlation Functionals: From Local Hybrids to Becke B05 Model. **2010**, 224, 545-567		8
1748	The applicability of TD-DFT methods to calculations of the electronic absorption spectrum of hexaamminoruthenium(II) in aqueous solution. **2010**, 84, 39-43		5
1747	A Computational Investigation of Organic Dyes for Dye-Sensitized Solar Cells: Benchmark, Strategies, and Open Issues. **2010**, 114, 7205-7212		302
1746	Fundamental gaps in finite systems from eigenvalues of a generalized Kohn-Sham method. **2010**, 105, 266802		338
1745	Overcoming systematic DFT errors for hydrocarbon reaction energies. **2010**, 127, 429-442		45
1744	The K-band max values of the ultraviolet visible spectra of some hydrazones in ethanol by a TD-DFT/PCM approach. **2010**, 494, 198-201		3
1743	A broken-symmetry study on the automerization of cyclobutadiene. Comparison with UNO- and DNO-MRCC methods. **2010**, 498, 253-258		18
1742	Approximate spin-projected spin-unrestricted density functional theory method: Application to the diradical character dependences of the (hyper)polarizabilities in p-quinodimethane models. **2010**, 501, 140-145		30
1741	DFT study of linear and nonlinear optical properties of donor-acceptor substituted stilbenes, azobenzenes and benzilideneanilines. *Journal of Molecular Modeling*, **2010**, 16, 659-68	2	46
1740	Theoretical studies of vibrationally resolved absorption and emission spectra: From a single chromophore to multichromophoric oligomers/aggregates. **2010**, 53, 297-309		16
1739	Theoretical studies on electronic spectroscopy and dynamics with the real-time time-dependent density functional theory. **2010**, 5, 11-28		7

1738	The Simulation of UV-Vis Spectroscopy with Computational Methods. **2010**, 151-171		6
1737	Enhancing the light driven modulation of the refractive index in organic photochromic materials: A quantum chemical strategy. **2010**, 214, 61-68		9
1736	Photolysis mechanism of a squarylium dye. **2010**, 214, 264-268		2
1735	High second-order NLO responses of dehydrogenated hydrogen cyanide borane(1) oligomers. **2010**, 961, 66-72		9
1734	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. **2010**, 372, 61-66		53
1733	Theoretical treatment of the electronic excited states of the DMSO molecule: A challenge for current theoretical methods. **2010**, 377, 136-141		2
1732	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. **2010**, 181, 1477-1489		3430
1731	Visible spectrum of naphthazarin investigated through Time-Dependent Density Functional Theory. **2010**, 493, 67-71		19
1730	Theoretical investigation on the second hyperpolarizabilities of open-shell singlet systems by spin-unrestricted density functional theory with long-range correction: Range separating parameter dependence. **2010**, 493, 195-199		56
1729	A critical analysis of the performance of new generation functionals on the calculation of the (hyper) polarizabilities of clusters of varying stoichiometry: Test case the SimGen (m + n = 7, n = 07) clusters. **2010**, 498, 134-139		17
1728	Divide-and-conquer self-consistent field calculation for open-shell systems: Implementation and application. **2010**, 500, 172-177		40
1727	Theoretical and computational studies of organometallic reactions: successful or not?. **2010**, 10, 29-45		29
1726	The role of exact-exchange in the theoretical description of organic-metal interfaces. *International Journal of Quantum Chemistry*, **2010**, 110, 2162-2171	2.1	16
1725	Assessing the performances of some recently proposed density functionals for the description of bond dissociations involving organic radicals. *International Journal of Quantum Chemistry*, **2010**, 110, 2320-2329	2.1	11
1724	UNO- and ULO-MRCC(Mk), AP-UCC and AP-UBD approaches to diradical systems. *International Journal of Quantum Chemistry*, **2010**, 110, 3015-3026	2.1	15
1723	Theoretical spectroscopy of carbocyanine dyes made accurate by frozen density correction to excitation energies obtained by TD-DFT. *International Journal of Quantum Chemistry*, **2010**, 110, 3095-3100	2.1	35
1722	An Additive Long-range Potential to Correct for the Charge-transfer Failure of Time-dependent Density Functional Theory. **2010**, 224, 311-324		9
1721	Hybrid functionals including random phase approximation correlation and second-order screened exchange. *Journal of Chemical Physics*, **2010**, 132, 094103	3.9	117

1720	Active-space completely-renormalized equation-of-motion coupled-cluster formalism: Excited-state studies of green fluorescent protein, free-base porphyrin, and oligoporphyrin dimer. *Journal of Chemical Physics*, **2010**, 132, 154103	3.9	56
1719	Constrained-pairing mean-field theory. III. Inclusion of density functional exchange and correlation effects via alternative densities. *Journal of Chemical Physics*, **2010**, 132, 024111	3.9	28
1718	Excited states and electronic spectra of extended tetraazaporphyrins. *Journal of Chemical Physics*, **2010**, 133, 144316	3.9	31
1717	Local response dispersion method. II. Generalized multicenter interactions. *Journal of Chemical Physics*, **2010**, 133, 194101	3.9	82
1716	Communication: Bond length alternation of conjugated oligomers: Another step on the fifth rung of Perdew's ladder of functional. *Journal of Chemical Physics*, **2010**, 133, 151104	3.9	19
1715	Range-dependent adiabatic connections. *Journal of Chemical Physics*, **2010**, 133, 164112	3.9	29
1714	The axial methionine ligand may control the redox reorganizations in the active site of blue copper proteins. *Journal of Chemical Physics*, **2010**, 133, 175101	3.9	12
1713	A one-electron model for the aqueous electron that includes many-body electron-water polarization: Bulk equilibrium structure, vertical electron binding energy, and optical absorption spectrum. *Journal of Chemical Physics*, **2010**, 133, 154506	3.9	75
1712	Electric field induced activation of H2--can DFT do the job?. **2010**, 46, 7942-4		94
1711	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. *Journal of Chemical Physics*, **2010**, 132, 094107	3.9	74
1710	Effect of chemical change on TDDFT accuracy: orbital overlap perspective of the hydrogenation of retinal. **2010**, 12, 2816-8		36
1709	Computational study of molecules with high intrinsic hyperpolarizabilities. *Journal of Physical Chemistry A*, **2010**, 114, 10676-83	2.8	17
1708	Electronic excitation energy calculation by the fragment molecular orbital method with three-body effects. *Journal of Chemical Physics*, **2010**, 133, 044113	3.9	16
1707	Stability of Hydrocarbons of the Polyhedrane Family Containing Bridged CH Groups: A Case of Failure of the Colle-Salvetti Correlation Density Functionals. *Journal of Chemical Theory and Computation*, **2010**, 6, 3442-55	6.4	16
1706	Assessment of the accuracy of long-range corrected functionals for describing the electronic and optical properties of silver clusters. *Journal of Chemical Physics*, **2010**, 132, 194302	3.9	43
1705	Range-separated local hybrids. *Journal of Chemical Physics*, **2010**, 132, 224106	3.9	34
1704	Challenges with range-separated exchange-correlation functionals in time-dependent density functional theory calculations. **2010**, 108, 2745-2750		16
1703	Effects of structural fluctuations on two-photon absorption activity of interacting dipolar chromophores. **2010**, 114, 10814-20		19

1702	Zooming into pi-stacked manifolds of nucleobases: ionized states of dimethylated uracil dimers. *Journal of Physical Chemistry A*, **2010**, 114, 2001-9	2.8	17
1701	Nonlinear Optical Effects Induced by Nanoparticles in Symmetric Molecules **2010**, 114, 20870-20876		13
1700	MkMRCC, APUCC, APUBD calculations of didehydronated species: comparison among calculated through-bond effective exchange integrals for diradicals. **2010**, 108, 2533-2541		10
1699	Calculations of alkane energies using long-range corrected DFT combined with intramolecular van der Waals correlation. **2010**, 12, 1440-3		56
1698	Toward an Accurate Modeling of the Water Zeolite Interaction: Calibrating the DFT Approach. **2010**, 1, 763-768		11
1697	Nonlinear optical properties of Ni(Me(6)pzS(2))MX (M = Ni, Pd, Pt; X = Me(2)timdt, mnt). *Journal of Physical Chemistry A*, **2010**, 114, 5838-45	2.8	11
1696	Understanding the Resonance Raman Scattering of Donor-Acceptor Complexes using Long-Range Corrected DFT. *Journal of Chemical Theory and Computation*, **2010**, 6, 2845-55	6.4	20
1695	Theoretical study on the excess electron binding mechanism in the [CH(3)NO(2).(H(2)O)(n)](-) (n = 1-6) anion clusters. *Journal of Physical Chemistry A*, **2010**, 114, 8939-47	2.8	11
1694	Ionization-Induced Structural Changes in Uracil Dimers and Their Spectroscopic Signatures. *Journal of Chemical Theory and Computation*, **2010**, 6, 705-17	6.4	19
1693	Shielding constants and chemical shifts in DFT: influence of optimized effective potential and Coulomb-attenuation. *Journal of Physical Chemistry A*, **2010**, 114, 7179-86	2.8	16
1692	Applications of Screened Hybrid Density Functionals with Empirical Dispersion Corrections to Rare Gas Dimers and Solids. *Journal of Chemical Theory and Computation*, **2010**, 6, 864-72	6.4	16
1691	How does a double-cage single molecule confine an excess electron? Unusual intercage excess electron transfer transition. *Journal of Physical Chemistry A*, **2010**, 114, 11782-7	2.8	15
1690	Reinvestigation of the reaction of ethylene and singlet oxygen by the approximate spin projection method. Comparison with multireference coupled-cluster calculations. *Journal of Physical Chemistry A*, **2010**, 114, 7967-74	2.8	37
1689	Exchange-Enhanced H-Abstraction Reactivity of High-Valent Nonheme Iron(IV)-Oxo from Coupled Cluster and Density Functional Theories. **2010**, 1, 1533-1540		96
1688	Nonradiative Deactivation in Benzylidene Malononitriles **2010**, 114, 5602-5610		26
1687	The Exchange-Energy Density Functional Based on the Modified Becke-Roussel Model. *Journal of Chemical Theory and Computation*, **2010**, 6, 647-61	6.4	6
1686	On Koopmans' theorem in density functional theory. *Journal of Chemical Physics*, **2010**, 133, 174101	3.9	258
1685	Linear and nonlinear optical properties of triphenylamine-functionalized C60: insights from theory and experiment. **2010**, 12, 373-81		39

1684	Tuned range-separated hybrids in density functional theory. *Annual Review of Physical Chemistry*, **2010**, 61, 85-109	15.7	562
1683	Electronic Transition Energies: A Study of the Performance of a Large Range of Single Reference Density Functional and Wave Function Methods on Valence and Rydberg States Compared to Experiment. *Journal of Chemical Theory and Computation*, **2010**, 6, 370-83	6.4	181
1682	Multireference character of 1,3-dipolar cycloaddition of ozone with ethylene and acrylonitrile. *Journal of Physical Chemistry A*, **2010**, 114, 12116-23	2.8	22
1681	Stress sensing in polycaprolactone films via an embedded photochromic compound. **2010**, 2, 1594-600		149
1680	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. *Journal of Chemical Theory and Computation*, **2010**, 6, 2071-85	6.4	335
1679	Effects of mercury(II) on structural properties, electronic structure and UV absorption spectra of a duplex containing thymine-mercury(II)-thymine nucleobase pairs. **2010**, 12, 909-17		31
1678	Density functional approximations for charge transfer excitations with intermediate spatial overlap. **2010**, 12, 12697-701		86
1677	Long-range density-matrix-functional theory: Application to a modified homogeneous electron gas. **2010**, 81,		26
1676	Describing Anions by Density Functional Theory: Fractional Electron Affinity. *Journal of Chemical Theory and Computation*, **2010**, 6, 2726-35	6.4	95
1675	Quantum chemical study on UV-vis spectra of microhydrated iodine dimer radical anion. *Journal of Physical Chemistry A*, **2010**, 114, 721-4	2.8	10
1674	Environmental effects in computational spectroscopy: accuracy and interpretation. *ChemPhysChem*, **2010**, 11, 1812-32	3.2	47
1673	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. **2010**, 12, 8016-23		113
1672	Hydrates of Cu2+ and CuCl+ in dilute aqueous solution: a density functional theory and polarized continuum model investigation. *Journal of Physical Chemistry A*, **2010**, 114, 8406-16	2.8	36
1671	Electric Field Gradients Calculated from Two-Component Hybrid Density Functional Theory Including Spin-Orbit Coupling. *Journal of Chemical Theory and Computation*, **2010**, 6, 2669-86	6.4	35
1670	Modeling the charge transfer between alkali metals and polycyclic aromatic hydrocarbons using electronic structure methods. *Journal of Physical Chemistry A*, **2010**, 114, 10326-33	2.8	50
1669	Optoelectronic and Excitonic Properties of Oligoacenes: Substantial Improvements from Range-Separated Time-Dependent Density Functional Theory. *Journal of Chemical Theory and Computation*, **2010**, 6, 3704-3712	6.4	213
1668	Ab Initio Study of Xe Adsorption on Graphene. **2010**, 114, 3544-3548		47
1667	Environmental broadening of the CTTS bands: the hexaammineruthenium(II) complex in aqueous solution. *Journal of Physical Chemistry A*, **2010**, 114, 12804-12	2.8	23

1666	Identification of the mechanism of enhanced exciton interaction in rigidly linked naphthalene dimers. **2010**, 12, 13070-5		10
1665	MkMRCC, APUCC and APUBD approaches to 1,n-didehydropolyene diradicals: the nature of through-bond exchange interactions. **2010**, 108, 2559-2578		11
1664	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. **2011**, 30, 115-160		106
1663	Exploring dynamical electron theory beyond the Born-Oppenheimer framework: from chemical reactivity to non-adiabatically coupled electronic and nuclear wavepackets on-the-fly under laser field. **2011**, 13, 4987-5016		56
1662	Ground and excited state properties of photoactive platinum(IV) diazido complexes: theoretical considerations. **2011**, 40, 7571-82		29
1661	Improved DFT description of intrastrand cross-link formation by inclusion of London dispersion corrections. **2011**, 115, 15138-44		21
1660	Molecular Structures, AcidBase Properties, and Formation of Group 6 Transition Metal Hydroxides. **2011**, 115, 8072-8103		50
1659	Bonding nature and vibrational signatures of oxirane:(water)(n=1-3). Assessment of the performance of the dispersion-corrected DFT methods compared to the ab initio results and Fourier transform infrared experimental data. *Journal of Physical Chemistry A*, **2011**, 115, 6688-701	2.8	12
1658	Conjugation of two nitronyl nitroxides-attached diarylethenes. **2011**, 115, 5685-92		14
1657	Energy and lifetime of temporary anion states of uracil by stabilization method. *Journal of Physical Chemistry A*, **2011**, 115, 10113-21	2.8	19
1656	Theoretical Investigations on the Photoinduced Phase Transition Mechanism of Tetrathiafulvalene-p-chloranil. *Journal of Chemical Theory and Computation*, **2011**, 7, 2233-9	6.4	5
1655	[CuCl3]- and [CuCl4]2- hydrates in concentrated aqueous solution: a density functional theory and ab initio study. *Journal of Physical Chemistry A*, **2011**, 115, 4416-26	2.8	36
1654	Theoretical study of Pt(PR3)(2)(AlCl3) (R = H, Me, Ph, or Cy) including an unsupported bond between transition metal and non-transition metal elements: geometry, bond strength, and prediction. *Journal of Physical Chemistry A*, **2011**, 115, 8520-7	2.8	9
1653	Charge-Transfer-Like Excitations in Time-Dependent Density Functional Theory: A Conundrum and Its Solution. *Journal of Chemical Theory and Computation*, **2011**, 7, 2408-15	6.4	204
1652	Improving band gap prediction in density functional theory from molecules to solids. **2011**, 107, 026403		139
1651	Experimental and theoretical studies of the photophysical properties of 2- and 2,7-functionalized pyrene derivatives. **2011**, 133, 13349-62		229
1650	Solvent effects in the excited-state tautomerization of 7-azaindole: a theoretical study. **2011**, 115, 15048-58		18
1649	Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks. *Journal of Chemical Theory and Computation*, **2011**, 7, 369-76	6.4	119

1648	TD-CI simulation of the electronic optical response of molecules in intense fields II: comparison of DFT functionals and EOM-CCSD. *Journal of Physical Chemistry A*, **2011**, 115, 11832-40	2.8	37
1647	Theoretical studies for excited-state tautomerization in the 7-azaindole-(CH3OH)n (n = 1 and 2) complexes in the gas phase. *Journal of Physical Chemistry A*, **2011**, 115, 13743-52	2.8	19
1646	Electronically excited states of vitamin B12: benchmark calculations including time-dependent density functional theory and correlated ab initio methods. *Journal of Physical Chemistry A*, **2011**, 115, 1280-92	2.8	86
1645	Design of Molecular Chains Based on the Planar Tetracoordinate Carbon Unit C2Al4. **2011**, 115, 13187-13192		25
1644	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, 2439-51	6.4	68
1643	Oscillator Strengths in ONIOM Excited State Calculations. *Journal of Chemical Theory and Computation*, **2011**, 7, 180-7	6.4	10
1642	Redox and Photoisomerization Switching the Second-Order Nonlinear Optical Properties of a Tetrathiafulvalene Derivative Across Six States: A DFT Study. **2011**, 115, 23946-23954		76
1641	Time-Dependent Density-Functional Description of the (1)La State in Polycyclic Aromatic Hydrocarbons: Charge-Transfer Character in Disguise?. *Journal of Chemical Theory and Computation*, **2011**, 7, 1296-306	6.4	148
1640	Ground Electronic State of Peptide Cation Radicals: A Delocalized Unpaired Electron?. **2011**, 2, 1426-1431		16
1639	Direct Simulation of Excited-State Intramolecular Proton Transfer and Vibrational Coherence of 10-Hydroxybenzo[h]quinoline in Solution. **2011**, 2, 2366-2371		49
1638	Resolutions of the Coulomb Operator: V. The Long-Range Ewald Operator. *Journal of Chemical Theory and Computation*, **2011**, 7, 2353-7	6.4	9
1637	Diffusion and aggregation of sodium fluorescein in aqueous solutions. **2011**, 115, 12896-904		63
1636	Evolution of Properties in Prolate (GaAs)n Clusters. **2011**, 115, 97-107		30
1635	TD-DFT Vibronic Couplings in Anthraquinones: From Basis Set and Functional Benchmarks to Applications for Industrial Dyes. *Journal of Chemical Theory and Computation*, **2011**, 7, 1882-92	6.4	96
1634	Density functional theory calculations of dynamic first hyperpolarizabilities for organic molecules in organic solvent: comparison to experiment. *Journal of Chemical Physics*, **2011**, 135, 134104	3.9	33
1633	Double-hybrid density-functional theory made rigorous. *Journal of Chemical Physics*, **2011**, 134, 064113	3.9	144
1632	Computational Study of Absorption Energies of Organic Sensitizers Used in Photovoltaic Applications. **2011**, 115, 19424-19430		40
1631	New cyanine dyes or not? Theoretical insights for model chains. *Journal of Physical Chemistry A*, **2011**, 115, 2442-5	2.8	8

1630	Peculiarities of the environmental influence on the optical properties of push-pull nonlinear optical molecules: a theoretical study. *Journal of Physical Chemistry A*, **2011**, 115, 12251-8	2.8	22
1629	Quantum chemistry studies of electronically excited nitrobenzene, TNA, and TNT. *Journal of Physical Chemistry A*, **2011**, 115, 12286-97	2.8	28
1628	Amylose□Vanillin Complexation Assessed by a Joint Experimental and Theoretical Analysis. **2011**, 115, 23315-23322		19
1627	Approximate Density Functionals: Which Should I Choose?. **2011**,		3
1626	Evaluation of a combination of local hybrid functionals with DFT-D3 corrections for the calculation of thermochemical and kinetic data. *Journal of Physical Chemistry A*, **2011**, 115, 8990-6	2.8	25
1625	Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. *Journal of Chemical Theory and Computation*, **2011**, 7, 456-66	6.4	104
1624	Di-8-ANEPPS emission spectra in phospholipid/cholesterol membranes: a theoretical study. **2011**, 115, 4160-7		39
1623	CO oxidation catalyzed by a single gold atom: benchmark calculations and the performance of DFT methods. **2011**, 13, 13358-69		36
1622	Time-Dependent Density Functional Tight Binding: New Formulation and Benchmark of Excited States. *Journal of Chemical Theory and Computation*, **2011**, 7, 3304-13	6.4	85
1621	Role of Many-Body Effects in Describing Low-Lying Excited States of □Conjugated Chromophores: High-Level Equation-of-Motion Coupled-Cluster Studies of Fused Porphyrin Systems. *Journal of Chemical Theory and Computation*, **2011**, 7, 2200-8	6.4	21
1620	Long-range-corrected hybrids using a range-separated Perdew-Burke-Ernzerhof functional and random phase approximation correlation. *Journal of Chemical Physics*, **2011**, 135, 094105	3.9	32
1619	A new parametrizable model of molecular electronic structure. *Journal of Chemical Physics*, **2011**, 135, 134120	3.9	40
1618	N?□and O?□Interactions rather than □directed□hydrogen bonding in the crystal packing of ethyl (Z)-2-cyano-3-[(4-alkoxyphenyl)amino]prop-2-enoates. **2011**, 13, 4496		11
1617	Design of Dye Acceptors for Photovoltaics from First-Principles Calculations. **2011**, 115, 9276-9282		69
1616	Structure of the aqueous electron: assessment of one-electron pseudopotential models in comparison to experimental data and time-dependent density functional theory. *Journal of Physical Chemistry A*, **2011**, 115, 14470-83	2.8	58
1615	Nonlinear Optical Switching Behavior in the Solid State: A Theoretical Investigation on Anils. **2011**, 23, 3993-4001		40
1614	Electric field polarization in conventional density functional theory: from quasilinear to two-dimensional and three-dimensional extended systems. *Journal of Chemical Physics*, **2011**, 135, 154101	3.9	27
1613	Scalar Relativistic Computations of Nuclear Magnetic Shielding and g-Shifts with the Zeroth-Order Regular Approximation and Range-Separated Hybrid Density Functionals. *Journal of Chemical Theory and Computation*, **2011**, 7, 3278-92	6.4	38

1612	Spin-orbit relativistic long-range corrected time-dependent density functional theory for investigating spin-forbidden transitions in photochemical reactions. *Journal of Chemical Physics*, **2011**, 135, 224106	3.9	14
1611	DFT study of trichloroethene reaction with permanganate in aqueous solution. **2011**, 45, 3006-11		25
1610	Quantum mechanical modeling of catalytic processes. **2011**, 2, 453-77		58
1609	Improved Prediction of Properties of Conjugated Oligomers with Range-Separated Hybrid Density Functionals. *Journal of Chemical Theory and Computation*, **2011**, 7, 2568-83	6.4	160
1608	A density functional theory for studying ionization processes in water clusters. *Journal of Physical Chemistry A*, **2011**, 115, 5735-44	2.8	48
1607	Doping-enhanced hyperpolarizabilities of silicon clusters: a global ab initio and density functional theory study of Si10 (Li, Na, K)n (n=1, 2) clusters. *Journal of Chemical Physics*, **2011**, 135, 044511	3.9	62
1606	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. **2011**, 83,		121
1605	Energy-Specific Linear Response TDHF/TDDFT for Calculating High-Energy Excited States. *Journal of Chemical Theory and Computation*, **2011**, 7, 3540-7	6.4	83
1604	Evaluation of the Nonlinear Optical Properties for Annulenes with H kel and M bius Topologies. *Journal of Chemical Theory and Computation*, **2011**, 7, 3935-43	6.4	76
1603	The pH-Controlled Plasmon-Assisted Surface Photocatalysis Reaction of 4-Aminothiophenol to p,p?-Dimercaptoazobenzene on Au, Ag, and Cu Colloids. **2011**, 115, 9629-9636		131
1602	Hemibonding of hydroxyl radical and halide anion in aqueous solution. *Journal of Physical Chemistry A*, **2011**, 115, 14620-8	2.8	29
1601	A study of TDDFT performance in modeling of spectral changes induced by interactions of ketocyanine dyes with inorganic ions. **2011**, 972, 32-38		11
1600	DFT studies on the electronic properties of organometallic-polyoxomolybdate anions [Cpn*Mo6O19](2)(n = 1 or 2): Revealing bonding features of Cp*Mo. **2011**, 976, 1-7		2
1599	Comparative study of hybrid functionals applied to structural and electronic properties of semiconductors and insulators. **2011**, 84,		56
1598	Theoretical study of metallasilatranes; Bonding nature and prediction of new metallasilatrane. **2011**, 76, 619-629		8
1597	Dispersion interactions in density-functional theory: an adiabatic-connection analysis. *Journal of Chemical Physics*, **2011**, 135, 194109	3.9	18
1596	Benchmark results for empirical post-GGA functionals: difficult exchange problems and independent tests. **2011**, 13, 19325-37		71
1595	Spin-adapted open-shell time-dependent density functional theory. III. An even better and simpler formulation. *Journal of Chemical Physics*, **2011**, 135, 194106	3.9	49

1594	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. *Journal of Chemical Theory and Computation*, **2011**, 7, 3567-77	6.4	322
1593	An examination of density functional theories on isomerization energy calculations of organic molecules. **2011**, 130, 851-857		24
1592	Modeling Fast Electron Dynamics with Real-Time Time-Dependent Density Functional Theory: Application to Small Molecules and Chromophores. *Journal of Chemical Theory and Computation*, **2011**, 7, 1344-55	6.4	177
1591	First-principles simulations of exciton diffusion in organic semiconductors. **2011**, 84,		51
1590	Evaluation of Nonlinear Optical Properties of Large Conjugated Molecular Systems by Long-Range-Corrected Density Functional Theory. **2011**, 475-491		
1589	Analysis of self-consistency effects in range-separated density-functional theory with M□ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2011**, 135, 034116	3.9	11
1588	The influence of density functional approximations on the description of LiH + NH3 -> LiNH2 + H2 reaction. **2011**, 511, 427-433		8
1587	Validity of describing reaction coordinate of intramolecular charge transfer of 1,3-dinitrobenzene anion radical using constrained density functional theory. **2011**, 511, 219-223		15
1586	The quantified NTO analysis for the electronic excitations of molecular many-body systems. **2011**, 514, 362-367		9
1585	Static NLO responses of fluorinated polyacetylene chains evaluated with long-range corrected density functionals. **2011**, 515, 78-84		23
1584	Accurate singlet and triplet excitation energies using the Localized Hartree□Fock Kohn□Sham potential. **2011**, 391, 19-26		12
1583	Excited-State Tautomerization in the 7-Azaindole-(H2O)n (n = 1 and 2) Complexes in the Gas Phase and in Solution: A Theoretical Study. *Journal of Chemical Theory and Computation*, **2011**, 7, 642-57	6.4	25
1582	Optical rotation calculated with time-dependent density functional theory: the OR45 benchmark. *Journal of Physical Chemistry A*, **2011**, 115, 10930-49	2.8	97
1581	A Qualitative Index of Spatial Extent in Charge-Transfer Excitations. *Journal of Chemical Theory and Computation*, **2011**, 7, 2498-506	6.4	657
1580	Insights into dehydrogenative coupling of alcohols and amines catalyzed by a (PNN)-Ru(II) hydride complex: unusual metal-ligand cooperation. *Inorganic Chemistry*, **2011**, 50, 10572-80	5.1	66
1579	Influence of Triplet Instabilities in TDDFT. *Journal of Chemical Theory and Computation*, **2011**, 7, 3578-85	6.4	226
1578	Dispersion, static correlation, and delocalisation errors in density functional theory: an electrostatic theorem perspective. *Journal of Chemical Physics*, **2011**, 135, 164110	3.9	8
1577	Long-range corrected hybrid functionals for □conjugated systems: dependence of the range-separation parameter on conjugation length. *Journal of Chemical Physics*, **2011**, 135, 204107	3.9	210

1576	Excited-State Electronic Structure with Configuration Interaction Singles and Tamm-Dancoff Time-Dependent Density Functional Theory on Graphical Processing Units. *Journal of Chemical Theory and Computation*, **2011**, 7, 1814-1823	6.4	154
1575	Size dependences of the diradical character and the second hyperpolarizabilities in dicyclopenta-fused acenes: relationships with their aromaticity/antiaromaticity. **2011**, 13, 20575-83		64
1574	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. **2011**, 6, 269-279		17
1573	Exchange functional by a range-separated exchange hole. **2011**, 83,		5
1572	Third-order nonlinear optical properties of open-shell supermolecular systems composed of acetylene linked phenalenyl radicals. *Journal of Physical Chemistry A*, **2011**, 115, 8767-77	2.8	30
1571	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. **2011**, 13, 16987-98		258
1570	DNA insertion in and wrapping around carbon nanotubes. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 902-919	7.9	5
1569	Long-range corrected DFT calculations of charge-transfer integrals in model metal-free phthalocyanine complexes. *Journal of Molecular Modeling*, **2011**, 17, 2143-9	2	21
1568	Assessment of the B97 family for excited-state calculations. **2011**, 128, 127-136		115
1567	Performance of density functional theory on homogeneous gold catalysis. **2011**, 128, 647-661		75
1566	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. **2011**, 130, 711-724		114
1565	Singlet–triplet energy gap for trimethylenemethane, oxyallyl diradical, and related species: single- and multireference computational results. **2011**, 130, 739-748		30
1564	Symmetry and broken symmetry in molecular orbital description of unstable molecules IV: comparison between single- and multi-reference computational results for antiaromtic molecules. **2011**, 130, 749-763		36
1563	An examination of density functionals on aldol, Mannich and α-aminoxylation reaction enthalpy calculations. **2011**, 130, 153-160		7
1562	Theoretical study of the excited states and the redox potentials of unusually distorted β-trifluoromethylporphycene. **2011**, 130, 175-185		4
1561	Finite-field evaluation of static (hyper)polarizabilities based on the linear-scaling divide-and-conquer method. **2011**, 130, 701-709		12
1560	Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. **2011**, 130, 251-260		34
1559	Applications and validations of the Minnesota density functionals. **2011**, 502, 1-13		568

1558	Performances of recently-proposed functionals for describing disulfide radical anions and similar systems. **2011**, 501, 245-251		18
1557	Donor–acceptor diethynylsilane oligomers: A second-order nonlinear optical material. **2011**, 49, 1410-1419		10
1556	Advances in local hybrid exchange-correlation functionals: from thermochemistry to magnetic-resonance parameters and hyperpolarizabilities. *International Journal of Quantum Chemistry*, **2011**, 111, 2625-2638	2.1	40
1555	Ab initio study of the structure, spectral, ionochromic, and fluorochromic properties of benzoazacrown-containing dyes as potential optical molecular sensors. *International Journal of Quantum Chemistry*, **2011**, 111, 2649-2662	2.1	8
1554	On the shape dependence of cluster (hyper)polarizabilities. A combined ab initio and DFT study on large fullerene-like gallium arsenide semiconductor clusters. *International Journal of Quantum Chemistry*, **2011**, 111, 788-796	2.1	14
1553	Absorption spectra of azobenzenes simulated with time-dependent density functional theory. *International Journal of Quantum Chemistry*, **2011**, 111, 4224-4240	2.1	32
1552	Theoretical and experimental studies on the mechanism of coloration of polyimides. *ChemPhysChem*, **2011**, 12, 1367-77	3.2	14
1551	Open-shell characters and second hyperpolarizabilities of one-dimensional graphene nanoflakes composed of trigonal graphene units. *ChemPhysChem*, **2011**, 12, 1697-707	3.2	45
1550	Thermochemical stabilities, electronic structures, and optical properties of C56X10 (X = H, F, and Cl) fullerene compounds. *Journal of Computational Chemistry*, **2011**, 32, 658-67	3.5	16
1549	Infinite Basis set extrapolation for Double Hybrid Density Functional Theory 1: effect of applying various extrapolation functions. *Journal of Computational Chemistry*, **2011**, 32, 1671-9	3.5	9
1548	Exchange coupling constants using Density Functional Theory: long-range corrected functionals. *Journal of Computational Chemistry*, **2011**, 32, 1998-2004	3.5	41
1547	Proton-coupled electron transfer of the phenoxyl/phenol couple: effect of Hartree-Fock exchange on transition structures. *Journal of Computational Chemistry*, **2011**, 32, 3081-91	3.5	11
1546	A semiempirical long-range corrected exchange correlation functional including a short-range Gaussian attenuation (LCgau-B97). *Journal of Computational Chemistry*, **2011**, 32, 3269-75	3.5	12
1545	Electronic and optical properties of families of polycyclic aromatic hydrocarbons: A systematic (time-dependent) density functional theory study. **2011**, 384, 19-27		114
1544	Twelve outstanding problems in ground-state density functional theory: A bouquet of puzzles. **2011**, 963, 2-6		36
1543	Accurate finite element method for atomic calculations based on density functional theory and Hartree–Fock method. **2011**, 182, 1245-1252		9
1542	Assessment of DFT functionals for the calculation of interaction-induced electric properties of molecular complexes. **2011**, 503, 39-44		13
1541	Photoinduced charge transfer in heterofullerene–donor hybrids: A theoretical study. **2011**, 506, 248-254		

1540	Computational study on second-order nonlinear optical (NLO) properties of a novel class of two-dimensional □and W-shaped sandwich metallocarborane-containing chromophores. **2011**, 696, 2380-2387		28
1539	Chemically accurate and computationally-efficient time-dependent density functional theory (TDDFT) modeling of the UV/Vis spectra of Pechmann dyes and related compounds. **2011**, 4, 1157-1166		2
1538	The performance and relationship among range-separated schemes for density functional theory. *Journal of Chemical Physics*, **2011**, 135, 074109	3.9	38
1537	Density functional study of multiplicity-changing valence and Rydberg excitations of p-block elements: delta self-consistent field, collinear spin-flip time-dependent density functional theory (DFT), and conventional time-dependent DFT. *Journal of Chemical Physics*, **2011**, 135, 044118	3.9	55
1536	Kojic acid derivatives as powerful chelators for iron(III) and aluminium(III). **2011**, 40, 5984-98		39
1535	Theoretical study of the origin of the large difference in the visible absorption spectra of organic dyes containing a thienylmethine unit and differing by the methine unit position. **2011**,		5
1534	O - H Bond Dissociation Energies. **2011**, 64, 394		18
1533	Nature's most squishy ion: The important role of solvent polarization in the description of the hydrated electron. **2011**, 30, 1-48		45
1532	Theoretical studies on the second-order nonlinear optical properties of donor□cceptor-substituted hexaphyrins(1.1.1.1.1.1) and their redox-switchability. **2011**, 109, 2625-2632		2
1531	Communication: Tailoring the optical gap in light-harvesting molecules. *Journal of Chemical Physics*, **2011**, 134, 151101	3.9	98
1530	Demonstration and interpretation of significant asymmetry in the low-resolution and high-resolution Q(y) fluorescence and absorption spectra of bacteriochlorophyll a. *Journal of Chemical Physics*, **2011**, 134, 024506	3.9	98
1529	The role of range-separated Hartree-Fock exchange in the calculation of magnetic exchange couplings in transition metal complexes. *Journal of Chemical Physics*, **2011**, 134, 034108	3.9	31
1528	An efficient, fragment-based electronic structure method for molecular systems: self-consistent polarization with perturbative two-body exchange and dispersion. *Journal of Chemical Physics*, **2011** , 134, 094118	3.9	72
1527	Communication: a new hybrid exchange correlation functional for band-gap calculations using a short-range Gaussian attenuation (Gaussian-Perdue-Burke-Ernzerhof). *Journal of Chemical Physics*, **2011**, 135, 071103	3.9	40
1526	Optical response of silver nanoclusters complexed with aromatic thiol molecules: a time-dependent density functional study. **2011**, 44, 035101		13
1525	Electronic excitation spectrum of the photosensitizer [Ir(ppy)2(bpy)]+. *Journal of Chemical Physics*, **2012**, 136, 214305	3.9	34
1524	Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. *Journal of Chemical Physics*, **2012**, 136, 154109	3.9	88
1523	Computational Investigations on Organic Sensitizers for Dye-Sensitized Solar Cell. **2012**, 9, 215-232		18

1522	Importance of the correlation contribution for local hybrid functionals: range separation and self-interaction corrections. *Journal of Chemical Physics*, **2012**, 136, 014111	3.9	62
1521	Nonspherical model density matrices for Rung 3.5 density functionals. *Journal of Chemical Physics*, **2012**, 136, 024111	3.9	18
1520	Dispersion-free component of non-covalent interaction via mutual polarization of fragment densities. *Journal of Chemical Physics*, **2012**, 136, 204109	3.9	8
1519	Electric dipole (hyper)polarizabilities of spatially confined LiH molecule. *Journal of Chemical Physics*, **2012**, 137, 094307	3.9	25
1518	Extension of local response dispersion method to excited-state calculation based on time-dependent density functional theory. *Journal of Chemical Physics*, **2012**, 137, 124106	3.9	16
1517	Nonempirical Rung 3.5 density functionals from the Lieb-Oxford bound. *Journal of Chemical Physics*, **2012**, 137, 224110	3.9	15
1516	Gaussian attenuation hybrid scheme applied to the Ernzerhof-Perdew exchange hole model (Gau-PBEh). *Journal of Chemical Physics*, **2012**, 137, 244105	3.9	9
1515	A non-self-consistent range-separated time-dependent density functional approach for large-scale simulations. **2012**, 24, 205801		15
1514	Laser-assisted field evaporation from insulators triggered by photoinduced hole accumulation. **2012**, 86,		25
1513	Failure of the random-phase-approximation correlation energy. **2012**, 85,		49
1512	Vibronic coupling simulations for linear and nonlinear optical processes: simulation results. *Journal of Chemical Physics*, **2012**, 136, 064110	3.9	30
1511	An excited state paired interacting orbital method. *Journal of Chemical Physics*, **2012**, 136, 064109	3.9	8
1510	INSIGHTS INTO THE SOLVATO-/THERMO-PROMOTED INTRAMOLECULAR ELECTRON TRANSFER IN A TTF-□TCNQ DYAD WITH AN EXTREMELY LOW HOMO□UMO GAP. **2012**, 11, 599-609		5
1509	Dynamic hyperpolarizability calculations of large systems: the linear-scaling divide-and-conquer approach. *Journal of Chemical Physics*, **2012**, 136, 084108	3.9	15
1508	TD-DFT Assessment of Functionals for Optical 0-0 Transitions in Solvated Dyes. *Journal of Chemical Theory and Computation*, **2012**, 8, 2359-72	6.4	342
1507	The Odd Electron Density Is the Guide toward Achieving Organic Molecules with Gigantic Third-Order Nonlinear Optical Responses. **2012**, 3, 3338-3342		19
1506	The □conjugated P-flowers C16(PH)8 and C16(PF)8 are potential materials for organic n-type semiconductors. **2012**, 14, 14832-41		21
1505	Performance of recent and high-performance approximate density functionals for time-dependent density functional theory calculations of valence and Rydberg electronic transition energies. *Journal of Chemical Physics*, **2012**, 137, 244104	3.9	145

1504	Accurate Spin-State Energetics of Transition Metal Complexes. 1. CCSD(T), CASPT2, and DFT Study of [M(NCH)6](2+) (M = Fe, Co). *Journal of Chemical Theory and Computation*, **2012**, 8, 4216-31	6.4	115
1503	Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS. *Journal of Chemical Theory and Computation*, **2012**, 8, 4189-203	6.4	70
1502	Attenuating Away the Errors in Inter- and Intramolecular Interactions from Second-Order M□ller-Plesset Calculations in the Small Aug-cc-pVDZ Basis Set. **2012**, 3, 3592-8		31
1501	Ferric complexes of 3-hydroxy-4-pyridinones characterized by density functional theory and Raman and UV-vis spectroscopies. *Inorganic Chemistry*, **2012**, 51, 4473-81	5.1	18
1500	A close inspection of the charge-transfer excitation by TDDFT with various functionals: An application of orbital- and density-based analyses. **2012**, 405, 93-99		22
1499	Electronic structure study of the triplet azulene-like molecules. **2012**, 545, 132-137		6
1498	Significant role of the DNA backbone in mediating the transition origin of electronic excitations of B-DNA--implication from long range corrected TDDFT and quantified NTO analysis. **2012**, 14, 9092-103		5
1497	Aza-boron-dipyrromethene dyes: TD-DFT benchmarks, spectral analysis and design of original near-IR structures. **2012**, 14, 157-64		92
1496	C?□Interaction of non-hydrogen bond type. *New Journal of Chemistry*, **2012**, 36, 44-47	3.6	7
1495	Understanding the absorption and emission spectra of borondipyrromethene dye and its substituted analogues. **2012**, 110, 445-456		10
1494	Theoretical Insight into the Second-Order NLO Response of the Bis{4-[2-(4-pyridyl)ethenyl]benzoato}-zinc(II) Metal□Organic Framework. **2012**, 116, 21973-21981		21
1493	Solvatochromic shifts of polar and non-polar molecules in ambient and supercritical water: a sequential quantum mechanics/molecular mechanics study including solute-solvent electron exchange-correlation. *Journal of Chemical Physics*, **2012**, 137, 214504	3.9	15
1492	Application of screened hybrid functionals to the bulk transition metals Rh, Pd, and Pt. **2012**, 86,		20
1491	Theoretical analysis of charge-transfer electronic spectra of methylated benzenes□TCNE complexes including solvent effects: approaching experiment. **2012**, 131, 1		11
1490	Four Bases Score a Run: Ab Initio Calculations Quantify a Cooperative Effect of H-Bonding and □Stacking on the Ionization Energy of Adenine in the AATT Tetramer. **2012**, 3, 2726-32		35
1489	Assessment of density functional theory for bonds formed between rare gases and open-shell atoms: a computational study of small molecules containing He, Ar, Kr and Xe. **2012**, 14, 553-61		8
1488	Predicting properties of organic optoelectronic materials: asymptotically corrected density functional study. *Journal of Physical Chemistry A*, **2012**, 116, 12153-62	2.8	12
1487	Assessment of Density Functional Theory in Predicting Structures and Free Energies of Reaction of Atmospheric Prenucleation Clusters. *Journal of Chemical Theory and Computation*, **2012**, 8, 2071-7	6.4	134

1486	DFT and TD-DFT study on the electronic structures and phosphorescent properties of 6-phenyl-2,2'-bipyridine tridentate iridium(III) complexes and their isomer. **2012**, 41, 8441-6		28
1485	Elucidating electronic transitions from orbitals of liquid n- and branched alkanes by far-ultraviolet spectroscopy and quantum chemical calculations. *Journal of Physical Chemistry A*, **2012**, 116, 11957-64	2.8	41
1484	(1)La and (1)Lb States of Indole and Azaindole: Is Density Functional Theory Inadequate?. *Journal of Chemical Theory and Computation*, **2012**, 8, 575-84	6.4	31
1483	Electronic excitations in epicocconone analogues: TDDFT methodological assessment guided by experiment. *Journal of Physical Chemistry A*, **2012**, 116, 8634-43	2.8	18
1482	Theoretical verification of nonthermal microwave effects on intramolecular reactions. *Journal of Physical Chemistry A*, **2012**, 116, 2177-83	2.8	13
1481	Superior performance of range-separated hybrid functionals for describing <- UV-vis signatures of three-electron two-center anions. *Journal of Physical Chemistry A*, **2012**, 116, 3237-46	2.8	9
1480	Energies and lifetimes of temporary anion states of chloromethanes by stabilized Koopmans' theorem in long-range corrected density functional theory. *Journal of Physical Chemistry A*, **2012**, 116, 12364-72	2.8	8
1479	Accurate thermochemistry of hydrocarbon radicals via an extended generalized bond separation reaction scheme. *Journal of Physical Chemistry A*, **2012**, 116, 3436-47	2.8	33
1478	Impact of Antidot Structure on the Multiradical Characters, Aromaticities, and Third-Order Nonlinear Optical Properties of Hexagonal Graphene Nanoflakes. **2012**, 116, 17787-17795		58
1477	Calculating Off-Site Excitations in Symmetric Donor-Acceptor Systems via Time-Dependent Density Functional Theory with Range-Separated Density Functionals. *Journal of Chemical Theory and Computation*, **2012**, 8, 2661-8	6.4	32
1476	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. *Journal of Chemical Theory and Computation*, **2012**, 8, 2824-34	6.4	58
1475	Synthesis and electronic structure of highly electron-accepting radiaannulene and its reduced species. **2012**, 53, 5385-5388		6
1474	BDE261: a comprehensive set of high-level theoretical bond dissociation enthalpies. *Journal of Physical Chemistry A*, **2012**, 116, 4975-86	2.8	58
1473	Importance of Correctly Describing Charge-Transfer Excitations for Understanding the Chemical Effect in SERS. **2012**, 3, 2470-5		74
1472	Constrained density functional theory. **2012**, 112, 321-70		366
1471	How Evenly Can Approximate Density Functionals Treat the Different Multiplicities and Ionization States of 4d Transition Metal Atoms?. *Journal of Chemical Theory and Computation*, **2012**, 8, 4112-26	6.4	34
1470	Electronic excitation spectra of the [Ir(ppy)2(bpy)]+ photosensitizer bound to small silver clusters Ag(n) (n = 1-6). **2012**, 14, 4977-84		6
1469	Overcoming low orbital overlap and triplet instability problems in TDDFT. *Journal of Physical Chemistry A*, **2012**, 116, 9783-9	2.8	162

1468	Polarons, bipolarons, and side-by-side polarons in reduction of oligofluorenes. **2012**, 134, 10852-63		67
1467	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. **2012**, 116, 11946-11955		193
1466	A Density Functional with Spherical Atom Dispersion Terms. *Journal of Chemical Theory and Computation*, **2012**, 8, 4989-5007	6.4	324
1465	Derivative discontinuity, bandgap and lowest unoccupied molecular orbital in density functional theory. *Journal of Chemical Physics*, **2012**, 136, 204111	3.9	129
1464	DFT and Proton Transfer Reactions: A Benchmark Study on Structure and Kinetics. *Journal of Chemical Theory and Computation*, **2012**, 8, 3082-8	6.4	69
1463	Molecular design of distorted push□pull porphyrins for dye-sensitized solar cells. **2012**, 131, 1		44
1462	Increasing the applicability of density functional theory. III. Do consistent Kohn-Sham density functional methods exist?. *Journal of Chemical Physics*, **2012**, 137, 134102	3.9	31
1461	Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. *Journal of Chemical Theory and Computation*, **2012**, 8, 4305-16	6.4	34
1460	□Frontier molecular orbitals in S = 2 ferryl species and elucidation of their contributions to reactivity. **2012**, 109, 14326-31		74
1459	Computational design of linear, flat, and tubular nanomolecules using planar tetracoordinate carbon C2Al4 units. **2012**, 992, 78-83		17
1458	Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory. *Journal of Chemical Physics*, **2012**, 137, 120901	3.9	813
1457	Electronic structures and second-order nonlinear optical properties of a series of functionalized Sc3N@Ih□80 derivatives. **2012**, 996, 51-56		1
1456	A Theoretical Investigation on the Oxidation of Carbon Monoxide by an Aqueous Molybdocene. **2012**, 2012, 4445-4453		6
1455	Density functional study of tetraphenylporphyrin long-range exciton coupling. **2012**, 1, 184-94		18
1454	Modeling adsorption in metal-organic frameworks with open metal sites: propane/propylene separations. **2012**, 28, 8537-49		64
1453	Absorption and fluorescence spectra of heterocyclic isomers from long-range-corrected density functional theory in polarizable continuum approach. *Journal of Physical Chemistry A*, **2012**, 116, 3048-55	2.8	33
1452	Nonmechanical Conductance Switching in a Molecular Tunnel Junction. **2012**, 3, 498-502		16
1451	Bathochromic Shift in Green Fluorescent Protein: A Puzzle for QM/MM Approaches. *Journal of Chemical Theory and Computation*, **2012**, 8, 112-24	6.4	84

1450	Donor–acceptor dyes incorporating a stable dibenzosilole–conjugated spacer for dye-sensitized solar cells. **2012**, 22, 10771		43
1449	A qualitative failure of B3LYP for textbook organic reactions. **2012**, 14, 7170-5		52
1448	Towards a Greater Accuracy in DFT Calculations: From GGA to Hybrid Functionals. **2012**, 3-15		
1447	A theoretical study of an unusual Y-shaped three-coordinate Pt complex: Pt(0)–disilane complex or Pt(II) disilyl complex?. **2012**, 134, 11749-59		34
1446	Excitation energies from range-separated time-dependent density and density matrix functional theory. *Journal of Chemical Physics*, **2012**, 136, 184105	3.9	19
1445	A multiconfigurational hybrid density-functional theory. *Journal of Chemical Physics*, **2012**, 137, 044104	3.9	65
1444	Density functional theory with fractional orbital occupations. *Journal of Chemical Physics*, **2012**, 136, 154104	3.9	99
1443	Optical absorption spectra of gold clusters Au(n) (n = 4, 6, 8,12, 20) from long-range corrected functionals with optimal tuning. *Journal of Chemical Physics*, **2012**, 137, 114302	3.9	52
1442	Characterization of the temporary anion states on perfluoroalkanes via stabilized Koopmans' theorem in long-range corrected density functional theory. *Journal of Physical Chemistry A*, **2012**, 116, 3224-36	2.8	12
1441	A pass too far: dissociation of internal energy selected paracyclophane cations, theory and experiment. **2012**, 14, 11920-9		14
1440	Complexes of tetracyclines with divalent metal cations investigated by stationary and femtosecond-pulsed techniques. **2012**, 14, 823-34		66
1439	Density-Functional Approximations for Exchange and Correlation. **2012**, 125-156		9
1438	Fullerene–Porphyrin Dyads. **2012**, 113-122		
1437	Nonlinear Optical Properties of Fullerene Derivatives. **2012**, 49-97		
1436	Range-Separated Exchange Functionals with Slater-Type Functions. *Journal of Chemical Theory and Computation*, **2012**, 8, 901-7	6.4	86
1435	Predicting Nuclear Resonance Vibrational Spectra of [Fe(OEP)(NO)]. *Journal of Chemical Theory and Computation*, **2012**, 8, 214-223	6.4	18
1434	Many-body Green's function study of coumarins for dye-sensitized solar cells. **2012**, 86,		48
1433	Experiment and theoretical modeling of the luminescence of silver nanoclusters dispersed in oxyfluoride glass. *Journal of Chemical Physics*, **2012**, 136, 174108	3.9	34

1432	Quantum Systems in Chemistry and Physics. **2012**,		2
1431	Fundamentals of Time-Dependent Density Functional Theory. **2012**,		277
1430	Improved semiconductor lattice parameters and band gaps from a middle-range screened hybrid exchange functional. **2012**, 24, 145504		62
1429	Resolutions of the Coulomb operator. VI. Computation of auxiliary integrals. *Journal of Chemical Physics*, **2012**, 136, 104102	3.9	9
1428	Rapid computation of intermolecular interactions in molecular and ionic clusters: self-consistent polarization plus symmetry-adapted perturbation theory. **2012**, 14, 7679-99		48
1427	Facet-Dependent Catalytic Activity of Gold Nanocubes, Octahedra, and Rhombic Dodecahedra toward 4-Nitroaniline Reduction. **2012**, 116, 23757-23763		179
1426	Assessment of DFT Exchange-Correlation Functionals for Evaluating the Multipolar Contributions to the Quadratic Nonlinear Optical Responses of Small Reference Molecules. *Journal of Chemical Theory and Computation*, **2012**, 8, 2044-52	6.4	42
1425	Tautomerism in 1-phenylazo-4-naphthols: Experimental results vs quantum-chemical predictions. **2012**, 92, 714-723		30
1424	Theoretical study of static (Hyper)polarizabilities of twisted intramolecular charge transfer chromophores. *International Journal of Quantum Chemistry*, **2012**, 112, 1086-1096	2.1	5
1423	Excited states of the green fluorescent protein chromophore: Performance of ab initio and semi-empirical methods. **2012**, 249, 392-400		29
1422	Range separated functionals in the density functional based tight-binding method: Formalism. **2012**, 249, 237-244		37
1421	Spectroscopic properties of mono- and bis-azopyrroles. *International Journal of Quantum Chemistry*, **2012**, 112, 2043-2050	2.1	1
1420	The Importance of the DFT method on the computation of the second hyperpolarizability of semiconductor clusters of increasing size: A critical analysis on prolate aluminum phosphide clusters. *International Journal of Quantum Chemistry*, **2012**, 112, 2115-2125	2.1	17
1419	Impurity hamiltonian for transition metal complexes based on the exact exchange for correlated electrons hybrid functional. *International Journal of Quantum Chemistry*, **2012**, 112, 2691-2700	2.1	
1418	Why are the Interaction Energies of Charge-Transfer Complexes Challenging for DFT?. *Journal of Chemical Theory and Computation*, **2012**, 8, 1629-40	6.4	141
1417	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2012**, 8, 1515-31	6.4	642
1416	Challenges for density functional theory. **2012**, 112, 289-320		1521
1415	Performance of the M11 and M11-L density functionals for calculations of electronic excitation energies by adiabatic time-dependent density functional theory. **2012**, 14, 11363-70		109

1414	Stable alkanes containing very long carbon-carbon bonds. **2012**, 134, 13641-50		153
1413	The role of the basis set and the level of quantum mechanical theory in the prediction of the structure and reactivity of cisplatin. *Journal of Computational Chemistry*, **2012**, 33, 2292-302	3.5	33
1412	Infinite Basis Set Extrapolation for Double Hybrid Density Functional Theory 2: Effect of Adding Diffuse Basis Functions. **2012**, 59, 1094-1103		4
1411	StructureProperty Relationships in PtII Diimine-Dithiolate Nonlinear Optical Chromophores Based on Arylethylene-1,2-dithiolate and 2-Thioxothiazoline-4,5-dithiolate. **2012**, 2012, 3577-3594		18
1410	Unexpectedly strong anion-interactions on the graphene flakes. *Journal of Computational Chemistry*, **2012**, 33, 1328-37	3.5	71
1409	Tuned Range-Separated Time-Dependent Density Functional Theory Applied to Optical Rotation. *Journal of Chemical Theory and Computation*, **2012**, 8, 245-56	6.4	92
1408	Time-dependent density functional theory (TDDFT) modelling of Pechmann dyes: from accurate absorption maximum prediction to virtual dye screening. **2012**, 10, 6682-92		52
1407	Time-dependent density functional theory benchmarking for the calculations of atomic spectra: efficiency of exc-ETDZ basis set. **2012**, 131, 1		7
1406	On the potential application of DFT methods in predicting the interaction-induced electric properties of molecular complexes. Molecular H-bonded chains as a case of study. *Journal of Molecular Modeling*, **2012**, 18, 3073-86	2	27
1405	Range-separated density functional theory: A 4-component relativistic study of the rare gas dimers He2, Ne2, Ar2, Kr2, Xe2, Rn2 and Uuo2. **2012**, 395, 54-62		34
1404	Probing microcluster formation between PACO and solvents containing oxygen donor sites mediated by the NH Bond. **2012**, 402, 96-104		4
1403	New range-separated hybrids based on the TCA density functional. **2012**, 519-520, 145-149		5
1402	Assessment of chemical core potentials for the computation on enthalpies of formation of transition-metal complexes. **2012**, 521, 150-156		11
1401	Increasing the applicability of DFT I: Non-variational correlation corrections from HartreeBock DFT for predicting transition states. **2012**, 524, 10-15		61
1400	Tuned CAM-B3LYP functional in the time-dependent density functional theory scheme for excitation energies and properties of diarylethene derivatives. **2012**, 235, 29-34		65
1399	Theoretical investigation on redox-switchable second-order nonlinear optical responses of push-pull Cp*CoEt2C2B4H3-expanded (metallo)porphyrins. *Journal of Computational Chemistry*, **2012**, 33, 211-9	3.5	26
1398	Electronic structure theory: present and future challenges. **2012**, 131, 1		7
1397	Theoretical study of electronic absorptions in aminopyridines - TCNE CT complexes by quantum chemical methods, including solvent. *Journal of Molecular Modeling*, **2013**, 19, 4639-50	2	5

1396	Influences of dispersion and long-range corrections on molecular structures of three types of lithium phthalocyanine dimer. *International Journal of Quantum Chemistry*, **2013**, 113, 272-276	2.1	19
1395	Antidot effects on the open-shell characters and second hyperpolarizabilities of rectangular graphene nanoflakes. *International Journal of Quantum Chemistry*, **2013**, 113, 605-611	2.1	3
1394	Self-consistent field treatment and analytical energy gradient of local response dispersion method. *International Journal of Quantum Chemistry*, **2013**, 113, 257-262	2.1	16
1393	SCC-DFTB calculation of the static first hyperpolarizability: from gas phase molecules to functionalized surfaces. *Journal of Chemical Physics*, **2013**, 138, 204107	3.9	13
1392	Nonlinear optical properties of DPO and DMPO: a theoretical and computational study. **2013**, 132, 1		21
1391	Alkyl mercury compounds: an assessment of DFT methods. **2013**, 132, 1		16
1390	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. *Journal of Chemical Theory and Computation*, **2013**, 9, 3872-7	6.4	248
1389	On asymptotic behavior of density functional theory. *Journal of Chemical Physics*, **2013**, 139, 024104	3.9	28
1388	Performance of conventional and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. **2013**, 15, 12821-8		101
1387	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. *Journal of Computational Chemistry*, **2013**, 34, 2079-90	3.5	27
1386	Long-range corrected density functionals combined with local response dispersion: A promising method for weak interactions. *Journal of Computational Chemistry*, **2013**, 34, 2353-9	3.5	5
1385	Influence of fluorination on UV spectra of polyurethane structural fragments. **2013**, 80, 319-325		
1384	Comparison of TD-DFT Methods for the Calculation of Two-Photon Absorption Spectra of Oligophenylvinylenes. **2013**, 117, 18170-18189		50
1383	Performance of DFT Methods in Momentum Space: Quantum Similarity Measures versus Moments of Momentum. *Journal of Chemical Theory and Computation*, **2013**, 9, 3908-16	6.4	
1382	Chemically intuitive indices for charge-transfer excitation based on SAC-CI and TD-DFT calculations. *Journal of Computational Chemistry*, **2013**, 34, 2498-501	3.5	24
1381	Comparative assessment of density functionals for excited-state dipole moments. **2013**, 584, 58-62		8
1380	Avoiding pitfalls of a theoretical approach: the harmonic oscillator measure of aromaticity index from quantum chemistry calculations. **2013**, 24, 1171-1184		27
1379	Polarizability of C60 fullerene dimer and oligomers: the unexpected enhancement and its use for rational design of fullerene-based nanostructures with adjustable properties. *RSC Advances*, **2013**, 3, 19430	3.7	39

1378	Assessing the quantum mechanical level of theory for prediction of linear and nonlinear optical properties of push-pull organic molecules. *Journal of Molecular Modeling*, **2013**, 19, 2079-90	2	14
1377	Computational Modeling of Isoindigo-Based Polymers Used in Organic Solar Cells. **2013**, 117, 17940-17954		27
1376	Electrostatic Potential of Insulin: Exploring the Limitations of Density Functional Theory and Force Field Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 3978-85	6.4	35
1375	Many-body Green's function GW and Bethe-Salpeter study of the optical excitations in a paradigmatic model dipeptide. *Journal of Chemical Physics*, **2013**, 139, 194308	3.9	44
1374	Photochromic and nonlinear optical properties of fulgides: A density functional theory study. **2013**, 1022, 82-85		26
1373	Density functional theory for comprehensive orbital energy calculations. *Journal of Chemical Physics*, **2013**, 139, 064102	3.9	20
1372	Using optimally tuned range separated hybrid functionals in ground-state calculations: consequences and caveats. *Journal of Chemical Physics*, **2013**, 138, 204115	3.9	140
1371	Evaluating push-pull dye efficiency using TD-DFT and charge transfer indices. **2013**, 15, 20210-9		53
1370	Structure and intermolecular vibrations of perylene•trans-1,2-dichloroethene, a weak charge-transfer complex. *Journal of Physical Chemistry A*, **2013**, 117, 10702-13	2.8	10
1369	Theoretical investigations of ferrocene/ferrocenium solvation in imidazolium-based room-temperature ionic liquids. **2013**, 15, 2669-83		20
1368	Optical absorption in donor-acceptor polymers--alternating vs. random. **2013**, 15, 20016-25		12
1367	Performance of modified Lennard□ones potential to seed ab initio calculations of small cadmium clusters. **2013**, 1021, 249-255		8
1366	Intermolecular interaction as the origin of red shifts in absorption spectra of zinc-phthalocyanine from first-principles. *Journal of Physical Chemistry A*, **2013**, 117, 11246-53	2.8	33
1365	Investigation of Linear and Nonlinear Raman Scattering for Isotopologues of Ru(bpy)32+. **2013**, 117, 20855-20866		14
1364	Theoretical Study on the Electronic Structure and Third-Order Nonlinear Optical Properties of Open-Shell Quinoidal Oligothiophenes. **2013**, 117, 21498-21508		23
1363	Ab initio modeling of excitonic and charge-transfer states in organic semiconductors: the PTB1/PCBM low band gap system. **2013**, 135, 18252-5		52
1362	Ground- and Excited-State Geometry Optimization of Small Organic Molecules with Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2013**, 9, 5513-25	6.4	44
1361	Polarization response of methane encapsulated in water cages. **2013**, 1013, 52-56		4

1360	Efficient Monomer-Based Quantum Chemistry Methods for Molecular and Ionic Clusters. **2013**, 9, 25-58		31
1359	Density-dependent onset of the long-range exchange: a key to donor-acceptor properties. *Journal of Physical Chemistry A*, **2013**, 117, 11580-6	2.8	18
1358	Quantum chemistry, reaction kinetics, and tunneling effects in the reaction of methoxy radicals with O(2). *Journal of Physical Chemistry A*, **2013**, 117, 14230-42	2.8	15
1357	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. **2013**, 132, 1		12
1356	Cation-cation interactions in [(UO2)2(OH)n](4-n) complexes. *Inorganic Chemistry*, **2013**, 52, 11269-79	5.1	8
1355	Electronic structure calculations for the study of D-□A organic sensitizers: Exploring polythiophene linkers. **2013**, 423, 157-166		6
1354	Spectral signatures of thieno[3,4-b]pyrazines: Theoretical interpretations and design of improved structures. **2013**, 99, 972-978		19
1353	Switching of emissive and NLO properties in push-pull chromophores with crescent PPV-like structures. **2013**, 15, 1666-74		38
1352	Solvent effect on excited states of merocyanines: A theoretical study using the RISM□SCF method. **2013**, 583, 69-73		6
1351	Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. **2013**, 15, 14581-94		79
1350	Evaluation of photodissociation spectroscopy as a structure elucidation tool for isolated clusters: a case study of Ag4(+) and Au4(+). **2013**, 15, 19715-23		34
1349	On the nature of unusual intensity changes in the infrared spectra of the enflurane···acetone complexes. **2013**, 15, 6001-7		13
1348	C□H···□ interactions as modulators of carbocation structure □ implications for terpene biosynthesis. **2013**, 4, 2512		37
1347	A theoretical study of luminescent vapochromic compounds including an AuCu2(NHC)2 core. **2013**, 42, 4809-21		7
1346	Charge-Transfer Excited States and Proton Transfer in Model Guanine-Cytosine DNA Duplexes in Water. **2013**, 4, 2540-2545		28
1345	Modeling Excited States and Alignment of Energy Levels in Dye-Sensitized Solar Cells: Successes, Failures, and Challenges. **2013**, 117, 3685-3700		117
1344	Charge Transfer or J-Coupling? Assignment of an Unexpected Red-Shifted Absorption Band in a Naphthalenediimide-Based Metal-Organic Framework. **2013**, 4, 453-8		55
1343	Theoretical Approach to the Study of Thiophene-Based Discotic Systems As Organic Semiconductors. **2013**, 117, 15-22		9

1342	Assessment of local response dispersion method for open-shell systems. **2013**, 556, 386-392		9
1341	Induced optical activity of DNA-templated cyanine dye aggregates: exciton coupling theory and TD-DFT studies. *Journal of Physical Chemistry A*, **2013**, 117, 5909-18	2.8	12
1340	Interfacial States in Donor-Acceptor Organic Heterojunctions: Computational Insights into Thiophene-Oligomer/Fullerene Junctions. *Journal of Chemical Theory and Computation*, **2013**, 9, 533-42	6.4	36
1339	Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2013**, 9, 263-72	6.4	321
1338	Reaction energetics on long-range corrected density functional theory: Diels-Alder reactions. *Journal of Computational Chemistry*, **2013**, 34, 379-86	3.5	30
1337	Assessment of long-range corrected functionals for the prediction of non-linear optical properties of organic materials. **2013**, 575, 122-125		53
1336	Computational investigation of first hyperpolarizability in substituted hydrazones. **2013**, 581, 42-46		3
1335	Modeling materials and processes in dye-sensitized solar cells: understanding the mechanism, improving the efficiency. **2014**, 352, 151-236		18
1334	Importance of spin□rbit coupling effect and solvent effect in electronic transition assignments of PtII complexes: In the case of cis/trans-[PtIICl2(NH3)2]. *Journal of Molecular Structure*, **2013**, 1035, 218-223	1.4	3
1333	Long-range corrected density functional theory with optimized one-parameter progressive correlation functional (LC-BOP12 and LCgau-BOP12). **2013**, 563, 15-19		16
1332	Tuning the NLO properties of polymethineimine chains by chemical substitution. **2013**, 415, 196-206		8
1331	Non-empirical tuning of CAM-B3LYP functional in time-dependent density functional theory for excitation energies of diarylethene derivatives. **2013**, 585, 201-206		22
1330	Ground and excited states of BF3+. Coupled cluster and density functional studies. **2013**, 423, 151-156		2
1329	Assessing the performance of density functional theory for the dynamic polarizabilities of amino acids: Treatment of correlation and role of exact exchange. *International Journal of Quantum Chemistry*, **2013**, 113, 1803-1811	2.1	7
1328	Electronic structure of the S1 state in methylcobalamin: insight from CASSCF/MC-XQDPT2, EOM-CCSD, and TD-DFT calculations. *Journal of Computational Chemistry*, **2013**, 34, 987-1004	3.5	49
1327	Long-range corrected functionals satisfy Koopmans' theorem: calculation of correlation and relaxation energies. *Journal of Computational Chemistry*, **2013**, 34, 958-64	3.5	46
1326	Modeling of phytochrome absorption spectra. *Journal of Computational Chemistry*, **2013**, 34, 1363-74	3.5	24
1325	Multi-configuration time-dependent density-functional theory based on range separation. *Journal of Chemical Physics*, **2013**, 138, 084101	3.9	72

1324	Understanding the Second-Order Nonlinear Optical Properties of One-Dimensional Ruthenium(II) Ammine Complexes. **2013**, 117, 1833-1848		25
1323	The calculations of excited-state properties with Time-Dependent Density Functional Theory. **2013**, 42, 845-56		1048
1322	Modeling Transition Metal Reactions with Range-Separated Functionals. *Journal of Chemical Theory and Computation*, **2013**, 9, 2286-99	6.4	20
1321	Atropisomers of arylmaleimides: stereodynamics and absolute configuration. **2013**, 78, 3709-19		26
1320	Effective fragment potential method in Q-CHEM: a guide for users and developers. *Journal of Computational Chemistry*, **2013**, 34, 1060-70	3.5	44
1319	On the performance of long-range-corrected density functional theory and reduced-size polarized LPol-n basis sets in computations of electric dipole (hyper)polarizabilities of π-conjugated molecules. *Journal of Computational Chemistry*, **2013**, 34, 819-26	3.5	24
1318	Nonprecious-metal-assisted photochemical hydrogen production from ortho-phenylenediamine. **2013**, 135, 8646-54		43
1317	DFT calculations of effective exchange integrals at the complete basis set limit on oxo-vanadium ring complex. **2013**, 66, 97-101		6
1316	Q-Chem: an engine for innovation. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 317-326	7.9	257
1315	Repulsion integrals involving Slater-type functions and Yukawa potential. **2013**, 132, 1		9
1314	Noncovalent interactions of metal cations and arenes probed with thallium(I) complexes. *Inorganic Chemistry*, **2013**, 52, 5749-56	5.1	14
1313	Trajectory-based nonadiabatic dynamics with time-dependent density functional theory. *ChemPhysChem*, **2013**, 14, 1314-40	3.2	143
1312	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. *Journal of Chemical Theory and Computation*, **2013**, 9, 2749-60	6.4	196
1311	Photophysics of push-pull distyrylfurans, thiophenes and pyridines by fast and ultrafast techniques. *ChemPhysChem*, **2013**, 14, 970-81	3.2	28
1310	BN Segment Doped Effect on the First Hyperpolarizibility of Heteronanotubes: Focused on an Effective Connecting Pattern. **2013**, 117, 10039-10044		24
1309	TD-DFT study on the charge-transfer excitations of anions possessing double or triple bonds. **2013**, 1014, 49-55		4
1308	Influence of the delocalization error and applicability of optimal functional tuning in density functional calculations of nonlinear optical properties of organic donor-acceptor chromophores. *ChemPhysChem*, **2013**, 14, 2450-61	3.2	110
1307	Calculating excited states of molecular aggregates by the renormalized excitonic method. *Journal of Physical Chemistry A*, **2013**, 117, 3655-65	2.8	16

1306	Intramolecular halogen-halogen bonds?. **2013**, 15, 11543-53		53
1305	Assessment of density functional methods with correct asymptotic behavior. **2013**, 15, 8352-61		44
1304	Modeling noncovalent radical-molecule interactions using conventional density-functional theory: beware erroneous charge transfer. *Journal of Physical Chemistry A*, **2013**, 117, 947-52	2.8	37
1303	Assessment of range-separated time-dependent density-functional theory for calculating C6 dispersion coefficients. *Journal of Chemical Physics*, **2013**, 138, 194106	3.9	17
1302	Non-covalent interactions and thermochemistry using XDM-corrected hybrid and range-separated hybrid density functionals. *Journal of Chemical Physics*, **2013**, 138, 204109	3.9	109
1301	Recent advances in the use of density functional theory to design efficient solar energy-based renewable systems. **2013**, 5, 022701		9
1300	Assessment of the performance of long-range-corrected density functionals for calculating the absorption spectra of silver clusters. *Journal of Physical Chemistry A*, **2013**, 117, 4267-78	2.8	41
1299	Performance of density functional theory in computing nonresonant vibrational (hyper)polarizabilities. *Journal of Computational Chemistry*, **2013**, 34, 1775-84	3.5	39
1298	Which density functional is close to CCSD accuracy to describe geometry and interaction energy of small non-covalent dimers? A benchmark study using Gaussian09. *Journal of Computational Chemistry*, **2013**, 34, 1341-53	3.5	92
1297	A Density Functional Theory Based Protocol to Compute the Redox Potential of Transition Metal Complex with the Correction of Pseudo-Counterion: General Theory and Applications. *Journal of Chemical Theory and Computation*, **2013**, 9, 2974-80	6.4	29
1296	Modeling catalytic promiscuity in the alkaline phosphatase superfamily. **2013**, 15, 11160-77		41
1295	TD-DFT benchmarks: A review. *International Journal of Quantum Chemistry*, **2013**, 113, 2019-2039	2.1	715
1294	Supramolecular step in design of nonlinear optical materials: Effect of □.□stacking aggregation on hyperpolarizability. *Journal of Chemical Physics*, **2013**, 139, 094310	3.9	70
1293	Binding in Radical-Solvent Binary Complexes: Benchmark Energies and Performance of Approximate Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 1568-79	6.4	41
1292	Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer. *Journal of Chemical Theory and Computation*, **2013**, 9, 3848-54	6.4	2
1291	Finite-field method with unbiased polarizable continuum model for evaluation of the second hyperpolarizability of an open-shell singlet molecule in solvents. *Journal of Computational Chemistry*, **2013**, 34, 2345-52	3.5	1
1290	Novel approach to excited-state calculations of large molecules based on divide-and-conquer method: application to photoactive yellow protein. **2013**, 117, 5565-73		31
1289	Dielectric constant of NiO and LDA+U. **2013**, 87,		10

1288	Theoretical study of the photoelectron spectrum of ethyl formate: Ab initio and density functional theory investigation. **2013**, 222, 2257-2266		7
1287	The Performance of Density Functionals for Sulfate-Water Clusters. *Journal of Chemical Theory and Computation*, **2013**, 9, 1368-80	6.4	61
1286	Assessment of Tuning Methods for Enforcing Approximate Energy Linearity in Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2013**, 9, 4414-20	6.4	29
1285	Probing the performances of HISS functionals for the description of excited states of molecular systems. **2013**, 132, 1		1
1284	Resonant and Nonresonant Hyperpolarizabilities of Spatially Confined Molecules: A Case Study of Cyanoacetylene. *Journal of Chemical Theory and Computation*, **2013**, 9, 3463-72	6.4	25
1283	Appropriate description of intermolecular interactions in the methane hydrates: an assessment of DFT methods. *Journal of Computational Chemistry*, **2013**, 34, 121-31	3.5	99
1282	Extreme density-driven delocalization error for a model solvated-electron system. *Journal of Chemical Physics*, **2013**, 139, 184116	3.9	75
1281	Interface dipoles of organic molecules on Ag(111) in hybrid density-functional theory. **2013**, 15, 123028		54
1280	Asymptotic correction schemes for semilocal exchange-correlation functionals. **2013**, 87,		10
1279	Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory. *Journal of Chemical Physics*, **2013**, 139, 134113	3.9	30
1278	Electronic excitations from a linear-response range-separated hybrid scheme. **2013**, 111, 1219-1234		20
1277	A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules. *Journal of Chemical Physics*, **2013**, 138, 244104	3.9	176
1276	Superphenalenyl: Theoretical Design of a Conjugated Planar Hydrocarbon Radical. **2013**, 42, 1386-1387		4
1275	Time-dependent Density Functional-based Tight-bind Method Efficiently Implemented with OpenMP Parallel and GPU Acceleration. **2013**, 26, 635-645		29
1274	DFT Study on the Co-Xe Bond in the HCo(CO)3Xe Adduct. **2014**, 2014, 1-5		
1273	Chiroptical properties and the racemization of pyrene and tetrathiafulvalene-substituted allene: substitution and solvent effects on racemization in tetrathiafulvalenylallene. *Molecules*, **2014**, 19, 2829-41	4.8	7
1272	Relativistic Density Functional Theory. **2014**, 13, 71-82		1
1271	Theoretical Study on Excess-Electron Transfer in DNA Based on the Marcus Theory. **2014**, 13, 242-249		

1270	Application of long-range corrected density-functional theory to excess electron attachment to biomolecules. **2014**, 1046, 99-106		13
1269	Symmetry-adapted perturbation theory with Kohn-Sham orbitals using non-empirically tuned, long-range-corrected density functionals. *Journal of Chemical Physics*, **2014**, 140, 044108	3.9	24
1268	Understanding molecular structure dependence of exciton diffusion in conjugated small molecules. **2014**, 104, 143303		7
1267	Local-hybrid functional based on the correlation length. *Journal of Chemical Physics*, **2014**, 141, 124120	3.9	26
1266	TDDFT assessment of functionals for optical 0-0 transitions in small radicals. *Journal of Physical Chemistry A*, **2014**, 118, 11033-46	2.8	12
1265	Practical auxiliary basis implementation of Rung 3.5 functionals. *Journal of Chemical Physics*, **2014**, 141, 034103	3.9	22
1264	Charge transfer mechanism of SERS for metal□molecule□metal junction supported by graphene and boron-doped graphene. *RSC Advances*, **2014**, 4, 63596-63602	3.7	9
1263	On the structures, lifetimes, and infrared spectra of alkylmercury hydrides. *ChemPhysChem*, **2014**, 15, 530-41	3.2	3
1262	Can short- and middle-range hybrids describe the hyperpolarizabilities of long-range charge-transfer compounds?. *Journal of Physical Chemistry A*, **2014**, 118, 11787-96	2.8	45
1261	Ab initio calculation of the electronic absorption spectrum of liquid water. *Journal of Chemical Physics*, **2014**, 140, 164511	3.9	6
1260	Increasing the applicability of density functional theory. IV. Consequences of ionization-potential improved exchange-correlation potentials. *Journal of Chemical Physics*, **2014**, 140, 18A534	3.9	56
1259	Tuned range-separated hybrid functionals in the symmetry-adapted perturbation theory. *Journal of Chemical Physics*, **2014**, 141, 134120	3.9	13
1258	Density Functional Theory Beyond the Generalized Gradient Approximation for Surface Chemistry. **2014**, 25-51		9
1257	Benchmarking the AK13 Exchange Functional: Ionization Potentials and Electron Affinities. *Journal of Chemical Theory and Computation*, **2014**, 10, 5625-9	6.4	15
1256	The formulation of a constricted variational density functional theory for double excitations. **2014**, 112, 661-668		8
1255	Application of the Stabilized Koopmans□Theorem to the Temporary Anion States of Chlorosilanes in Long-Range Corrected Density Functional Theory. **2014**, 61, 1313-1325		2
1254	Constricted Variational Density Functional Theory Approach to the Description of Excited States. **2016**, 368, 61-95		5
1253	Surface Hopping Dynamics with DFT Excited States. **2016**, 368, 415-44		48

1252	8th Congress on Electronic Structure: Principles and Applications (ESPA 2012). **2014**,		
1251	Competing Deactivation Channels for Excited Stacked Cytosines. **2014**, 2014, 1-9		1
1250	Testing an excited-state energy density functional and the associated potential with the ionization potential theorem. **2014**, 47, 115005		7
1249	Free base phthalocyanine: Influence of thermal effects and dimerization on the electronic absorption spectrum. **2014**, 595-596, 97-102		6
1248	A Brief Compendium of Time-Dependent Density Functional Theory. **2014**, 44, 154-188		67
1247	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. **2014**, 372, 20120476		514
1246	Halogen bonds with benzene: an assessment of DFT functionals. *Journal of Computational Chemistry*, **2014**, 35, 386-94	3.5	65
1245	Strategies for Designing Diarylethenes as Efficient Nonlinear Optical Switches. **2014**, 118, 4334-4345		31
1244	Assessing long-range corrected functionals with physically-adjusted range-separated parameters for calculating the polarizability and the second hyperpolarizability of polydiacetylene and polybutatriene chains. **2014**, 16, 7083-8		57
1243	Assessment of the global and range-separated hybrids for computing the dynamic second-order hyperpolarizability of solution-phase organic molecules. **2014**, 133, 1		5
1242	A computational study of the nonlinear optical properties of carbazole derivatives: theory refines experiment. **2014**, 133, 1		30
1241	What makes differences between intra- and inter-molecular charge transfer excitations in conjugated long-chained polyene? EOM-CCSD and LC-BOP study. **2014**, 133, 1		8
1240	Novel metal organic framework linkers for light harvesting applications. **2014**, 5, 2081-2090		136
1239	RETRACTED: DFT flavor of coordination chemistry. **2014**, 272, 1-29		145
1238	Density Functional Theory in Quantum Chemistry. **2014**,		90
1237	Helical Carbon Segment in Carbon Boron Nitride Heteronanotubes: Structure and Nonlinear Optical Properties. **2014**, 79, 732-736		16
1236	Dramatic changes in electronic structure revealed by fractionally charged nuclei. *Journal of Chemical Physics*, **2014**, 140, 044110	3.9	22
1235	DFT studies on the tetranuclear cubane complex [Ni4(ampd)4(Cl4)]·MeCN. **2014**, 55, 30-37		4

1234	Energy decomposition scheme based on the generalized Kohn-Sham scheme. *Journal of Physical Chemistry A*, **2014**, 118, 2531-42	2.8	91
1233	Introducing constricted variational density functional theory in its relaxed self-consistent formulation (RSCF-CV-DFT) as an alternative to adiabatic time dependent density functional theory for studies of charge transfer transitions. *Journal of Chemical Physics*, **2014**, 140, 18A502	3.9	23
1232	Perspective: Fifty years of density-functional theory in chemical physics. *Journal of Chemical Physics* , **2014**, 140, 18A301	3.9	826
1231	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. **2014**, 1-23		15
1230	Substituent effects on absorption spectra of pH indicators: An experimental and computational study of sulfonphthaleine dyes. **2014**, 102, 241-250		61
1229	Achieving High-Accuracy Intermolecular Interactions by Combining Coulomb-Attenuated Second-Order M□ ller-Plesset Perturbation Theory with Coupled Kohn-Sham Dispersion. *Journal of Chemical Theory and Computation*, **2014**, 10, 2054-63	6.4	13
1228	Thermally-assisted-occupation density functional theory with generalized-gradient approximations. *Journal of Chemical Physics*, **2014**, 140, 18A521	3.9	49
1227	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. *Journal of Chemical Theory and Computation*, **2014**, 10, 1934-1952	6.4	109
1226	Electronic responses of long chains to electrostatic fields: Hartree-Fock vs. density-functional theory: a model study. *Journal of Chemical Physics*, **2014**, 140, 054117	3.9	8
1225	Trihalide cations MF3 +, MCl3 + and MBr +3 , M = B, Al, Ga: pseudo Jahn□ eller coupling, electronic spectra and ionization potentials of MX3. **2014**, 133, 1		2
1224	NIR Emission in Borondifluoride Complexes of 2?-Hydroxychalcone Derivatives Containing an Acetonaphthone Ring. **2014**, 118, 11906-11918		22
1223	Quantum Mechanics for Organic Chemistry. **2014**, 1-60		1
1222	Charge transport and optical properties of cross-conjugated organic molecules: A theoretical study. **2014**, 15, 1607-1623		13
1221	Electronic Energy Gaps for □Conjugated Oligomers and Polymers Calculated with Density Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 1035-47	6.4	111
1220	Density functional theory prediction for the second-order nonlinear optical responses of phenanthroline-fused phthalocyanine derivatives. **2014**, 18, 58-66		2
1219	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. *Journal of Chemical Theory and Computation*, **2014**, 10, 102-21	6.4	55
1218	25th anniversary article: Design of polymethine dyes for all-optical switching applications: guidance from theoretical and computational studies. **2014**, 26, 68-83		84
1217	Long-range correction for density functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 375-390	7.9	98

1216	Critical role of deep hydrogen tunneling to accelerate the antioxidant reaction of ubiquinol and vitamin E. **2014**, 118, 937-50		19
1215	Theoretical and computational studies of conformation, natural bond orbital and nonlinear optical properties of cis-N-phenylbenzohydroxamic acid. **2014**, 1028, 65-71		8
1214	Experimental and theoretical studies of the second- and third-order NLO properties of a semi-organic compound: 6-Aminoquinolinium iodide monohydrate. **2014**, 428, 67-74		29
1213	Electronic structure of conducting organic polymers: insights from time-dependent density functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 601-622	7.9	70
1212	Axial chirality of 4-arylpyrazolo[3,4-b]pyridines. Conformational analysis and absolute configuration. **2014**, 79, 11039-50		23
1211	A perspective on the relative merits of time-dependent and time-independent density functional theory in studies of the electron spectra due to transition metal complexes. An illustration through applications to copper tetrachloride and plastocyanin. *International Journal of Quantum Chemistry*, **2014**, 114, 1019-1029	2.1	18
1210	BODIPY-bridged push-pull chromophores for nonlinear optical applications. *ChemPhysChem*, **2014**, 15, 2693-700	3.2	62
1209	Double hybrid density-functional theory using the coulomb-attenuating method. *International Journal of Quantum Chemistry*, **2014**, 114, 1199-1211	2.1	25
1208	Gas-phase valence-electron photoemission spectroscopy using density functional theory. **2014**, 347, 137-91		35
1207	Visible light-induced diastereoselective E/Z-photoisomerization equilibrium of the C=C benzofuran-3-one-hydantoin dyad. **2014**, 27, 756-763		6
1206	Impact of ground- and excited-state aromaticity on cyclopentadiene and silole excitation energies and excited-state polarities. **2014**, 20, 9295-303		50
1205	Status in calculating electronic excited states in transition metal oxides from first principles. **2014**, 347, 47-98		14
1204	Effect of Donor-Acceptor Substitution on Optoelectronic Properties of Conducting Organic Polymers. *Journal of Chemical Theory and Computation*, **2014**, 10, 4921-37	6.4	24
1203	Self-interaction corrections in density functional theory. *Journal of Chemical Physics*, **2014**, 140, 18A513	3.9	52
1202	Structure-sensitive bend elastic constants between piconewton and subnanonewton in diphenylacetylene-core-based liquid crystals. **2014**, 90, 042506		3
1201	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbon-tetracyanoethylene complexes. **2014**, 16, 20586-97		37
1200	The structural and energetic aspects of substrate binding and the mechanism of action of the DapE-encoded N-succinyl-L,L-diaminopimelic acid desuccinylase (DapE) investigated using a hybrid QM/MM method. **2014**, 16, 26348-58		14
1199	A double-QM/MM method for investigating donor-acceptor electron-transfer reactions in solution. **2014**, 16, 19530-9		12

1198	Receding mechanism of NLO response of polyanion [M8O26]4[(M = Cr, Mo, W) and the closed loops theory analysis. *New Journal of Chemistry*, **2014**, 38, 2619-2628	3.6	3
1197	Specific coordination phenomena of alkaline earth metal ions with aromatic sulfonate ions in alcohols and binary solvents of acetonitrile[lcohols. *Journal of Molecular Liquids*, **2014**, 199, 445-453	6	6
1196	Excited states using the simplified Tamm-Dancoff-Approach for range-separated hybrid density functionals: development and application. **2014**, 16, 14408-19		58
1195	Quantum-chemical insights into mixed-valence systems: within and beyond the Robin-Day scheme. **2014**, 43, 5067-88		132
1194	Theoretical study on excited states of bacteriochlorophyll a in solutions with density functional assessment. **2014**, 118, 10906-18		29
1193	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 4599-608	6.4	36
1192	Computational study of the working mechanism and rate acceleration of overcrowded alkene-based light-driven rotary molecular motors. *RSC Advances*, **2014**, 4, 10240	3.7	19
1191	Spin density distribution after electron transfer from triethylamine to an [Ir(ppy)2(bpy)]+ photosensitizer during photocatalytic water reduction. **2014**, 16, 4789-96		37
1190	Phosphorus(V) tetraazaporphyrins: porphyrinoids showing an exceptionally strong CT band between the Soret and Q bands. **2014**, 5, 2466-2474		23
1189	Photocurrent spectroscopic studies of diketopyrrolopyrrole-based statistical copolymers. **2014**, 16, 4291-8		6
1188	Theoretical study on diradical characters and nonlinear optical properties of 1,3-diradical compounds. *Journal of Physical Chemistry A*, **2014**, 118, 10837-48	2.8	20
1187	The derivative discontinuity of the exchange-correlation functional. **2014**, 16, 14378-87		61
1186	Theoretical studies on the quinoidal thiophene based dyes for dye sensitized solar cell and NLO applications. **2014**, 16, 21496-505		18
1185	Absorption spectra of alkali-C[hanoclusters. **2014**, 16, 22399-408		2
1184	On the performance of the Kohn-Sham orbital approach in the calculation of electron transfer parameters. The three state model. **2014**, 16, 17154-62		4
1183	Substituted diphenyl butadiynes: a computational study of geometries and electronic transitions using DFT/TD-DFT. **2014**, 16, 14015-28		23
1182	Analysis of the Resonant Raman Spectra of Viologens and of Their Radical Cations Using Range-Separated Hybrid Density Functionals. **2014**, 118, 12469-12484		11
1181	Manifestation of intrinsic defects in the band structures of quaternary chalcogenide Ag2In2SiSe6 and Ag2In2GeSe6 crystals. **2014**, 16, 9534-9544		7

1180	Solvatochromic Shift of Brooker's Merocyanine: Hartree-Fock Exchange in Time Dependent Density Functional Calculation and Hydrogen Bonding Effect. *Journal of Chemical Theory and Computation*, **2014**, 10, 4535-47	6.4	19
1179	Unveiling solvents effect on excited-state polarizabilities with the corrected linear-response model. *Journal of Physical Chemistry A*, **2014**, 118, 5652-6	2.8	11
1178	Dinuclear Ru/Ni, Ir/Ni, and Ir/Pt complexes with bridging phenanthroline-5,6-dithiolate: synthesis, structure, and electrochemical and photophysical behavior. *Inorganic Chemistry*, **2014**, 53, 8859-73	5.1	14
1177	A balanced procedure for the treatment of cluster-ligand interactions on gold phosphine systems in catalysis. *Journal of Computational Chemistry*, **2014**, 35, 986-97	3.5	23
1176	Prediction of Accurate Thermochemistry of Medium and Large Sized Radicals Using Connectivity-Based Hierarchy (CBH). *Journal of Chemical Theory and Computation*, **2014**, 10, 4342-50	6.4	15
1175	Assessment of Exchange-Correlation Functionals in Reproducing the Structure and Optical Gap of Organic-Protected Gold Nanoclusters. **2014**, 118, 7532-7544		45
1174	Polaron Structure and Transport in Fullerene Materials: Insights from First-Principles Calculations. **2014**, 118, 21785-21797		6
1173	Two-Photon Absorption in Fluorescent Protein Chromophores: TDDFT and CC2 Results. *Journal of Chemical Theory and Computation*, **2014**, 10, 3260-9	6.4	25
1172	B97X-V: a 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. **2014**, 16, 9904-24		384
1171	Effect of fluorination on electronic properties of polythienothiophene-co-benzodithiophenes and their fullerene complexes. **2014**, 6, 15889-96		13
1170	Multilithiation Effect on the First Hyperpolarizability of Carbon–Boron–Nitride Heteronanotubes: Activating Segment versus Connecting Pattern. **2014**, 118, 14185-14191		27
1169	Third-order nonlinear optical properties of one-dimensional open-shell molecular aggregates composed of phenalenyl radicals. **2014**, 20, 11129-36		42
1168	Polarizabilities from Long-Range Corrected DFT Calculations. **2014**, 59, 3160-3166		9
1167	Assessment of various electronic structure methods for characterizing temporary anion states: application to the ground state anions of N2, C2H2, C2H4, and C6H6. *Journal of Physical Chemistry A* , **2014**, 118, 7489-97	2.8	46
1166	DFT reinvestigation of DNA strand breaks induced by electron attachment. **2014**, 118, 11137-44		30
1165	Molecular double core-hole electron spectroscopy for probing chemical bonds: C60 and chain molecules revisited. **2014**, 440, 64-68		12
1164	Synthesis and photophysical properties of two-photon chromophores containing 1H-benzimidazole residue. **2014**, 111, 162-175		13
1163	Performance of the M06 family of functionals in prediction of the charge transfer transition energies of the naphthalene–TCNE and pyrene–TCNE molecular complexes. **2014**, 610-611, 19-22		7

1162	Accuracy of density functionals in the description of dispersion interactions and IR spectra of phosphates and phosphorylated compounds. *Journal of Molecular Modeling*, **2014**, 20, 2426	2	9
1161	Benchmarking DFT and TD-DFT Functionals for the Ground and Excited States of Hydrogen-Rich Peptide Radicals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3308-18	6.4	28
1160	Optimum Exchange for Calculation of Excitation Energies and Hyperpolarizabilities of Organic Electro-optic Chromophores. *Journal of Chemical Theory and Computation*, **2014**, 10, 3821-31	6.4	87
1159	Excited State Geometries and Vertical Emission Energies of Solvated Dyes for DSSC: A PCM/TD-DFT Benchmark Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 3925-33	6.4	69
1158	Multiscale Modelling of Organic and Hybrid Photovoltaics. **2014**,		12
1157	Ultraviolet□visible absorption, Raman, vibration spectra of pure silver and Ag□Cu clusters: A density functional theory study. **2014**, 451, 96-105		11
1156	Experimental and theoretical electronic structure of quinacridone. **2014**, 90,		56
1155	Metropolis Evaluation of the Hartree-Fock Exchange Energy. *Journal of Chemical Theory and Computation*, **2014**, 10, 4317-23	6.4	11
1154	Benchmarking of Density Functionals for the Accurate Description of Thiol-Disulfide Exchange. *Journal of Chemical Theory and Computation*, **2014**, 10, 4842-56	6.4	26
1153	Promising density functional theory methods for predicting the structures of uranyl complexes. *RSC Advances*, **2014**, 4, 50261-50270	3.7	4
1152	Distinguishing between keto-enol and acid-base forms of firefly oxyluciferin through calculation of excited-state equilibrium constants. *Journal of Computational Chemistry*, **2014**, 35, 2184-94	3.5	16
1151	Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. **2014**, 133, 1		5
1150	Optical spectroscopy of the bulk and interfacial hydrated electron from ab initio calculations. *Journal of Physical Chemistry A*, **2014**, 118, 7507-15	2.8	48
1149	Derivation of the RPA (Random Phase Approximation) Equation of ATDDFT (Adiabatic Time Dependent Density Functional Ground State Response Theory) from an Excited State Variational Approach Based on the Ground State Functional. *Journal of Chemical Theory and Computation*, **2014** , 10, 3380-6	6.4	11
1148	Theoretical study (CC2, DFT and PCM) of charge transfer complexes between antithyroid thioamides and TCNE: electronic CT transitions. *Journal of Molecular Modeling*, **2014**, 20, 2312	2	4
1147	Simultaneous Determination of Structures, Vibrations, and Frontier Orbital Energies from a Self-Consistent Range-Separated Hybrid Functional. **2014**, 5, 2734-41		43
1146	Synthesis, chiral resolution, and absolute configuration of dissymmetric 4,15-difunctionalized [2.2]paracyclophanes. **2014**, 79, 6679-87		28
1145	Photoexcitation of Light-Harvesting C-P-C60 Triads: A FLMO-TD-DFT Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 2436-48	6.4	28

1144	Unrestricted density functional theory based on the fragment molecular orbital method for the ground and excited state calculations of large systems. *Journal of Chemical Physics*, **2014**, 140, 144101	3.9	18
1143	Time-dependent density functional study of UV-visible absorption spectra of small noble metal clusters (Cun, Agn, Aun, n = 2, 20). *RSC Advances*, **2014**, 4, 13001	3.7	36
1142	Electronic Structures of Platinum(II) Complexes with 2-Arylpyridine and 1,3-Diketonate Ligands: A Relativistic Density Functional Study on Photoexcitation and Phosphorescent Properties. **2014**, 118, 12443-12449		9
1141	Prediction of the linear and nonlinear optical properties of tetrahydronaphthalone derivatives via long-range corrected hybrid functionals. **2014**, 112, 3165-3172		19
1140	Size dependence of the structural, electronic, and optical properties of (CdSe)n, n = 6, 60, nanocrystals. *RSC Advances*, **2014**, 4, 14613-14623	3.7	17
1139	Evaluation of the Linear and Second-Order NLO Properties of Molecular Crystals within the Local Field Theory: Electron Correlation Effects, Choice of XC Functional, ZPVA Contributions, and Impact of the Geometry in the Case of 2-Methyl-4-nitroaniline. *Journal of Chemical Theory and Computation* , **2014**, 10, 2114-24	6.4	46
1138	Computational study on redox-switchable second-order nonlinear optical properties of ferrocene-tetrathiafulvalene hybrid. *RSC Advances*, **2014**, 4, 38300-38309	3.7	7
1137	Novel [2 + 1] Concerted Reaction Path for Disilacyclobutenes with Acetylene. **2014**, 33, 763-770		5
1136	Implementation of nuclear gradients of range-separated hybrid density functionals and benchmarking on rotational constants for organic molecules. *Journal of Computational Chemistry*, **2014**, 35, 1509-16	3.5	41
1135	Electronic and optical properties of dye-sensitized TiO interfaces. **2014**, 347, 1-45		16
1134	Exciton diffusion in disordered small molecules for organic photovoltaics: insights from first-principles simulations. **2014**, 26, 185006		6
1133	Open-shell characters and second hyperpolarizabilities for hexagonal graphene nanoflakes including boron nitride domains. **2014**, 595-596, 220-225		9
1132	Electron-correlation based externally predictive QSARs for mutagenicity of nitrated-PAHs in Salmonella typhimurium TA100. **2014**, 101, 42-50		23
1131	Charge transfer optical absorption and fluorescence emission of 4-(9-acridyl)julolidine from long-range-corrected time dependent density functional theory in polarizable continuum approach. **2014**, 128, 370-6		14
1130	Effects of the basis set and of the exchange-correlation functional on the Inelastic Electron Tunneling signatures of 1,4-benzenedithiol. **2014**, 119, 34-41		3
1129	A simplified time-dependent density functional theory approach for electronic ultraviolet and circular dichroism spectra of very large molecules. **2014**, 1040-1041, 45-53		138
1128	Delocalization error and "functional tuning" in Kohn-Sham calculations of molecular properties. **2014**, 47, 2592-602		196
1127	Theoretical Study on the Ligand Exchange Reactions of Hypervalent Antimony and Tellurium Compounds. **2014**, 33, 1218-1226		6

1126	DFT Calculation of Static First Hyperpolarizabilities and Linear Optical Properties of Metal Alkynyl Complexes. **2014**, 33, 2434-2447		24
1125	Accurate Model for Predicting Adsorption of Olefins and Paraffins on MOFs with Open Metal Sites. **2014**, 53, 15475-15487		48
1124	Reactivity index based on orbital energies. *Journal of Computational Chemistry*, **2014**, 35, 1093-100	3.5	12
1123	Theoretical Study of the Local and Charge-Transfer Excitations in Model Complexes of Pentacene-C60 Using Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 2379-88	6.4	65
1122	How does LCDFT compare to SAC-CI for the treatment of valence and Rydberg excited states of organic compounds?. *Journal of Physical Chemistry A*, **2014**, 118, 1741-7	2.8	12
1121	Applications of Time Dependent and Time Independent Density Functional Theory to the First □to □ Transition in Cyanine Dyes. *Journal of Chemical Theory and Computation*, **2014**, 10, 3299-307	6.4	73
1120	Cluster Approach To Model Titanium Dioxide as Isolated or Organic Dye Sensitized Nanoobjects. **2014**, 118, 6009-6018		16
1119	Absorption and fluorescence signatures of 1,2,3-triazole based regioisomers: challenging compounds for TD-DFT. **2014**, 16, 9064-73		22
1118	Orbital gap predictions for rational design of organic photovoltaic materials. **2014**, 15, 1509-1520		95
1117	Theoretical investigation of local proton conductance in the proton exchange membranes. **2014**, 608, 11-16		8
1116	On the stability of [Pb(Proline)]2+ complexes. Reconciling theory with experiment. **2014**, 598, 91-95		6
1115	Synthesis and photophysical properties of the 2-(3-(2-Alkyl-6,8-diaryl-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)propyl)-6,8-diarylquinazolin-4(3H)-ones. *Molecules*, **2014**, 19, 9712-35	4.8	4
1114	Modeling OPV Performance□Morphology, Transport and Recombination. **2014**, 515-554		
1113	Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: A Potential Tetraradicaloid Hydrocarbon. **2015**, 127, 2118-2122		26
1112	UV Action Spectroscopy of Gas-Phase Peptide Radicals. **2015**, 6, 4722-7		25
1111	The Quantum Chemistry of Loosely-Bound Electrons. **2015**, 391-517		24
1110	Surface calculations with asymptotically long-ranged potentials in the full-potential linearized augmented plane-wave method. **2015**, 92,		7
1109	Theoretical Study on the Mechanism of the Ligand Coupling Reaction of Hypervalent Pentacoordinate Antimony Compounds. **2015**, 88, 1584-1590		1

1108	Theoretical Study of Extremely Long yet Stable Carbon–Carbon Bonds: Effect of Attractive C···H Interactions and Small Radical Stabilization of Diamondoids. **2015**, 88, 1636-1641		13
1107	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. *Journal of Chemical Physics*, **2015**, 143, 241101	3.9	40
1106	Long-range correction for tight-binding TD-DFT. *Journal of Chemical Physics*, **2015**, 143, 134120	3.9	43
1105	Size-dependent error of the density functional theory ionization potential in vacuum and solution. *Journal of Chemical Physics*, **2015**, 143, 244105	3.9	25
1104	Assessing the accuracy of some popular DFT methods for computing harmonic vibrational frequencies of water clusters. *Journal of Chemical Physics*, **2015**, 143, 214103	3.9	40
1103	Subspace formulation of time-dependent density functional theory for large-scale calculations. *Journal of Chemical Physics*, **2015**, 143, 064110	3.9	17
1102	Implementation and benchmark of a long-range corrected functional in the density functional based tight-binding method. *Journal of Chemical Physics*, **2015**, 143, 184107	3.9	53
1101	How well do static electronic dipole polarizabilities from gas-phase experiments compare with density functional and MP2 computations?. *Journal of Chemical Physics*, **2015**, 143, 144302	3.9	21
1100	Long-range corrected density functional theory with accelerated Hartree-Fock exchange integration using a two-Gaussian operator [LC-ΩPBE(2Gau)]. *Journal of Chemical Physics*, **2015**, 143, 144112	3.9	15
1099	Tuned range separated hybrid functionals for solvated low bandgap oligomers. *Journal of Chemical Physics*, **2015**, 143, 034101	3.9	39
1098	Perspective: Treating electron over-delocalization with the DFT+U method. *Journal of Chemical Physics*, **2015**, 142, 240901	3.9	113
1097	Polarizable embedding with a multiconfiguration short-range density functional theory linear response method. *Journal of Chemical Physics*, **2015**, 142, 114113	3.9	25
1096	Near-UV photodissociation of phosphopeptide cation-radicals. **2015**, 390, 71-80		9
1095	Second-Order Nonlinear Optical Properties of a Dithienylethene-Indolinooxazolidine Hybrid: A Joint Experimental and Theoretical Investigation. **2015**, 21, 18749-57		25
1094	Modulation of Energy Conversion Processes in Carbonaceous Molecular Bearings. **2015**, 10, 2404-10		14
1093	Three-dimensional reference interaction site model self-consistent field analysis of solvent and substituent effects on the absorption spectra of Brooker's merocyanine. *Journal of Computational Chemistry*, **2015**, 36, 1655-63	3.5	4
1092	Structural Dependence of Electronic Properties in A-A-D-A-A-Type Organic Solar Cell Material. **2015**, 2015, 1-7		2
1091	. **2015**,		2

1090	Switching of carbene spin states: effect of hydrogen bond donors. **2015**, 1		1
1089	Applicability of optimal functional tuning in density functional calculations of ionization potentials and electron affinities of adenine-thymine nucleobase pairs and clusters. **2015**, 17, 4337-45		27
1088	Electron transport in carbon wires in contact with Ag electrodes: a detailed first principles investigation. **2015**, 17, 18413-25		17
1087	On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies. *Journal of Chemical Physics*, **2015**, 142, 194114	3.9	35
1086	Tuning Range-Separated Density Functional Theory for Photocatalytic Water Splitting Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 1700-9	6.4	50
1085	Electric Property Variations in Nanosized Hexagonal Boron Nitride/Graphene Hybrids. **2015**, 119, 11872-11885		25
1084	Global hybrids from the semiclassical atom theory satisfying the local density linear response. *Journal of Chemical Theory and Computation*, **2015**, 11, 122-31	6.4	20
1083	The Electronic Structure of Amorphous Carbon Nanodots. **2015**, 119, 7258-65		47
1082	Computational Molecular Electronic Spectroscopy with TD-DFT. **2016**, 368, 347-75		25
1081	Electric properties of the low-lying excited states of benzonitrile: geometry relaxation and solvent effects. **2015**, 134, 1		11
1080	Analytic second derivative of the energy for density functional theory based on the three-body fragment molecular orbital method. *Journal of Chemical Physics*, **2015**, 142, 124101	3.9	10
1079	Assessment of hybrid, meta-hybrid-GGA, and long-range corrected density functionals for the estimation of enthalpies of formation, barrier heights, and ionisation potentials of selected C1–C5 oxygenates. **2015**, 113, 1630-1635		3
1078	Intersystem Crossing Pathway in Quinoline-Pyrazole Isomerism: A Time-Dependent Density Functional Theory Study on Excited-State Intramolecular Proton Transfer. *Journal of Physical Chemistry A*, **2015**, 119, 6269-74	2.8	81
1077	Toward assessment of density functionals for vibronic coupling in two-photon absorption: A case study of 4-nitroaniline. *Journal of Computational Chemistry*, **2015**, 36, 1124-31	3.5	12
1076	On Predicting the Excited-State Properties of Thermally Activated Delayed Fluorescence Emitters. **2015**, 119, 13535-13544		125
1075	Combining Near-UV Photodissociation with Electron Transfer. Reduction of the Diazirine Ring in a Photomethionine-Labeled Peptide Ion. **2015**, 26, 1367-81		9
1074	Quantum chemical study of the electronic properties of an Iridium-based photosensitizer bound to medium-sized silver clusters. **2015**, 457, 1-6		4
1073	Electronic excitation energies in dimers between radical ions presenting long, multicenter bonding. *Journal of Chemical Theory and Computation*, **2015**, 11, 2651-60	6.4	5

1072	Interaction of a Ni(II) tetraazaannulene complex with elongated fullerenes as simple models for carbon nanotubes. *Journal of Molecular Modeling*, **2015**, 21, 146	2	12
1071	Development of asymmetrical near infrared squaraines with large Stokes shift. *RSC Advances*, **2015**, 5, 106868-106876	3.7	14
1070	Nicholas Charles Handy. 17 June 1941 – 2 October 2012. **2015**, 61, 145-160		1
1069	Benchmarking Ground-State Geometries and Vertical Excitation Energies of a Selection of P-Type Semiconducting Molecules with Different Polarity. *Journal of Physical Chemistry A*, **2015**, 119, 12876-91	2.8	22
1068	A weight averaged approach for predicting amide vibrational bands of a sphingomyelin bilayer. **2015**, 17, 29113-23		11
1067	Applications of Time-Dependent and Time-Independent Density Functional Theory to Electronic Transitions in Tetrahedral d(0) Metal Oxides. *Journal of Chemical Theory and Computation*, **2015**, 11, 4041-53	6.4	11
1066	The molecular structure of tris(dipivaloylmethanato) lanthanides, Ln(thd)3 (Ln = La–Lu): Peculiarities and regularities. **2015**, 1055, 78-87		12
1065	Local scaling correction for reducing delocalization error in density functional approximations. **2015**, 114, 053001		59
1064	Theoretical study on the stability of double-decker type metal phthalocyanines, M(Pc)2 and M(Pc)2(+) (M = Ti, Sn and Sc): a critical assessment on the performance of density functionals. **2015**, 17, 6478-83		8
1063	Probing peptide cation-radicals by near-UV photodissociation in the gas phase. Structure elucidation of histidine radical chromophores formed by electron transfer reduction. **2015**, 119, 3948-61		19
1062	Absorption Spectra of Aryl Thiol-Coated Silver Nanoclusters: A Time-Dependent Density-Functional Study. **2015**, 119, 4268-4277		12
1061	Calculating Electron-Transfer Coupling with Density Functional Theory: The Long-Range-Corrected Density Functionals. **2015**, 119, 7480-90		24
1060	Delocalization and the vibrational spectroscopy of conjugated materials: computational insights on Raman frequency dispersion in thiophene, furan, and pyrrole oligomers. **2015**, 119, 3583-94		27
1059	Theoretical design of solvatochromism switching by photochromic reactions using donor-acceptor disubstituted diarylethene derivatives with oxidized thiophene rings. **2015**, 17, 6484-94		4
1058	First principle calculations of the electronic and vibrational properties of the 3-(1,1-dicyanoethenyl)-1-phenyl-4,5-dihydro-1H-pyrazole molecule. *Journal of Physical Chemistry A*, **2015**, 119, 1347-58	2.8	14
1057	NLO Properties of Unidirectional Lengthening [Pt3(CO)3(μ-CO)3] 2− Clusters: A TDDFT Study. **2015**, 26, 1511-1526		
1056	Role of Excess Electrons in Nonlinear Optical Response. **2015**, 6, 612-9		140
1055	Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: a potential tetraradicaloid hydrocarbon. **2015**, 54, 2090-4		77

1054	Applications of time-dependent and time-independent density functional theory to Rydberg transitions. *Journal of Physical Chemistry A*, **2015**, 119, 5107-16	2.8	15
1053	Efficient implementation of the pair atomic resolution of the identity approximation for exact exchange for hybrid and range- separated density functionals. *Journal of Chemical Theory and Computation*, **2015**, 11, 518-27	6.4	41
1052	Structural, electronic and reactivity studies on group 15 analogues of N-heterocyclic carbene. **2015**, 26, 859-871		9
1051	Charge-transfer matrix elements by FMO-LCMO approach: Hole transfer in DNA with parameter tuned range-separated DFT. **2015**, 621, 96-101		20
1050	Quantum chemical study on HKrCN, HXeCN, and related rare gas compounds. *Journal of Physical Chemistry A*, **2015**, 119, 2672-82	2.8	4
1049	X-ray absorption in insulators with non-Hermitian real-time time-dependent density functional theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 646-54	6.4	31
1048	On the performance of range-separated hybrid in computations of dynamic quadratic polarizability of solution-phase organic molecules: a comparison to MP2(Full) calculation. **2015**, 134, 1		3
1047	Electron transfer reduction of the diazirine ring in gas-phase peptide ions. On the peculiar loss of [NH4O] from photoleucine. **2015**, 26, 415-31		7
1046	Charge transfer or biradicaloid character: assessing TD-DFT and SAC-CI for squarylium dye derivatives. *RSC Advances*, **2015**, 5, 18813-18821	3.7	12
1045	A theoretical perspective on charge transfer in photocatalysis. The example of Ir-based systems. **2015**, 304-305, 133-145		40
1044	Direct and indirect effects of dispersion interactions on the electric properties of weakly bound complexes. *Journal of Physical Chemistry A*, **2015**, 119, 3112-24	2.8	11
1043	Gaussian-based cutoff scheme on Hartree–Fock exchange term of dielectric-dependent potential. **2015**, 634, 83-87		5
1042	Ultrafast excited state hydrogen atom transfer in salicylideneaniline driven by changes in aromaticity. **2015**, 17, 31608-12		40
1041	Choosing a density functional for static molecular polarizabilities. **2015**, 635, 257-261		34
1040	Theoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamics. **2015**, 6, 2746-2753		43
1039	Nonlinear optical properties of rhenium(I) complexes: Influence of the extended π-conjugated connectors and proton abstraction. **2015**, 61, 196-203		7
1038	Toward an Experimental Quantum Chemistry: Exploring a New Energy Partitioning. **2015**, 137, 10282-91		24
1037	Improving Rydberg Excitations within Time-Dependent Density Functional Theory with Generalized Gradient Approximations: The Exchange-Enhancement-for-Large-Gradient Scheme. *Journal of Chemical Theory and Computation*, **2015**, 11, 3123-30	6.4	26

1036	Fluorescence Enhancement/Quenching Based on Metal Orbital Control: Computational Studies of a 6-Thienyllumazine-Based Mercury Sensor. *Journal of Physical Chemistry A*, **2015**, 119, 8106-16	2.8	38
1035	Range separated hybrids of pair coupled cluster doubles and density functionals. **2015**, 17, 22412-22		34
1034	Theoretical studies of molecular orientation and charge recombination in poly-paraphenylenevinylene light-emitting diodes. **2015**, 17, 20923-31		7
1033	Far- and Deep-Ultraviolet Spectroscopy. **2015**,		31
1032	Balancing Exchange Mixing in Density-Functional Approximations for Iron Porphyrin. *Journal of Chemical Theory and Computation*, **2015**, 11, 3022-8	6.4	21
1031	Performance of the M06 family of functionals in predicting the charge transfer transition energies of molecular complexes of TCNE with a series of methylated indoles. **2015**, 1068, 123-127		4
1030	Ab initio theoretical reinvestigation of the ground and excited state properties of silylated coumarins: Good candidates for solid state dye lasers and dye-sensitized solar cells. **2015**, 150, 806-13		5
1029	A Chemically Meaningful Measure of Electron Localization. *Journal of Chemical Theory and Computation*, **2015**, 11, 3617-28	6.4	13
1028	Reliable Prediction with Tuned Range-Separated Functionals of the Singlet-Triplet Gap in Organic Emitters for Thermally Activated Delayed Fluorescence. *Journal of Chemical Theory and Computation*, **2015**, 11, 3851-8	6.4	256
1027	Charge-transfer excited states in phosphorescent organo-transition metal compounds: a difficult case for time dependent density functional theory?. *RSC Advances*, **2015**, 5, 63318-63329	3.7	63
1026	Electronic and photophysical properties of 2-(2?-hydroxyphenyl)benzoxazole and its derivatives enhancing in the excited-state intramolecular proton transfer processes: A TD-DFT study on substitution effect. **2015**, 167, 132-139		16
1025	1,8-Bis(phenylethynyl)anthracene - gas and solid phase structures. **2015**, 13, 8893-905		10
1024	Designating Oxygen Anions in Al□TQ-21 as Br□nsted Acid Sites Using DFT Calculations. **2015**, 119, 16568-16577		
1023	Anharmonic simulations of the vibrational spectrum of sulfated compounds: application to the glycosaminoglycan fragment glucosamine 6-sulfate. **2015**, 17, 25705-13		29
1022	Theoretical study on reaction mechanisms of nitrite reduction by copper nitrite complexes: toward understanding and controlling possible mechanisms of copper nitrite reductase. **2015**, 119, 5392-403		11
1021	Electronic Properties of Zigzag Graphene Nanoribbons Studied by TAO-DFT. *Journal of Chemical Theory and Computation*, **2015**, 11, 2003-11	6.4	56
1020	Theoretical analysis of the SP bond in a family of compounds that involve a P2S2 ring: role of the PBE0-1/5 exchange□correlation functional. **2015**, 1062, 36-43		3
1019	Infrared spectra of small anionic water clusters from density functional theory and wavefunction theory calculations. **2015**, 17, 12698-707		4

1018	Diradical character and second hyperpolarizability of multidecker inverse sandwich complexes of Mg and Ca. **2015**, 628, 1-8		12
1017	Quantum-Chemical Characterization of the Properties and Reactivities of Metal-Organic Frameworks. **2015**, 115, 6051-111		197
1016	Time-dependent density functional theory calculations of the solvatochromism of some azo sulfonamide fluorochromes. *Journal of Molecular Modeling*, **2015**, 21, 118	2	29
1015	van der Waals forces in density functional theory: a review of the vdW-DF method. **2015**, 78, 066501		477
1014	Why do TD-DFT excitation energies of BODIPY/Aza-BODIPY families largely deviate from experiment? Answers from electron correlated and multireference methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 2619-32	6.4	128
1013	Distributed Atomic Polarizabilities of Amino Acids and their Hydrogen-Bonded Aggregates. *Journal of Physical Chemistry A*, **2015**, 119, 3285-98	2.8	26
1012	Reaction mechanism of the anomalous formal nucleophilic borylation of organic halides with silylborane: combined theoretical and experimental studies. **2015**, 137, 4090-9		62
1011	Regarding the use and misuse of retinal protonated Schiff base photochemistry as a test case for time-dependent density-functional theory. *Journal of Chemical Physics*, **2015**, 142, 144104	3.9	14
1010	Assessment of long-range corrected and conventional DFT functional for the prediction of second--order NLO properties and other molecular properties of N-(2-cyanoethyl)-N-butylaniline--a vibrational spectroscopy study. **2015**, 146, 66-79		6
1009	Second hyperpolarizability of multimetallocenes [Cp⁅Mn⁅Cp] of Be, Mg and Ca. **2015**, 14, 1550002		6
1008	On the origin and variation of colors in lobster carapace. **2015**, 17, 16723-32		26
1007	Structural changes in non-planar octaaryl substituted phthalocyanine phosphorus complexes. **2015**, 19, 500-509		8
1006	New trans-stilbene derivatives with large two-photon absorption cross-section and non-linear optical susceptibility values--a theoretical investigation. **2015**, 17, 12299-309		4
1005	Tuning the electronic and phosphorescence properties of blue-emitting iridium(III) complexes through different cyclometalated ligand substituents: a theoretical investigation. **2015**, 44, 8577-89		26
1004	A new pentacoordinate polymeric copper(II) complex with 2-amino-2-methyl-1,3-propandiol: Structural investigations using XRD and DFT. **2015**, 56, 92-101		7
1003	Toward the complete range separation of non-hybrid exchange-correlation functional. *Journal of Computational Chemistry*, **2015**, 36, 871-7	3.5	6
1002	Efficient method of evaluation for Gaussian Hartree-Fock exchange operator for Gau-PBE functional. *Journal of Chemical Physics*, **2015**, 143, 024102	3.9	4
1001	0-0 Energies Using Hybrid Schemes: Benchmarks of TD-DFT, CIS(D), ADC(2), CC2, and BSE/GW formalisms for 80 Real-Life Compounds. *Journal of Chemical Theory and Computation*, **2015**, 11, 5340-59	6.4	166

1000	Benchmarking Electronic Excitation Energies and Transitions in Peptide Radicals. *Journal of Physical Chemistry A*, **2015**, 119, 10101-11	2.8	19
999	Double role of squarylium dye: Fluorescence probe for biomolecule determination and photosensitizer in dyeing photoinitiating system. *Journal of Molecular Liquids*, **2015**, 212, 196-202	6	3
998	H-atom loss and migration in hydrogen-rich peptide cation radicals: The role of chemical environment. **2015**, 390, 28-38		6
997	Theoretical investigation of stabilities and optical properties of Si12C12 clusters. *Journal of Chemical Physics*, **2015**, 142, 034303	3.9	16
996	Local hybrid functionals with orbital-free mixing functions and balanced elimination of self-interaction error. *Journal of Chemical Physics*, **2015**, 142, 074112	3.9	26
995	Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. *Journal of Chemical Physics*, **2015**, 142, 184104	3.9	31
994	Density matrix renormalization group with efficient dynamical electron correlation through range separation. *Journal of Chemical Physics*, **2015**, 142, 224108	3.9	74
993	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. *Journal of Chemical Physics*, **2015**, 143, 054107	3.9	404
992	Tuning range-separated DFT functionals for accurate orbital energy modeling of conjugated molecules. **2015**, 1070, 14-20		9
991	A first principles approach to the electronic properties of liquid and supercritical CO2. *Journal of Chemical Physics*, **2015**, 142, 024504	3.9	13
990	Density-functional errors in ionization potential with increasing system size. *Journal of Chemical Physics*, **2015**, 142, 184106	3.9	48
989	Interplay between Open-Shell Character, Aromaticity, and Second Hyperpolarizabilities in Indenofluorenes. *Journal of Physical Chemistry A*, **2015**, 119, 10620-7	2.8	33
988	Chromophore-protein coupling beyond nonpolarizable models: understanding absorption in green fluorescent protein. *Journal of Chemical Theory and Computation*, **2015**, 11, 4825-39	6.4	54
987	Structure of P3HT crystals, thin films, and solutions by UV/Vis spectral analysis. **2015**, 17, 28616-25		50
986	Oxocomplexes of Mo(VI) and W(VI) with 8-hydroxyquinoline-5-sulfonate in solution: structural studies and the effect of the metal ion on the photophysical behaviour. **2015**, 44, 19076-89		10
985	Molecules relevant for organic photovoltaics: a range-separated density functional study. **2015**, 113, 2930-2938		4
984	Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 4226-37	6.4	39
983	The first hyperpolarizability of nitrobenzene in benzene solutions: investigation of the effects of electron correlation within the sequential QM/MM approach. **2015**, 17, 23634-42		28

982	Fine-Tuning of Magnetic Properties in Nickel(II) Trinuclear EMACs via Modifications of Equatorial Ligands. *Journal of Physical Chemistry A*, **2015**, 119, 9363-72	2.8	1
981	Assessment of DFT methods for studying acid gas capture by ionic liquids. **2015**, 17, 26875-91		22
980	Unusual bonding modes of perfluorobenzene in its polymeric (dimeric, trimeric and tetrameric) forms: entirely negative fluorine interacting cooperatively with entirely negative fluorine. **2015**, 17, 31624-45		28
979	Crystalline Alloys of Organic Donors and Acceptors Based on TIPS-Pentacene. **2015**, 119, 20823-20832		13
978	Understanding structural and electronic properties of dithienyl benzothiadiazole and its complex with C70. **2015**, 75, 73-77		6
977	Properties of noncovalent tetraphenylporphine⋯C60 dyads as studied by different long-range and dispersion-corrected DFT functionals. **2015**, 17, 27399-408		8
976	Antioxidant properties can be tuned in the presence of an external electric field: accurate computation of OH BDE with range-separated density functionals. *RSC Advances*, **2015**, 5, 78229-78237	3.7	6
975	Inter-Excited-State Phosphorescence in the Four-Component Relativistic Kohn-Sham Approximation: A Case Study on Lumiflavin. *Journal of Physical Chemistry A*, **2015**, 119, 11911-21	2.8	6
974	Scaling correction approaches for reducing delocalization error in density functional approximations. **2015**, 58, 1825-1844		10
973	DFT calculations of thiosemicarbazide, arylisothiocynates, and 1-aryl-2,5-dithiohydrazodicarbonamides as corrosion inhibitors of copper in an aqueous chloride solution. **2015**, 26, 291-308		56
972	Path integral Monte Carlo study of hydrogen tunneling effect on dielectric properties of molecular crystal 5-Bromo-9-hydroxyphenalenone. **2015**, 446, 118-126		1
971	Reptation Quantum Monte Carlo calculation of charge transfer: The NaCl dimer. **2015**, 618, 236-240		4
970	Local response dispersion method: A density-dependent dispersion correction for density functional theory. *International Journal of Quantum Chemistry*, **2015**, 115, 309-324	2.1	10
969	Accurate and efficient quantum chemistry calculations for noncovalent interactions in many-body systems: the XSAPT family of methods. *Journal of Physical Chemistry A*, **2015**, 119, 235-52	2.8	65
968	Local response dispersion method in periodic systems: Implementation and assessment. *Journal of Computational Chemistry*, **2015**, 36, 303-11	3.5	2
967	Pigment violet 19 - a test case to define a simple method to simulate the vibronic structure of absorption spectra of organic pigments and dyes in solution. **2015**, 14, 444-56		10
966	Understanding the effect of heteroatoms on structural and electronic properties of conjugated polymers. **2015**, 56, 293-299		10
965	Models of charge pair generation in organic solar cells. **2015**, 17, 2311-2325		135

964	Accurate ab initio description of adsorption on coordinatively unsaturated Cu(2+) and Fe(3+) sites in MOFs. *Journal of Chemical Theory and Computation*, **2015**, 11, 230-8	6.4	31
963	Linearity condition for orbital energies in density functional theory (V): Extension to excited state calculations. **2015**, 618, 30-36		3
962	FIrpic: archetypal blue phosphorescent emitter for electroluminescence. **2015**, 44, 8318-29		148
961	Chemical reaction analyses based on orbitals and orbital energies. *International Journal of Quantum Chemistry*, **2015**, 115, 270-282	2.1	10
960	Binding of nucleobases with graphene and carbon nanotube: a review of computational studies. **2015**, 33, 1567-97		25
959	Can gap tuning schemes of long-range corrected hybrid functionals improve the description of hyperpolarizabilities?. **2015**, 119, 1202-12		47
958	Intrinsic reaction coordinate: Calculation, bifurcation, and automated search. *International Journal of Quantum Chemistry*, **2015**, 115, 258-269	2.1	212
957	DFT and TD-DFT assessment of the structural and optoelectronic properties of an organic-Ag14 nanocluster. *Journal of Physical Chemistry A*, **2015**, 119, 5088-98	2.8	27
956	Statistical Significance of the Maximum Hardness Principle Applied to Some Selected Chemical Reactions. *Molecules*, **2016**, 21,	4.8	6
955	Orbital Energy-Based Reaction Analysis of SN2 Reactions. *Computation*, **2016**, 4, 23	2.2	3
954	The Influence of One-Electron Self-Interaction on d-Electrons. *Computation*, **2016**, 4, 33	2.2	10
953	Hyperconjugative interactions are the main responsible for the anomeric effect: a direct relationship between the hyperconjugative anomeric effect, global hardness and zero-point energy. **2016**, 27, 1753-1768		11
952	Diradical Character Tuning for the Third-Order Nonlinear Optical Properties of Quinoidal Oligothiophenes by Introducing Thiophene-S,S-dioxide Rings. **2016**, 22, 1493-500		18
951	Relationship between orbital energy gaps and excitation energies for long-chain systems. *Journal of Computational Chemistry*, **2016**, 37, 1451-62	3.5	8
950	Theoretical Study on Electronic Structure of Bathocuproine: Renormalization of the Band Gap in the Crystalline State and the Large Exciton Binding Energy. **2016**, 63, 513-520		2
949	First principles study of thieno[2,3-b]indole-based organic dyes for dye-sensitized solar cells: Screen novel linkers and explore the interface between photosensitizers and TiO2. **2016**, 326, 193-202		28
948	Mapping Long-Lived Dark States in Copper Porphyrin Nanostructures. **2016**, 120, 16977-16984		5
947	Electronic Properties of Cyclacenes from TAO-DFT. *Scientific Reports*, **2016**, 6, 37249	4.9	37

946	Evolution of DFT studies in view of a scientometric perspective. **2016**, 8, 52		25
945	Polarization response of clathrate hydrates capsulated with guest molecules. *Journal of Chemical Physics*, **2016**, 144, 204308	3.9	10
944	Synthesis of meta-methoxyphenyl substituted tetraazaporphyrin and corrolazine phosphorus(V) complexes. **2016**, 20, 1075-1081		1
943	Calculations of electric dipole moments and static dipole polarizabilities based on the two-component normalized elimination of the small component method. *Journal of Chemical Physics*, **2016**, 145, 184104	3.9	15
942	Towards quantifying the role of exact exchange in the prediction hydrogen bond spin-spin coupling constants involving fluorine. *Journal of Chemical Physics*, **2016**, 145, 084301	3.9	8
941	Increasing the applicability of density functional theory. V. X-ray absorption spectra with ionization potential corrected exchange and correlation potentials. *Journal of Chemical Physics*, **2016**, 145, 034108	3.9	20
940	Multi-electron coincidence spectroscopy: double photoionization from molecular inner-shell orbitals. **2016**, 49, 182002		13
939	The growth of zinc phthalocyanine thin films by pulsed laser deposition. **2016**, 31, 163-172		14
938	The QTP family of consistent functionals and potentials in Kohn-Sham density functional theory. *Journal of Chemical Physics*, **2016**, 145, 034107	3.9	55
937	Tight-binding approximations to time-dependent density functional theory - A fast approach for the calculation of electronically excited states. *Journal of Chemical Physics*, **2016**, 144, 184103	3.9	28
936	Rungs 1 to 4 of DFT Jacob's ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. *Journal of Chemical Physics*, **2016**, 144, 204120	3.9	142
935	Blind test of density-functional-based methods on intermolecular interaction energies. *Journal of Chemical Physics*, **2016**, 145, 124105	3.9	76
934	Excess electrons in methanol clusters: Beyond the one-electron picture. *Journal of Chemical Physics*, **2016**, 145, 164313	3.9	4
933	Perspective: Kohn-Sham density functional theory descending a staircase. *Journal of Chemical Physics*, **2016**, 145, 130901	3.9	186
932	Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. *Journal of Chemical Physics*, **2016**, 145, 204101	3.9	21
931	Orientation hydrogen-bonding effect on vibronic spectra of isoquinoline in water solvent: Franck-Condon simulation and interpretation. *Journal of Chemical Physics*, **2016**, 145, 164314	3.9	32
930	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. *Journal of Chemical Physics*, **2016**, 144, 074106	3.9	93
929	Ionisation potential theorem in the presence of the electric field: Assessment of range-separated functional in the reproduction of orbital and excitation energies. *Journal of Chemical Physics*, **2016**, 144, 164113	3.9	5

928	Global and local curvature in density functional theory. *Journal of Chemical Physics*, **2016**, 145, 054109	3.9	34
927	Surface tension of ab initio liquid water at the water-air interface. *Journal of Chemical Physics*, **2016**, 144, 204705	3.9	30
926	Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. *Journal of Chemical Physics*, **2016**, 145, 044109	3.9	12
925	On the applicability of one- and many-electron quantum chemistry models for hydrated electron clusters. *Journal of Chemical Physics*, **2016**, 144, 154311	3.9	14
924	Ability of density functional theory methods to accurately model the reaction energy pathways of the oxidation of CO on gold cluster: A benchmark study. **2016**, 135, 1		11
923	The optical signature of 2,6-bis((E)-2-(benzoxazol-2-yl)vinyl)naphthalene (BBVN) laser dye: a TDDFT study. *New Journal of Chemistry*, **2016**, 40, 4911-4921	3.6	1
922	Electronic and Optical Properties of the Narrowest Armchair Graphene Nanoribbons Studied by Density Functional Methods. **2016**, 69, 960		7
921	Systematic Error Estimation for Chemical Reaction Energies. *Journal of Chemical Theory and Computation*, **2016**, 12, 2762-73	6.4	61
920	Stochastic Optimally Tuned Range-Separated Hybrid Density Functional Theory. *Journal of Physical Chemistry A*, **2016**, 120, 3071-8	2.8	29
919	Diindeno-fusion of an anthracene as a design strategy for stable organic biradicals. **2016**, 8, 753-9		217
918	Spin-Free CC2 Implementation of Induced Transitions between Singlet Ground and Triplet Excited States. *Journal of Chemical Theory and Computation*, **2016**, 12, 1892-904	6.4	9
917	A Local CC2 and TDA-DFT Double Hybrid Study on BODIPY/aza-BODIPY Dimers as Heavy Atom Free Triplet Photosensitizers for Photodynamic Therapy Applications. *Journal of Physical Chemistry A*, **2016**, 120, 2550-60	2.8	47
916	Assessment of the LFAs-PBE exchange□correlation potential for high-order harmonic generation of aligned H2+ molecules. *RSC Advances*, **2016**, 6, 33318-33325	3.7	2
915	Investigation of Multiconfigurational Short-Range Density Functional Theory for Electronic Excitations in Organic Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 2203-13	6.4	21
914	Dispersion-Corrected Mean-Field Electronic Structure Methods. **2016**, 116, 5105-54		738
913	ZIF-8 as Nonlinear Optical Material: Influence of Structure and Synthesis. **2016**, 28, 3203-3209		46
912	Porphyrin-rhodamine conjugates as new materials with sensing ability. **2016**, 135, 113-126		7
911	Global hybrid exchange energy functional with correct asymptotic behavior of the corresponding potential. **2016**, 135, 1		5

910	Tautomerization mechanism and spectral properties of porphyrin□glucose complexes as models of antibacterial material. **2016**, 135, 1		9
909	Time-dependent quantum simulation of coronene photoemission spectra. **2016**, 18, 13604-15		4
908	The fragment molecular orbital method combined with density-functional tight-binding and the polarizable continuum model. **2016**, 18, 22047-61		47
907	Prototype Dithiolene Radical Anion (S?CH-CH?S(□)) As Derived from Electron Attachment to 1,4-Dithiane: Experimental and Computational Studies on Electronic Structure. *Journal of Physical Chemistry A*, **2016**, 120, 3570-7	2.8	4
906	The Optical Signature of Charges in Conjugated Polymers. **2016**, 2, 309-15		58
905	Low-Lying □ States of Heteroaromatic Molecules: A Challenge for Excited State Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 2652-60	6.4	47
904	Super/hyperhalogen aromatic heterocyclic compounds. *RSC Advances*, **2016**, 6, 47145-47150	3.7	15
903	Noble gas endohedral fullerenes, Ng@C60 (Ng=Ar, Kr): a particular benchmark for assessing the account of non-covalent interactions by density functional theory calculations. **2016**, 135, 1		7
902	Charge Delocalization in Oligomers of Poly(2,5-bis(3-alkylthiophene-2-yl)thieno[3,2-b]thiophene) (PBTTT). **2016**, 120, 9671-9677		24
901	Connecting effect on the first hyperpolarizability of armchair carbon-boron-nitride heteronanotubes: pattern versus proportion. **2016**, 18, 13954-9		15
900	Computational studies of electronic structures and photophysical properties of luminescent iridium(III) complexes based on amidinate/bis(pyridylphenyl) ligands. **2016**, 33, 281-289		20
899	Critical Assessment of Time-Dependent Density Functional Theory for Excited States of Open-Shell Systems: II. Doublet-Quartet Transitions. *Journal of Chemical Theory and Computation*, **2016**, 12, 2517-27	6.4	17
898	Spectroscopic and nonlinear optical properties of new chalcone fluorescent probes for bioimaging applications: a theoretical and experimental study. *Journal of Molecular Modeling*, **2016**, 22, 125	2	23
897	Theoretical study on activation mechanism of fluorine substitution reactions of Keggin-MAl12 in aqueous solutions. **2016**, 69, 2864-2871		1
896	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. **2016**, 52, 13840-13860		15
895	Encyclopedia of Geochemistry. **2016**, 1-7		0
894	Synthetic, Optical and Theoretical Study of Alternating Ethylenedioxythiophene-Pyridine Oligomers: Evolution from Planar Conjugated to Helicoidal Structure towards a Chiral Configuration. *ChemPhysChem*, **2016**, 17, 4090-4101	3.2	5
893	Electronic and vibrational spectroscopic studies of jet-cooled 5-cyanoindole and its water clusters, 5CI□H2O) , (n= 0□). **2016**, 658, 63-70		4

892	Benchmarking the DFT methodology for assessing antioxidant-related properties: quercetin and edaravone as case studies. *Journal of Molecular Modeling*, **2016**, 22, 250	2	18
891	Spin-state energies of heme-related models from spin-flip TDDFT calculations. **2016**, 18, 29486-29494		8
890	Refractive indices of organo-metallic and -metalloid compounds: A long-range corrected DFT study. *Journal of Computational Chemistry*, **2016**, 37, 2759-2769	3.5	2
889	Quantum confinement effects on optical transitions in nanodiamonds containing nitrogen vacancies. **2016**, 94,		28
888	Synthesis, spectroscopic, physicochemical properties and binding site analysis of 4-(1H-phenanthro[9,10-d]-imidazol-2-yl)-benzaldehyde fluorescent probe for imaging in cell biology: Experimental and theoretical study. **2016**, 164, 112-122		14
887	DFT/ and TD-DFT/PCM calculations of molecular structure, spectroscopic characterization, NLO and NBO analyses of 4-(4-chlorophenyl) and 4-[4-(dimethylamino) phenyl]-2-oxo-1,2,5,6-tetrahydrobenzo[h]quinoline-3-carbonitrile dyes. *Journal of Molecular Liquids*, **2016**, 223, 29-47	6	24
886	Electronically Excited States of Borylenes. *Journal of Physical Chemistry A*, **2016**, 120, 6332-41	2.8	15
885	Electronic stopping power in liquid water for protons and α particles from first principles. **2016**, 94,		27
884	Benchmark Calculations of Energetic Properties of Groups 4 and 6 Transition Metal Oxide Nanoclusters Including Comparison to Density Functional Theory. *Journal of Chemical Theory and Computation*, **2016**, 12, 3689-710	6.4	24
883	Simulating Nuclear and Electronic Quantum Effects in Enzymes. **2016**, 577, 389-418		6
882	Recent application of calculations of metal complexes based on density functional theory. *RSC Advances*, **2016**, 6, 77375-77395	3.7	35
881	Separation of dynamic and nondynamic correlation. **2016**, 18, 24015-23		53
880	The Excitation Spectra of Naphthalene Dimers: Frenkel and Charge-transfer Excitons. **2016**, 63, 20-32		3
879	Theoretical predication for transition energies of thermally activated delayed fluorescence molecules. **2016**, 27, 1445-1452		33
878	Insights on the Auxochromic Properties of the Guanidinium Group. *Journal of Physical Chemistry A*, **2016**, 120, 7088-100	2.8	13
877	Experimental and Theoretical Infrared Spectroscopic Study on Hydrated Nafion Membrane. **2016**, 49, 6621-6629		38
876	First hyperpolarizability of para-aminoaniline induced by a variety of gold nano particles. **2016**, 18, 24343-9		1
875	Explicitly correlated frequency-independent second-order green's function for accurate ionization energies. *Journal of Computational Chemistry*, **2016**, 37, 2447-53	3.5	15

874	1,2-Dimethoxyethane Degradation Thermodynamics in Li-O Redox Environments. **2016**, 22, 17188-17203		22
873	Using Density Functional Theory To Study Neutral and Ionized Stacked Thymine Dimers. *Journal of Physical Chemistry A*, **2016**, 120, 7704-7713	2.8	7
872	Range-Separation Parameter in Tuned Exchange-Correlation Functionals: Successive Ionizations and the Fukui Function. *Journal of Chemical Theory and Computation*, **2016**, 12, 4879-4884	6.4	6
871	The Origin of Relative Stability of Di-μ-oxo M□M Chiral Salen Complexes [M□M = Ti(IV)□Ti(IV), V(IV)□V(IV), Cr(IV)□Cr(IV), and Mn(IV)□Mn(IV)]: A Quantum-Chemical Analysis. **2016**, 89, 447-454		1
870	On describing the optoelectronic characteristics of poly(benzodithiophene-co-quinoxaline)-fullerene complexes: the influence of optimally tuned density functionals. **2016**, 18, 27654-27670		6
869	Formation of thiophene sandwiches through cation□interaction: A DFT study. **2016**, 1095, 83-92		8
868	Employing Range Separation on the meta-GGA Rung: New Functional Suitable for Both Covalent and Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2016**, 12, 3662-73	6.4	9
867	[Al2O4](-), a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 3796-806	6.4	15
866	Spin-Forbidden Transitions between Electronic States in the Active Site of Rubredoxin. *Journal of Physical Chemistry A*, **2016**, 120, 8691-8698	2.8	6
865	Benchmarking Quantum Chemical Methods for Optical Absorption in Boron Wheels. **2016**, 1, 578-585		8
864	Where Does the Density Localize? Convergent Behavior for Global Hybrids, Range Separation, and DFT+U. *Journal of Chemical Theory and Computation*, **2016**, 12, 5931-5945	6.4	50
863	Study of Structure□Third-Order Susceptibility Relation of Indandione Derivatives. **2016**, 120, 27515-27522		11
862	Role of Kekul□ 'and Non-Kekul□ 'Structures in the Radical Character of Alternant Polycyclic Aromatic Hydrocarbons: A TAO-DFT Study. *Scientific Reports*, **2016**, 6, 30562	4.9	46
861	Structure of N?-(adamantan-2-ylidene)benzohydrazide, a potential antibacterial agent, in solution: Molecular dynamics simulations, quantum chemical calculations and Ultraviolet□isible spectroscopy studies. **2016**, 128, 1933-1942		4
860	Electronic excitation and injection of Ru-N3 dye anchored to TiO2 surface. **2016**, 1097, 8-14		1
859	Does the DFT Self-Interaction Error Affect Energies Calculated in Proteins with Large QM Systems?. *Journal of Chemical Theory and Computation*, **2016**, 12, 5667-5679	6.4	12
858	Absorption and Emission Spectra of Anthracene-9-Carboxylic Acid in Solution Within the Polarizable Continuum Model: A Long-Range Corrected Time Dependent Density Functional Study. **2016**, 72, 61-94		1
857	Reply to the 'Comment on "Theoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamics"' by E. M. Cabaleiro-Lago, J. Rodriguez-Otero and A. Gil, , 2016, , DOI: 10.1039/C5SC04676A. **2016**, 7, 2929-2932		13

856	Highly efficient implementation of pseudospectral time-dependent density-functional theory for the calculation of excitation energies of large molecules. *Journal of Computational Chemistry*, **2016**, 37, 1425-41	3.5	17
855	Doubly N-Methylated Porphyrinoids. **2016**, 18, 3006-9		7
854	A New Method To Evaluate Excited States Lifetimes Based on Green's Function: Application to Dye-Sensitized Solar Cells. *Journal of Chemical Theory and Computation*, **2016**, 12, 3074-86	6.4	5
853	First principles optimally tuned range-separated density functional theory for prediction of phosphorus-hydrogen spin-spin coupling constants. **2016**, 18, 18431-40		17
852	Density Functional Theory Calculation of pKa's of Thiols in Aqueous Solution Using Explicit Water Molecules and the Polarizable Continuum Model. *Journal of Physical Chemistry A*, **2016**, 120, 5726-35	2.8	115
851	Why HS□and CN□can be detected by different chemosensors with similar structures: a quantum mechanics and molecular dynamics study. *RSC Advances*, **2016**, 6, 63548-63558	3.7	2
850	Absorption Band Shapes of a Push-Pull Dye Approaching the Cyanine Limit: A Challenging Case for First Principle Calculations. *Journal of Physical Chemistry A*, **2016**, 120, 5581-9	2.8	22
849	Theoretical studies on oxidation-switchable second-order nonlinear optical responses of Metallosalen-Keggin polyoxometalate derivatives. *RSC Advances*, **2016**, 6, 53438-53443	3.7	2
848	Structure and Frontier Molecular Orbital (FMO) energies of □Keggin-type polyoxometalate [PW12O40]3□A systematical study with different functionals of density functional theory. **2016**, 1089, 28-34		8
847	Steric Effects Govern the Photoactivation of Phytochromes. *ChemPhysChem*, **2016**, 17, 954-7	3.2	17
846	Theoretical study of excited states of DNA base dimers and tetramers using optimally tuned range-separated density functional theory. *Journal of Computational Chemistry*, **2016**, 37, 684-93	3.5	25
845	Mechanistic Study of Photocatalytic Hydrogen Generation with Simple Iron Carbonyls as Water Reduction Catalysts. **2016**, 8, 404-411		14
844	Quantum Mechanical and Experimental Validation that Cyclobis(paraquat-p-phenylene) Forms a 1:1 Inclusion Complex with Tetrathiafulvalene. **2016**, 22, 2736-45		6
843	Ill-advised self-interaction contribution in modelling anionic attack along a reaction path. **2016**, 114, 1066-1075		3
842	Calculation of Zn, Cd, Hg adsorption on graphene with incremental CCSD(T) and range-separated hybrid DFT*. **2016**, 114, 1098-1109		1
841	Electronic structure and spectral properties of aurones as visible range fluorescent probes: a DFT/TDDFT study. *RSC Advances*, **2016**, 6, 7002-7010	3.7	20
840	Quantum chemical study of dissociative electron attachment to d -ribose and d -fructose. **2016**, 1075, 70-76		4
839	Describing excited states of [n]cycloparaphenylenes by hybrid and double-hybrid density functionals: from isolated to weakly interacting molecules. **2016**, 135, 1		12

838	Coordination phenomena of alkali metal, alkaline earth metal, and indium ions with the 1,3,6-naphthalenetrisulfonate ion in protic and aprotic solvents. *Journal of Molecular Liquids*, **2016**, 214, 369-377	6	4
837	Molecular structure, linear and nonlinear optical properties of some cyclic phosphazenes: A theoretical investigation. *Journal of Molecular Structure*, **2016**, 1106, 343-351	3.4	17
836	Excitation Spectra of Nucleobases with Multiconfigurational Density Functional Theory. *Journal of Physical Chemistry A*, **2016**, 120, 36-43	2.8	18
835	Ab initio calculations of static dipole polarizabilities and Cauchy moments for the halomethanes, CHmClnF4−m−n. **2016**, 644, 20-24		3
834	Ligand Exchange Reaction of Au(I) R-N-Heterocyclic Carbene Complexes with Cysteine. *Journal of Physical Chemistry A*, **2016**, 120, 2250-9	2.8	21
833	Exploring the limits of recent exchange−correlation functionals in modeling lithium/benzene interaction. **2016**, 135, 1		20
832	Gaussian-based range-separation approach on Hartree−Fock exchange interaction and second-order perturbation theory. **2016**, 647, 132-138		3
831	Adsorption and Self-Assembly of Anticancer Antibiotic Doxorubicin on Single-Walled Carbon Nanotubes. **2016**, 11, 1650038		17
830	Dipole properties of PH3, PF3, PF5, PCl3, SiCl4, GeCl4, and SnCl4. **2016**, 114, 1657-1663		4
829	Structure, Ionization, and Fragmentation of Neutral and Positively Charged Hydrogenated Carbon Clusters: C(n)H(m)(q+) (n = 1-5, m = 1-4, q = 0-3). *Journal of Physical Chemistry A*, **2016**, 120, 588-605	2.8	19
828	Why Is MP2-Water "Cooler" and "Denser" than DFT-Water?. **2016**, 7, 680-4		39
827	Distinguishing Bonds. **2016**, 138, 3731-44		32
826	Ferromagnetic ground state for a hypothetical iron-based extended metal atom chain. *Journal of Molecular Modeling*, **2016**, 22, 63	2	4
825	Polymer Optical Constants from Long-Range Corrected DFT Calculations. **2016**, 120, 2507-16		7
824	Theoretical investigation of [Ru(tpy)2]2+, [Ru(tpy)(bpy)(H2O)]2+ and [Ru(tpy)(bpy)(Cl)]+ complexes in acetone revisited: Inclusion of strong spin−orbit couplings to quantum chemistry calculations. **2016**, 15, 1650001		0
823	Charge generation in organic photovoltaics: a review of theory and computation. **2016**, 1, 10-24		73
822	Palladium-atom catalyzed formic acid decomposition and the switch of reaction mechanism with temperature. **2016**, 18, 10005-17		19
821	Improving the Description of the Optical Properties of Carotenoids by Tuning the Long-Range Corrected Functionals. *Journal of Physical Chemistry A*, **2016**, 120, 4944-50	2.8	25

820	Critical Assessment of TD-DFT for Excited States of Open-Shell Systems: I. Doublet-Doublet Transitions. *Journal of Chemical Theory and Computation*, **2016**, 12, 238-60	6.4	28
819	Combinations of coupled cluster, density functionals, and the random phase approximation for describing static and dynamic correlation, and van der Waals interactions. **2016**, 114, 997-1018		22
818	The van der Waals interactions in rare-gas dimers: the role of interparticle interactions. **2016**, 18, 3011-22		5
817	Coumarin-based donor–acceptor organic dyes for a dye-sensitized solar cell: photophysical properties and electron injection mechanism. **2016**, 135, 1		19
816	Solvent effects on excited-state electron-transfer rate of pyrene-labeled deoxyuridine: A theoretical study. **2016**, 644, 25-30		4
815	A simple and efficient dispersion correction to the Hartree-Fock theory (3): A comprehensive performance comparison of HF-Dtq with MP2 and DFT-Ds. **2016**, 26, 589-593		3
814	Computational insights into the photophysical and electroluminescence properties of homoleptic fac-Ir(C^N)3 complexes employing different phenyl-derivative-featuring phenylimidazole-based ligands for promising phosphors in OLEDs. **2016**, 45, 3034-47		6
813	Accurate atomic quantum defects from particle–particle random phase approximation. **2016**, 114, 1189-1198		4
812	Tuning the color and phosphorescent properties of iridium(III) complexes with phosphine-silanolate ancillary ligand: A theoretical investigation. **2016**, 28, 100-110		11
811	Computation of Second Harmonic Generation for Crystalline Urea and KDP. An ab Initio Approach through the Coupled Perturbed Hartree-Fock/Kohn-Sham Scheme. *Journal of Chemical Theory and Computation*, **2016**, 12, 107-13	6.4	21
810	N-Alkylthienopyrroledione versus benzothiadiazole pulling units in push-pull copolymers used for photovoltaic applications: density functional theory study. **2016**, 18, 1017-24		10
809	An Ab Initio QM/MM-Based Approach to Efficiently Evaluate Vertical Excitation Energies in Condensed Phases Including the Nonequilibrium Solvation Effect. **2016**, 120, 1670-8		9
808	Bond-bending isomerism of AuI: competition between covalent bonding and aurophilicity. **2016**, 7, 475-481		14
807	Synthesis, crystal structure, spectral characterization, and theoretical study of glycolato peroxido complexes of vanadium(V). **2016**, 27, 605-615		5
806	Theoretical investigation of curved π-conjugated fullerene flakes: open-shell character, aromaticity, and third-order nonlinear optical property. **2017**, 30, e3581		4
805	l-Histidinium thiocyanurate: Experimental and theoretical studies of a new nonlinear optical material. **2017**, 172, 168-173		0
804	Polarizability as a tool to determine the electrostatic shielding effect of nanocarbon cages: a polarizability distribution study on noble gas endohedral fullerenes. **2017**, 19, 4751-4757		2
803	Optical and vibrational properties of phosphorylcholine-based contact lenses-Experimental and theoretical investigations. **2017**, 176, 83-90		4

802	Nonempirically tuning range-separated functionals for dipole polarizabilities of nanostructures containing hydrogen bonds. **2017**, 136, 1		7
801	Coupled Cluster Studies of Ionization Potentials and Electron Affinities of Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry A*, **2017**, 121, 1328-1335	2.8	8
800	Photoactive Semiconducting Oxides for Energy and Environment: Experimental and Theoretical Insights. **2017**, 983-1030		
799	Two Photon Absorption in Biological Molecules. **2017**, 1875-1893		2
798	Assessment of range-separated exchange functionals and nonempirical functional tuning for calculating the static second hyperpolarizabilities of streptocyanines. *Journal of Computational Chemistry*, **2017**, 38, 594-600	3.5	6
797	Singularity Correction for Long-Range-Corrected Density Functional Theory with Plane-Wave Basis Sets. *Journal of Physical Chemistry A*, **2017**, 121, 2035-2045	2.8	1
796	Development of New Density Functional Approximations. *Annual Review of Physical Chemistry*, **2017**, 68, 155-182	15.7	32
795	Impact of Diradical/Ionic Character on Third-Order Nonlinear Optical Property in Asymmetric Phenalenyl Dimers. **2017**, 2, 2084-2087		8
794	Nucleophilic Aromatic Substitution Reactions Described by the Local Electron Attachment Energy. **2017**, 82, 3072-3083		29
793	Spectroscopic, DFT and Z-scan supported investigation of dicyanoisophorone based push-pull NLOphoric styryl dyes. **2017**, 66, 494-511		33
792	Theoretical approaches for predicting the color of rigid dyes in solution. *Journal of Computational Chemistry*, **2017**, 38, 998-1004	3.5	12
791	Time-Dependent Extension of the Long-Range Corrected Density Functional Based Tight-Binding Method. *Journal of Chemical Theory and Computation*, **2017**, 13, 1737-1747	6.4	46
790	Simulation of the UV/Visible Absorption Spectra of Fluorescent Protein Chromophore Models. **2017**, 1, 281-296		13
789	Computational Study of Oxidation of Guanine by Singlet Oxygen ( ) and Formation of Guanine:Lysine Cross-Links. **2017**, 23, 5804-5813		21
788	Benchmark, DFT assessments, cooperativity, and energy decomposition analysis of the hydrogen bonds in HCN/HNC oligomeric complexes. *Journal of Molecular Modeling*, **2017**, 23, 56	2	6
787	A density functional theory study of double proton transfer reactions in formamide, formamide-formic acid and formic acid dimers. **2017**, 55, 719-728		2
786	In search of the best DFT functional for dealing with organic anionic species. **2017**, 19, 9189-9198		25
785	A theoretical study on quasi-one-dimensional open-shell singlet ladder oligomers: multi-radical nature, aromaticity and second hyperpolarizability. **2017**, 4, 779-789		16

784	When does a functional correctly describe both the structure and the energy of the transition state?. *Journal of Molecular Modeling*, **2017**, 23, 65	2	5
783	Detection of NO 2 by hexa- peri -hexabenzocoronene nanographene: A DFT study. **2017**, 20, 758-764		13
782	Nonequilibrium Chemical Effects in Single-Molecule SERS Revealed by Ab Initio Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2017**, 121, 1344-1350	2.8	12
781	Computational evaluation of the remarkable electro-optical responses of the multilithiated pristine and heterosubstituted sumanenes. **2017**, 678, 51-58		6
780	The Quantum Chemistry of Open-Shell Species. **2017**, 151-224		35
779	Investigation of the solvent effect, molecular structure, electronic properties and adsorption mechanism of Tegafur anticancer drug on Graphene nanosheet surface as drug delivery system by molecular dynamics simulation and density functional approach. **2017**, 88, 159-169		37
778	Femtosecond time-resolved photoelectron spectroscopy of the benzyl radical. **2017**, 19, 12365-12374		7
777	Quantum Chemical Estimation of Acetone Physisorption on Graphene Using Combined Basis Set and Size Extrapolation Schemes. **2017**, 121, 8999-9010		2
776	Benzene and Pyridine on Silicon (001): A Trial Ground for Long-Range Corrections in Density Functional Theory. **2017**, 121, 10484-10500		1
775	About the nature of halogen bond interaction under the spatial confinement. *Journal of Chemical Physics*, **2017**, 146, 154304	3.9	1
774	The role of the long-range exchange corrections in the description of electron delocalization in aromatic species. *Journal of Computational Chemistry*, **2017**, 38, 1640-1654	3.5	47
773	Development of an excited-state calculation method for large systems using dynamical polarizability: A divide-and-conquer approach at the time-dependent density functional level. *Journal of Chemical Physics*, **2017**, 146, 124123	3.9	18
772	Decomposition of Effective Exchange Integrals of Radical Dimers Using Bond Energy Density Analysis. **2017**, 46, 879-882		1
771	Comparing the performance of TD-DFT and SAC-CI methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. *Journal of Computational Chemistry*, **2017**, 38, 1084-1092	3.5	13
770	Assessment of range-separated functionals in the presence of implicit solvent: Computation of oxidation energy, reduction energy, and orbital energy. *Journal of Chemical Physics*, **2017**, 146, 164102	3.9	14
769	Assessing the role of Hartree-Fock exchange, correlation energy and long range corrections in evaluating ionization potential, and electron affinity in density functional theory. *Journal of Computational Chemistry*, **2017**, 38, 1844-1852	3.5	9
768	PubChemQC Project: A Large-Scale First-Principles Electronic Structure Database for Data-Driven Chemistry. **2017**, 57, 1300-1308		73
767	Classical andab InitioPlasmonics Meet at Sub-nanometric Noble Metal Rods. **2017**, 4, 1484-1493		43

766	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. *Journal of Chemical Theory and Computation*, **2017**, 13, 2696-2704	6.4	28
765	DFT study of host-dopant systems of DPVBi with organophosphorus □conjugated materials. **2017**, 1113, 61-71		2
764	Rhodium-rhodium interactions in [Rh(□diketonato)(CO)2] complexes. *Journal of Molecular Structure*, **2017**, 1144, 280-289	3.4	10
763	Heteroatom effect on photophysical properties of 2-(2?-hydroxyphenyl)benzimidazole and its derivatives as fluorescent dyes: A TD-DFT study. **2017**, 188, 275-282		20
762	DFT and TD-DFT theoretical studies on photo-induced electron transfer process on [Cefamandole].C60 nano-complex. **2017**, 75, 42-48		21
761	DFT calculations of the tautomerization and NLO properties of 5-amino-7-(pyrrolidin-1-yl)-2,4,4-trimethyl-1,4-dihydro-1,6-naphthyridine-8-carbonitrile (APNC). *Journal of Molecular Structure*, **2017**, 1143, 397-404	3.4	16
760	Quadratic nonlinear optical (NLO) properties of borazino (B3N3)-doped nanographenes. **2017**, 5, 8273-8287		24
759	Radical Reactions Affecting Polar Groups in Threonine Peptide Ions. **2017**, 121, 6557-6569		8
758	Coupled Cluster and Density Functional Studies of Atomic Fluorine Chemisorption on Coronene as Model Systems for Graphene Fluorination. **2017**, 121, 14888-14898		6
757	Theoretical Study on the Open-Shell Singlet Nature and the Second Hyperpolarizabilities of Corannulene Derivatives with Two Phenoxyl Radicals. *Journal of Physical Chemistry A*, **2017**, 121, 4171-4179	2.8	3
756	Shedding Light on the Accuracy of Optimally Tuned Range-Separated Approximations for Evaluating Oxidation Potentials. *Journal of Physical Chemistry A*, **2017**, 121, 4189-4201	2.8	9
755	Local Descriptors of Dynamic and Nondynamic Correlation. *Journal of Chemical Theory and Computation*, **2017**, 13, 2705-2711	6.4	28
754	Lithium enhanced second hyperpolarizability of inverse sandwich compounds (M-C 4 X 4 -M; X = H, Li) of beryllium, magnesium and calcium. **2017**, 1112, 46-51		1
753	Accurate excitation energies of molecules and oligomers from a semilocal density functional. *Journal of Chemical Physics*, **2017**, 146, 234102	3.9	9
752	Performance of TD-DFT for Excited States of Open-Shell Transition Metal Compounds. *Journal of Physical Chemistry A*, **2017**, 121, 3929-3942	2.8	20
751	Unraveling factors leading to efficient norbornadiene□quadricyclane molecular solar-thermal energy storage systems. **2017**, 5, 12369-12378		46
750	New insight into strong correlated states realised in a ferroelectric and paraelectric chalcogenide Sn2P2S6 crystal. *RSC Advances*, **2017**, 7, 27770-27779	3.7	9
749	Light-induced relaxation dynamics of the ferricyanide ion revisited by ultrafast XUV photoelectron spectroscopy. **2017**, 19, 14248-14255		24

748	Charge-Transfer Excitations: A Challenge for Time-Dependent Density Functional Theory That Has Been Met. **2017**, 7, 1700440		102
747	The mechanical and thermodynamic properties of □Si1□C. *RSC Advances*, **2017**, 7, 28499-28505	3.7	7
746	Electronic Structure of Open-Shell Singlet Molecules: Diradical Character Viewpoint. **2017**, 375, 47		40
745	Effects of the locality of a potential derived from hybrid density functionals on Kohn-Sham orbitals and excited states. **2017**, 19, 10177-10186		10
744	First-principles studies of carrier injection in polyethylene (PE) and ethylene-vinyl acetate copolymer (EVA) oligomers. **2017**, 24, 574-582		15
743	Opinion: Quantum solutions for a sustainable energy future. **2017**, 1,		12
742	Improved Infrared Spectra Prediction by DFT from a New Experimental Database. **2017**, 23, 8414-8423		40
741	Role of exact exchange in thermally-assisted-occupation density functional theory: A proposal of new hybrid schemes. *Journal of Chemical Physics*, **2017**, 146, 044102	3.9	27
740	DFT Calculations and Molecular Dynamics Simulation Study on the Adsorption of 5-Fluorouracil Anticancer Drug on Graphene Oxide Nanosheet as a Drug Delivery Vehicle. **2017**, 27, 805-817		57
739	Exploring the Linear Optical Properties of Borazine (B3N3) Doped Graphenes. 0D Flakes vs 2D Sheets. **2017**, 121, 709-722		18
738	Optimized Long-Range Corrected Density Functionals for Electronic and Optical Properties of Bare and Ligated CdSe Quantum Dots. *Journal of Chemical Theory and Computation*, **2017**, 13, 110-116	6.4	7
737	On the applicability of time-dependent density functional theory (TDDFT) and semiempirical methods to the computation of excited-state potential energy surfaces of perylene-based dye-aggregates. *International Journal of Quantum Chemistry*, **2017**, 117, e25337	2.1	24
736	Singlet fission in pancake-bonded systems. **2017**, 19, 5737-5745		20
735	Evaluation of Spin-Orbit Couplings with Linear-Response Time-Dependent Density Functional Methods. *Journal of Chemical Theory and Computation*, **2017**, 13, 515-524	6.4	152
734	Synthesis, structural characterization and computational study of a novel amino chalcone: a potential nonlinear optical material. *New Journal of Chemistry*, **2017**, 41, 1744-1754	3.6	50
733	Unifying Exchange Sensitivity in Transition-Metal Spin-State Ordering and Catalysis through Bond Valence Metrics. *Journal of Chemical Theory and Computation*, **2017**, 13, 5443-5457	6.4	34
732	Exchange-correlation energies of atoms from efficient density functionals: influence of the electron density. **2017**, 50, 245004		
731	NLOphoric multichromophoric auxiliary methoxy aided triphenylamine D-□A chromophores □ Spectroscopic and computational studies. **2017**, 73, 602-616		22

730	The ionic versus metallic nature of 2D electrides: a density-functional description. **2017**, 19, 27343-27352		10
729	Evaluation of the Factors Impacting the Accuracy of C NMR Chemical Shift Predictions using Density Functional Theory-The Advantage of Long-Range Corrected Functionals. *Journal of Chemical Theory and Computation*, **2017**, 13, 5798-5819	6.4	49
728	Interrogating the Becke'05 density functional for non-locality information. *Journal of Chemical Physics*, **2017**, 147, 154103	3.9	12
727	Diffusion of Fission Gas in Uranium Dioxide: A First-Principles Study. **2017**,		
726	Theoretical Investigation of the HO-Induced Degradation Mechanism of Hydrated Nafion Membrane via Ether-Linkage Dissociation. **2017**, 2, 4053-4064		24
725	Do fractionally incremented nuclear charges improve time-dependent density functional theory excitation energies as reliably as fractional orbital populations?. **2017**, 136, 1		1
724	Molecular attochemistry in non-polar liquid environments: ultrafast charge migration dynamics through gold-thiolate and gold-selenolate linkages. **2017**, 19, 26679-26696		2
723	Interpretation of the □□k- X[combining tilde] transition of hydrated protons in aqueous solutions observed in the far-UV region with quantum chemical calculations. **2017**, 19, 21490-21499		3
722	DFTBaby: A software package for non-adiabatic molecular dynamics simulations based on long-range corrected tight-binding TD-DFT(B). **2017**, 221, 174-202		41
721	Combining Density Functional Theory and Green's Function Theory: Range-Separated, Nonlocal, Dynamic, and Orbital-Dependent Hybrid Functional. *Journal of Chemical Theory and Computation*, **2017**, 13, 5317-5331	6.4	8
720	The extent of charge transfer: A qualitative computational study on electronic transitions of unsymmetrical squarylium dyes. **2017**, 1118, 123-132		0
719	A General Route to Include Pauli Repulsion and Quantum Dispersion Effects in QM/MM Approaches. *Journal of Chemical Theory and Computation*, **2017**, 13, 4854-4870	6.4	44
718	Solvatochromism and preferential solvation of Brooker's merocyanine in water-methanol mixtures. *Journal of Computational Chemistry*, **2017**, 38, 2411-2419	3.5	9
717	Design of a sub phthalocyanine-based hybrid donor of photovoltaic materials and its theoretical investigation. **2017**,		1
716	Assessment of Methodology and Chemical Group Dependences in the Calculation of the pK for Several Chemical Groups. *Journal of Chemical Theory and Computation*, **2017**, 13, 4791-4803	6.4	23
715	Theoretical study on steric deconjugation of poly(3-hexylthiophene) through bromination. **2017**, 687, 60-65		2
714	Optimal Tuning of Range-Separated Hybrids for Solvated Molecules with Time-Dependent Density Functional Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 4972-4983	6.4	16
713	Improving the Performance of Long-Range-Corrected Exchange-Correlation Functional with an Embedded Neural Network. *Journal of Physical Chemistry A*, **2017**, 121, 7273-7281	2.8	24

712	Enhanced Luminescence of Asymmetrical Seven-Coordinate EuIII Complexes Including LMCT Perturbation. **2017**, 2017, 3843-3848		34
711	Correlation functional in screened-exchange density functional theory procedures. *Journal of Computational Chemistry*, **2017**, 38, 2307-2315	3.5	9
710	Prediction of the lowest charge-transfer excited-state energy at the donor-acceptor interface in a condensed phase using ground-state DFT calculations with generalized Kohn-Sham functionals. *Journal of Molecular Modeling*, **2017**, 23, 235	2	11
709	Calculations of n->π* Transition Energies: Comparisons Between TD-DFT, ADC, CC, CASPT2, and BSE/GW Descriptions. *Journal of Physical Chemistry A*, **2017**, 121, 6122-6134	2.8	17
708	Assessment of Density Functionals for Computing Thermodynamic Properties of Lanthanide Complexes. *ChemPhysChem*, **2017**, 18, 2688-2696	3.2	16
707	Rational design of doubly-bridged chromophores for singlet fission and triplet–triplet annihilation. *RSC Advances*, **2017**, 7, 34830-34845	3.7	12
706	A new nonempirical tuning scheme with single self-consistent field calculation: Comparison with global and IP-tuned range-separated functional. *Journal of Computational Chemistry*, **2017**, 38, 2258-2267	3.5	12
705	Using non-empirically tuned range-separated functionals with simulated emission bands to model fluorescence lifetimes. **2017**, 19, 21046-21057		7
704	Solvent effects on the excited state characteristics of adenine–thymine base pairs. *RSC Advances*, **2017**, 7, 33426-33440	3.7	8
703	The Role of Super-Atom Molecular Orbitals in Doped Fullerenes in a Femtosecond Intense Laser Field. *Scientific Reports*, **2017**, 7, 121	4.9	6
702	Enhanced NLO response in BODIPY-coumarin hybrids: density functional theory approach. **2017**, 129, 1349-1361		10
701	Roaming-Mediated CHNH Elimination from the Ionization of Aromatic Ethylamines. **2017**, 6, 40-45		2
700	Third-Order Nonlinear Optical Properties of One-Dimensional Quinoidal Oligothiophene Derivatives Involving Phenoxyl Groups. **2017**, 6, 506-513		4
699	An open-source framework for analyzing N-electron dynamics. II. Hybrid density functional theory/configuration interaction methodology. *Journal of Computational Chemistry*, **2017**, 38, 2378-2387	3.5	25
698	Charge transfer excitations in TDDFT: A ghost-hunter index. *Journal of Computational Chemistry*, **2017**, 38, 2151-2156	3.5	30
697	Quantifying the Performances of DFT for Predicting Vibrationally Resolved Optical Spectra: Asymmetric Fluoroborate Dyes as Working Examples. *Journal of Chemical Theory and Computation*, **2017**, 13, 4347-4356	6.4	14
696	Self-interaction effects on charge-transfer collisions. **2017**, 95,		16
695	Attosecond Charge Migration with TDDFT: Accurate Dynamics from a Well-Defined Initial State. **2017**, 8, 3991-3996		45

694	Resolving Discrepancy between Theory and Experiment in 4-Nitrotoluene Oxidation. *Journal of Physical Chemistry A*, **2017**, 121, 6638-6645	2.8	4
693	Charge transfer in time-dependent density functional theory. **2017**, 29, 423001		68
692	Valence electronic structure of cobalt phthalocyanine from an optimally tuned range-separated hybrid functional. *Journal of Chemical Physics*, **2017**, 147, 044301	3.9	39
691	Electronic Structure Rearrangements in Hybrid Ribozyme/Protein Catalysis. **2017**, 86, 044801		2
690	Theoretical determination of the ionization potential and the electron affinity of organic semiconductors. **2017**,		3
689	Vanadium NMR Chemical Shifts of (Imido)vanadium(V) Dichloride Complexes with Imidazolin-2-iminato and Imidazolidin-2-iminato Ligands: Cooperation with Quantum-Chemical Calculations and Multiple Linear Regression Analyses. *Journal of Physical Chemistry A*, **2017**, 121, 9099-9105	2.8	3
688	Molecular Engineering of Mn Diamine Diketonate Precursors for the Vapor Deposition of Manganese Oxide Nanostructures. **2017**, 23, 17954-17963		27
687	A Linear-Scaling Divide-and-Conquer Quantum Chemical Method for Open-Shell Systems and Excited States. **2017**, 297-321		2
686	Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory. *RSC Advances*, **2017**, 7, 50496-50507	3.7	25
685	Ultrafast kinetics of linkage isomerism in Na[Fe(CN)NO] aqueous solution revealed by time-resolved photoelectron spectroscopy. **2017**, 4, 044031		8
684	Electronic structure of BN-aromatics: Choice of reliable computational tools. *Journal of Chemical Physics*, **2017**, 147, 164306	3.9	7
683	Coupled-cluster based approach for core-level states in condensed phase: Theory and application to different protonated forms of aqueous glycine. *Journal of Chemical Physics*, **2017**, 147, 014107	3.9	31
682	NLO properties of 1, 4-naphthoquinone, Juglone and Lawsone by DFT and Z-scan technique □A detailed study. **2017**, 72, 549-558		25
681	The application of TD-DFT to excited states of a family of TPD molecules interesting for optoelectronic use. **2017**, 136, 1		1
680	Design new hole transport materials for efficient perovskite solar cells by suitable combination of donor and core groups. **2017**, 49, 255-261		31
679	A Theoretical Investigation on Intramolecular Hydrogen Bond: The ESIPT Mechanism of dmahf Sensor. **2017**, 28, 937-947		8
678	Synthesis, photophysical properties and systematic evaluations of new phenanthroimidazole fluorescent probe for bioimaging: Experimental and theoretical study. **2017**, 166, 74-85		17
677	Tuning Nonlinear Optical Properties by Altering the Diradical and Charge-Transfer Characteristics of Chichibabin's Hydrocarbon Derivatives. *ChemPhysChem*, **2017**, 18, 142-148	3.2	10

676	Design of novel tellurium and selenium containing semiconducting polymers using quantum mechanical tools. **2017**, 1099, 45-54		2
675	Theoretical perspective of FIrpic derivatives: relationship between structures and photophysical properties. **2017**, 171, 425-431		4
674	Open-Shell-Character-Based Molecular Design Principles: Applications to Nonlinear Optics and Singlet Fission. **2017**, 17, 27-62		100
673	Fractional-charge and fractional-spin errors in range-separated density-functional theory. **2017**, 115, 161-173		16
672	Experimental and theoretical studies of the influence of solvent polarity on the spectral properties of two push-pull oxazol-5-(4H)-one compounds. **2017**, 171, 258-267		17
671	Benchmarking singlet and triplet excitation energies of molecular semiconductors for singlet fission: Tuning the amount of HF exchange and adjusting local correlation to obtain accurate functionals for singlet□triplet gaps. **2017**, 482, 319-338		36
670	A Theoretical Guideline for Designing Effective Host Materials Based on 4,4?-Bis(9-carbazolyl)-1,1?-biphenyl Derivatives for Blue Phosphorescent Devices. **2017**, 90, 195-204		2
669	Chiroptical Properties of Imines Derived from R-(+)-Norbornenone: The Role of Electronegativity Differences. *Journal of Physical Chemistry A*, **2017**, 121, 8247-8250	2.8	1
668	Communication: Recovering the flat-plane condition in electronic structure theory at semi-local DFT cost. *Journal of Chemical Physics*, **2017**, 147, 191101	3.9	21
667	On low-lying excited states of extended nanographenes. *Journal of Computational Chemistry*, **2017**, 38, 2020-2029	3.5	11
666	Nonempirical Simulations of Inhomogeneous Broadening of Electronic Transitions in Solution: Predicting Band Shapes in One- and Two-Photon Absorption Spectra of Chalcones. *Molecules*, **2017**, 22,	4.8	8
665	Chemical Tuning and Absorption Properties of Iridium Photosensitizers for Photocatalytic Applications. **2017**, 5, 23		7
664	Electronic Structure of Open-Shell Singlet Molecules: Diradical Character Viewpoint. **2017**, 1-67		2
663	Characterization of the Photochemical Properties of 5-Benzyluracil via Time-Dependent Density Functional Theory. *Journal of Physical Chemistry A*, **2017**, 121, 3909-3917	2.8	10
662	Curved □Receptors. **2017**, 311-328		17
661	Theoretical study on p-type D-□A sensitizers with modified □spacers for dye-sensitized solar cells. *Journal of Molecular Modeling*, **2018**, 24, 68	2	5
660	Quantum-mechanical condensed matter simulations with CRYSTAL. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1360	7.9	795
659	Long-range-corrected Rung 3.5 density functional approximations. *Journal of Chemical Physics*, **2018**, 148, 104112	3.9	13

658	Kohn□Sham approach for fast hybrid density functional calculations in real-space numerical grid methods. **2018**, 230, 21-26		3
657	Plane-Wave Implementation and Performance of □ -la-Carte Coulomb-Attenuated Exchange-Correlation Functionals for Predicting Optical Excitation Energies in Some Notorious Cases. *Journal of Chemical Theory and Computation*, **2018**, 14, 3184-3195	6.4	8
656	Dielectric Screening Meets Optimally Tuned Density Functionals. **2018**, 30, e1706560		76
655	Diagrams for comprehensive molecular orbital-based chemical reaction analyses: reactive orbital energy diagrams. **2018**, 20, 14211-14222		3
654	Density-functional theoretical study of fluorination effect on the electronic structure and electron drift mobilities of symmetric pentacene derivatives. **2018**, 240, 67-76		9
653	Long-Range Corrected DFT Calculations of First Hyperpolarizabilities and Excitation Energies of Metal Alkynyl Complexes. *ChemPhysChem*, **2018**, 19, 1537-1546	3.2	8
652	Computational Investigation of the Influence of □Bridge Conjugation Order of Thiophene and Thiazole Units in Triphenylamine Based Dyes in Dye-Sensitized Solar Cells. **2018**, 3, 3582-3590		6
651	Self-Interaction Error in Density Functional Theory: An Appraisal. **2018**, 9, 2353-2358		86
650	Double-helix PLi chains: novel potential nonlinear optical materials. **2018**, 20, 12618-12623		8
649	Nonlinear Optical Response of ICT Molecules. **2018**, 149-195		1
648	Dipole moments of molecules with multi-reference character from optimally tuned range-separated density functional theory. *Journal of Computational Chemistry*, **2018**, 39, 1508-1516	3.5	9
647	Is the choice of a standard zeroth-order hamiltonian in CASPT2 ansatz optimal in calculations of excitation energies in protonated and unprotonated schiff bases of retinal?. *Journal of Computational Chemistry*, **2018**, 39, 1470-1480	3.5	1
646	Revisiting absorption and electronic circular dichroism spectra of cholesterol in solution: a joint experimental and theoretical study. **2018**, 20, 5274-5284		3
645	Comparison of experimental photonic and refractive index characteristics of the TBADN films with their theoretical counterparts. **2018**, 696, 12-18		3
644	Theoretical study on electronic and absorption characters of p-type D-A-□A triaryamine sensitizer. **2018**, 96, 425-429		4
643	Understanding and Calibrating Density-Functional-Theory Calculations Describing the Energy and Spectroscopy of Defect Sites in Hexagonal Boron Nitride. *Journal of Chemical Theory and Computation*, **2018**, 14, 1602-1613	6.4	42
642	Calculation of linear and nonlinear optical properties of azobenzene derivatives with Kohn-Sham and coupled-cluster methods. **2018**, 20, 7303-7316		16
641	Conformational Relaxation and Thermally Activated Delayed Fluorescence in Anthraquinone-Based Intramolecular Charge-Transfer Compound. **2018**, 122, 3727-3737		43

640	The influence of anchoring group position in ruthenium dye molecule on performance of dye-sensitized solar cells. **2018**, 150, 335-346		7
639	Performance of range-separated hybrid exchange-correlation functionals for the calculation of magnetic exchange coupling constants of organic diradicals. *Journal of Computational Chemistry*, **2018**, 39, 780-787	3.5	9
638	A Chemical View on X-ray Photoelectron Spectroscopy: the ESCA Molecule and Surface-to-Bulk XPS Shifts. *ChemPhysChem*, **2018**, 19, 169-174	3.2	17
637	Using Density Based Indexes and Wave Function Methods for the Description of Excited States: Excited State Proton Transfer Reactions as a Test Case. *Journal of Physical Chemistry A*, **2018**, 122, 375-382	2.8	10
636	Mechanism of HO Decomposition by Triphenylphosphine Oxide. **2018**, 3, 259-265		13
635	Inclusion of aggregation effect to evaluate the performance of organic dyes in dye-sensitized solar cells. **2018**, 439, 160-167		5
634	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. **2018**, 5, 203-215		71
633	Ab initio calculation of nonlinear optical properties for chiral carbon nanotubes. Second harmonic generation and dc-Pockels effect. **2018**, 137, 1		4
632	Where Does the Density Localize in the Solid State? Divergent Behavior for Hybrids and DFT+U. *Journal of Chemical Theory and Computation*, **2018**, 14, 670-683	6.4	37
631	Photophysics and peripheral ring size dependent aggregate emission of cross-conjugated enediynes: applications to white light emission and vapor sensing. **2018**, 20, 4167-4180		6
630	A general range-separated double-hybrid density-functional theory. *Journal of Chemical Physics*, **2018**, 148, 164105	3.9	25
629	Computational Identification of Pyrrole Ring C as the Preferred Donor for Excited-State Proton Transfer in Bacteriophytochromes. **2018**, 2, 453-457		12
628	An experimental and DFT study of the packing and structure of dithenoylmethane monocarbonylphosphine Rhodium(I) complex [Rh((CHS)COCHCO(CHS))(CO)(PPh)]. **2018**, 83, 33-41		
627	35Cl Nuclear Magnetic Resonance Analysis of Pentacoordinate Titanium n-Butoxide Derivatives. **2018**, 47, 183-185		1
626	Short-range density functional correlation within the restricted active space CI method. *Journal of Chemical Physics*, **2018**, 148, 124118	3.9	12
625	A rational design of hole-transport small molecules based on fluorene with different modified groups for organic lead-halide perovskite solar cells. **2018**, 154, 275-281		16
624	Computational studies of the nonlinear optical properties of organometallic complexes. **2018**, 375, 389-409		20
623	Long-range corrected density functional through the density matrix expansion based semilocal exchange hole. **2018**, 20, 8991-8998		17

622	Quantum modeling of ultrafast photoinduced charge separation. **2018**, 30, 013002		20
621	Unusual response to environmental polarity in a nonlinear-optical benzylidene-type chromophore containing a 1,3-bis(dicyanomethylidene)indane acceptor fragment. **2017**, 20, 404-413		4
620	Photophysical properties of acetylene-linked syn bimane oligomers: a molecular photonic wire. **2018**, 20, 1150-1163		
619	Investigation of the Electronic Excited-State Equilibrium Geometries of Three Molecules Undergoing ESIPT: A RI-CC2 and TDDFT Study. *Journal of Physical Chemistry A*, **2018**, 122, 972-984	2.8	12
618	Exploring the properties of carbazole-based derivatives as hole transport materials from first principle and MD simulation. **2018**, 54, 14-20		12
617	Tunability of Open-Shell Character, Charge Asymmetry, and Third-Order Nonlinear Optical Properties of Covalently Linked (Hetero)Phenalenyl Dimers. **2018**, 24, 1913-1921		3
616	First principles study on interface between dual-channel anchorable organic dyes and TiO2 for dye-sensitized solar cells. **2018**, 149, 908-914		19
615	The crucial role of a spacer material on the efficiency of charge transfer processes in organic donor-acceptor junction solar cells. **2017**, 10, 451-459		5
614	Exploration of H binding to the [NiFe]-hydrogenase active site with multiconfigurational density functional theory. **2018**, 20, 794-801		14
613	Rigorous and Empirical Approaches to Correlated Single-Particle Theories. **2018**, 1-20		1
612	Design of zinc porphyrin-perylene diimide donor-bridge-acceptor chromophores for large second-order nonlinear optical response: A theoretical exploration. *International Journal of Quantum Chemistry*, **2018**, 118, e25536	2.1	5
611	Relativistic Time-Dependent Density Functional Theory for Molecular Properties. **2018**, 223-247		
610	On the Performance of Hybrid Functionals for Non-linear Optical Properties and Electronic Excitations in Chiral Molecular Crystals: The Case of Butterfly-Shaped Dicinnamalacetone. *ChemPhysChem*, **2018**, 19, 82-92	3.2	8
609	Screening of the structural, topological, and electronic properties of the functionalized Graphene nanosheets as potential Tegafur anticancer drug carriers using DFT method. **2018**, 36, 2517-2529		38
608	Assessment of DFT for endohedral complexes' dipole moment: PNO-LCCSD-F12 as a reference method. **2018**, 20, 29374-29388		3
607	Analysis of charge transfer transitions in stacked □electron donor-acceptor complexes. **2018**, 20, 26957-26967		9
606	Ab initio molecular dynamics study of solvated electrons in methanol clusters. **2018**, 20, 28741-28750		6
605	Second-order nonlinear optical properties of Stenhouse photoswitches: insights from density functional theory. **2018**, 20, 27658-27667		24

604	Base-free glucose dehydration catalysed by NHC-stabilised heterohalo cyclopentadienyl Cr(III) complexes. *New Journal of Chemistry*, **2018**, 42, 19193-19204	3.6	11
603	Optical properties of size selected neutral Ag clusters: electronic shell structures and the surface plasmon resonance. **2018**, 10, 20821-20827		21
602	Constricted Variational Density Functional Theory Approach to the Description of Excited States. **2018**,		
601	A scarce CC?CN □hole interaction in (E)-isomers of 3-[(4-halogenphenyl)amino]-2-cyanoprop-2-enoates. *New Journal of Chemistry*, **2018**, 42, 19995-20000	3.6	1
600	Analytical evaluation of relativistic molecular integrals. II: Method of computation for molecular auxiliary functions involved. **2018**, 29, 765-775		7
599	Theoretical Elucidation of Am(III)/Cm(III) Separation Mechanism with Diamide-type Ligands Using Relativistic Density Functional Theory Calculation. *Inorganic Chemistry*, **2018**, 57, 14513-14523	5.1	13
598	Fundamental Gaps of Condensed-Phase Organic Semiconductors from Single-Molecule Calculations using Polarization-Consistent Optimally Tuned Screened Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2018**, 14, 6287-6294	6.4	52
597	Can Adsorption on Graphene be Used for Isotopic Enrichment? A DFT Perspective. *Molecules*, **2018**, 23,	4.8	7
596	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. **2018**, 1-47		2
595	Coupling to Charge Transfer States is the Key to Modulate the Optical Bands for Efficient Light Harvesting in Purple Bacteria. **2018**, 9, 6892-6899		39
594	First-order nonadiabatic couplings in extended systems by time-dependent density functional theory. *Journal of Chemical Physics*, **2018**, 149, 244103	3.9	5
593	Effective quenching and excited-state relaxation of a Cu(I) photosensitizer addressed by time-resolved spectroscopy and TDDFT calculations. **2018**, 515, 557-563		5
592	On the many-electron self-interaction error of the semilocal exchange hole based meta-GGA level range-separated hybrid with the B88 hybrids. **2018**, 713, 1-9		11
591	Efficient lattice constants and energy bandgaps for condensed systems from a meta-GGA level screened range-separated hybrid functional. *Journal of Chemical Physics*, **2018**, 149, 094105	3.9	10
590	Impact of non-empirically tuning the range-separation parameter of long-range corrected hybrid functionals on ionization potentials, electron affinities, and fundamental gaps. *Journal of Computational Chemistry*, **2018**, 39, 2378-2384	3.5	8
589	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. **2018**, 9, 6149-6163		76
588	Tuned Range-Separated Density Functional Theory and Dyson Orbital Formalism for Photoelectron Spectra. *Journal of Chemical Theory and Computation*, **2018**, 14, 5870-5880	6.4	9
587	Factors affecting cyclic durability of all-solid-state lithium batteries using poly(ethylene oxide)-based polymer electrolytes and recommendations to achieve improved performance. **2018**, 20, 26098-26104		9

586	Observation of the First Spin Crossover in an Iron(II) Complex with an S Coordination Environment: Tris[bis(N,N-diethylamino)carbeniumdithiocarboxylato]iron(II) Hexafluorophosphate. **2018**, 24, 17955-17963		2
585	Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. *Journal of Chemical Theory and Computation*, **2018**, 14, 5653-5672	6.4	22
584	Davydov-type excitonic effects on the absorption spectra of parallel-stacked and herringbone aggregates of pentacene: Time-dependent density-functional theory and time-dependent density-functional tight binding. *Journal of Chemical Physics*, **2018**, 149, 134111	3.9	11
583	Tuning the Nonlinear Optical Response of Graphitic Carbon Nitride by Doping Li Atoms. **2018**, 122, 26635-26641		11
582	Range-Separated Hybrid Functionals with Variational Fitted Exact Exchange. *Journal of Chemical Theory and Computation*, **2018**, 14, 5608-5616	6.4	14
581	Quantum Chemical Study of Axial Ligand Effect on the Electronic Properties of Type I Copper Protein. **2018**, 47, 1172-1175		0
580	Assessment of a range-separated orbital-optimised random-phase approximation electron correlation method. **2018**, 137, 1		6
579	A Density Functional Theory Study on the Diffusion of Fission Gas Atoms in Uranium Dioxide. **2018**, 4,		1
578	Theoretical and experimental investigation of multifunctional highly conjugated organic push-pull ligands for NLO applications. **2018**, 86, 304-310		10
577	Rational Design of High-Efficiency Organic Dyes in Dye-Sensitized Solar Cells by Multiscale Simulations. **2018**, 122, 25219-25228		27
576	Theoretical investigations on hydrogen peroxide decomposition in aquo. **2018**, 20, 24992-24999		9
575	Open-Shell Characters, Aromaticities and Third-Order Nonlinear Optical Properties of Carbon Nanobelts Composed of Five- and Six-Membered Rings. **2018**, 7, 2320-2329		2
574	Heteroleptic ‡diketonate Ln(III) complexes decorated with pyridyl substituted pyridazine ligands: synthesis, structure and luminescence properties. **2018**, 5, 3015-3027		13
573	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. **2018**, 1-47		7
572	Concyclic CH-□arrays for single-axis rotations of a bowl in a tube. **2018**, 9, 3779		41
571	Dinitrogen Fixation by Vanadium Complexes with a Triamidoamine Ligand. *Inorganic Chemistry*, **2018**, 57, 11884-11894	5.1	16
570	Chemical Reactivity Properties, p Values, AGEs Inhibitor Abilities and Bioactivity Scores of the Mirabamides A?H Peptides of Marine Origin Studied by Means of Conceptual DFT. **2018**, 16,		34
569	Why the lowest electronic excitations of rhodamines are overestimated by time-dependent density functional theory. *International Journal of Quantum Chemistry*, **2018**, 118, e25780	2.1	21

568	Identification of tautomeric intermediates of a novel thiazolylazonaphthol dye - A density functional theory study. **2018**, 203, 324-332		4
567	Relativistic time-dependent density functional theories. **2018**, 47, 4481-4509		37
566	Accurate Treatment of Charge-Transfer Excitations and Thermally Activated Delayed Fluorescence Using the Particle-Particle Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2018**, 14, 3196-3204	6.4	9
565	Insights into geometries, stabilities, electronic structures, reactivity descriptors, and magnetic properties of bimetallic Ni Cu (m = 1, 2; n = 3-13) clusters: Comparison with pure copper clusters. *Journal of Computational Chemistry*, **2018**, 39, 1878-1889	3.5	8
564	Benchmarking the Performance of Exchange-Correlation Functionals for Predicting Two-Photon Absorption Strengths. *Journal of Chemical Theory and Computation*, **2018**, 14, 3677-3685	6.4	30
563	Blue M2: an intermediate melanoidin studied via conceptual DFT. *Journal of Molecular Modeling*, **2018**, 24, 138	2	19
562	Benchmarking DFT methods on linear and nonlinear electric properties of spatially confined molecules. *International Journal of Quantum Chemistry*, **2018**, 118, e25666	2.1	11
561	Quantum chemical approach for positron annihilation spectra of atoms and molecules beyond plane-wave approximation. *Journal of Chemical Physics*, **2018**, 148, 184110	3.9	5
560	Reproduction of the UV-vis spectra of boron subphthalocyanine chloride in different solvents using time-dependent generalized Kohn–Sham density functionals with first solvation shell. **2018**, 22, 670-678		6
559	Simple computational screening of potential singlet fission molecules. **2018**, 137, 1		2
558	Constructive effects of the interfacial properties: A strategy to design hole transport materials for high performance perovskite solar cells. **2018**, 62, 591-597		10
557	Large-scale ab initio calculations of Raman scattering spectra within time-dependent density functional perturbation theory. *Journal of Chemical Physics*, **2018**, 148, 244103	3.9	3
556	Band-edge levels of the NaCl(100) surface: Self-consistent hybrid density functional theory compared to many-body perturbation theory. **2018**, 97,		9
555	The valence and Rydberg states of difluoromethane: A combined experimental vacuum ultraviolet spectrum absorption and theoretical study by ab initio configuration interaction and density functional computations. *Journal of Chemical Physics*, **2018**, 148, 214304	3.9	5
554	Comparison of the Transition Dipole Moments Calculated by TDDFT with High Level Wave Function Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 5303-5309	6.4	11
553	Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states. *Journal of Chemical Physics*, **2018**, 149, 044116	3.9	36
552	Can Popular DFT Approximations and Truncated Coupled Cluster Theory Describe the Potential Energy Surface of the Beryllium Dimer?. **2018**, 71, 804		5
551	Indolino-Oxazolidine Acido- and Photochromic System Investigated by NMR and Density Functional Theory Calculations. **2018**, 83, 10409-10419		8

550	Communication: Correct charge transfer in CT complexes from the Becke'05 density functional. *Journal of Chemical Physics*, **2018**, 148, 211101	3.9	13
549	Computational modelling of singlet excitation energy transfer: a DFT/TD-DFT study of the ground and excited state properties of a syn bimane dimer system using non-empirically tuned range-separated functionals. *New Journal of Chemistry*, **2018**, 42, 13732-13743	3.6	1
548	Accelerating Kohn-Sham response theory using density fitting and the auxiliary-density-matrix method. *International Journal of Quantum Chemistry*, **2018**, 118, e25639	2.1	8
547	The LDA-1/2 Method Applied to Atoms and Molecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 4678-4686	6.4	5
546	How well can density functional theory and pair-density functional theory predict the correct atomic charges for dissociation and accurate dissociation energetics of ionic bonds?. **2018**, 20, 23072-23078		10
545	Theoretical investigation of the defect position effect on the NLO properties of N and B doped graphenes. **2018**, 367, 39-44		1
544	Evaluation of Aromaticity for Open-Shell Singlet Dicyclopenta-Fused Acenes and Polyacenes Based on a Magnetically Induced Current. **2018**, 24, 13457-13466		10
543	Theoretical Study on Open-Shell Singlet Character and Second Hyperpolarizabilities in Cofacial Stacked Dimers Composed of Weak Open-Shell Antiaromatic Porphyrins. *ChemPhysChem*, **2018**, 19, 2863-2871	3.2	4
542	Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes. **2018**, 10, 16499-16507		26
541	Structural, elastic, electronic and thermodynamic properties of ZrB2 under high-pressure: First-principle study. **2018**, 32, 1850200		1
540	Effect of end group of amorphous perfluoro-polymer electrets on electron trapping. **2018**, 19, 486-494		17
539	Accuracy of TD-DFT Geometries: A Fresh Look. *Journal of Chemical Theory and Computation*, **2018**, 14, 3715-3727	6.4	40
538	The effect of electronic excitation on London dispersion. **2018**, 96, 730-737		4
537	Range-Separated Double-Hybrid Functional from Nonempirical Constraints. *Journal of Chemical Theory and Computation*, **2018**, 14, 4052-4062	6.4	32
536	Charge Transfer Excitations with Range Separated Functionals Using Improved Virtual Orbitals. *Journal of Chemical Theory and Computation*, **2018**, 14, 3667-3676	6.4	1
535	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1378	7.9	60
534	Effect of chain length and donor–acceptor substitution on the electrical responsive properties of conjugated biphenyls: a DFT-based computational study. **2019**, 117, 23-33		1
533	Angular dependence of strong field ionization of N2 by time-dependent configuration interaction using density functional theory and the Tamm-Dancoff approximation. *Journal of Chemical Physics*, **2019**, 151, 054102	3.9	10

532	The key to the yellow-to-cyan tuning in the green fluorescent protein family is polarisation. **2019**, 21, 18988-18998		14
531	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells.. *RSC Advances*, **2019**, 9, 26402-26418	3.7	68
530	Quantum-chemical study of oxophosphorus dipyrromethene (PODIPY) fluorophore coordination environment. **2019**, 1164, 112553		1
529	On combining the conductor-like screening model and optimally tuned range-separated hybrid density functionals. *Journal of Chemical Physics*, **2019**, 150, 174117	3.9	6
528	Importance of van der Waals Descriptions on Accurate Isomerization Energy Calculations of Thiourea Compounds: LCgau-BOP+LRD Method. *Journal of Physical Chemistry A*, **2019**, 123, 7034-7041	2.8	2
527	Cost-effective density functional theory (DFT) calculations of equilibrium isotopic fractionation in large organic molecules. **2019**, 21, 17555-17570		8
526	B2PLYP and B2GPPLYP: The First Two Double-Hybrid Density Functionals with Long-Range Correction Optimized for Excitation Energies. *Journal of Chemical Theory and Computation*, **2019**, 15, 4735-4744	6.4	55
525	Machine-learned electron correlation model based on correlation energy density at complete basis set limit. *Journal of Chemical Physics*, **2019**, 151, 024104	3.9	17
524	Axial Chirality at the Boron-Carbon Bond: Synthesis, Stereodynamic Analysis, and Atropisomeric Resolution of 6-Aryl-5,6-dihydrodibenzo[][1,2]azaborinines. **2019**, 84, 12253-12258		9
523	Toward photophysical characteristics of triplet-triplet annihilation photon upconversion: a promising protocol from the perspective of optimally tuned range-separated hybrids. **2019**, 21, 17126-17141		6
522	Role of solvent-anion charge transfer in oxidative degradation of battery electrolytes. **2019**, 10, 3360		26
521	Enhanced intramolecular charge transfer of organic dyes containing hydantoin donor: A DFT study. **2019**, 383, 111979		7
520	Brominated Azaphilones from the Sponge-Associated Fungus Strain 4.14.6a. **2019**, 82, 2159-2166		21
519	Charge Transfer and Delocalization in Ladder-Type Fused Bithiophene Imide Oligomers. **2019**, 123, 20093-20104		4
518	DFT and spatial confinement: a benchmark study on the structural and electrical properties of hydrogen bonded complexes. **2019**, 21, 17253-17273		4
517	Towards density functional approximations from coupled cluster correlation energy densities. *Journal of Chemical Physics*, **2019**, 150, 244116	3.9	4
516	Cross-Comparisons between Experiment, TD-DFT, CC, and ADC for Transition Energies. *Journal of Chemical Theory and Computation*, **2019**, 15, 4581-4590	6.4	34
515	Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of para-nitroaniline. **2019**, 18, 1950030		32

514	Restoring the iso-orbital limit of the kinetic energy density in relativistic density functional theory. *Journal of Chemical Physics*, **2019**, 151, 174114	3.9	5
513	Steric Switching From Photochemical to Thermal N Splitting: A Computational Analysis of the Isomerization Reaction {(Cp)(Am)Mo}(□□-N) -> {(Cp)(Am)Mo}(□N). **2019**, 7, 352		3
512	Stability of "No-Pair Ferromagnetic" Lithium Clusters. *Journal of Physical Chemistry A*, **2019**, 123, 9721-9728	2.8	0
511	Simple exchange hole models for long-range-corrected density functionals. *Journal of Chemical Physics*, **2019**, 151, 094106	3.9	3
510	Molecular and Supramolecular Interactions in Systems with Nitroxide-Based Radicals. **2019**, 20,		4
509	Application of quantum chemical methods in polymer chemistry. **2019**, 38, 343-403		10
508	Isotropic Site-Site Dispersion Potential Determined from Localized Frequency-Dependent Density Susceptibility. **2019**, 92, 1694-1700		
507	Limitations of Global Hybrids in Predicting the Geometries and Torsional Energy Barriers of Dimeric Systems and the Role of Hartree Fock and DFT Exchange. *Journal of Computational Chemistry*, **2019**, 40, 2810-2818	3.5	5
506	Machine Learning for Predicting Electron Transfer Coupling. *Journal of Physical Chemistry A*, **2019**, 123, 7792-7802	2.8	20
505	Electrostatics-Assisted Building-Up Procedure for Capturing Energy Minima of Metal Clusters: Test Case of Ag Clusters. *Journal of Physical Chemistry A*, **2019**, 123, 7872-7880	2.8	2
504	Singlet-Fission-Induced Enhancement of Third-Order Nonlinear Optical Properties of Pentacene Dimers. **2019**, 4, 16181-16190		9
503	Roles of silver nanoclusters in surface-enhanced Raman spectroscopy. *Journal of Chemical Physics*, **2019**, 151, 094102	3.9	8
502	Locating Minimum Energy Crossings of Different Spin States Using the Fragment Molecular Orbital Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 6074-6084	6.4	8
501	Charge-transfer excited states in the donor/acceptor interface from large-scale GW calculations. *Journal of Chemical Physics*, **2019**, 151, 114109	3.9	3
500	Chemical-Reactivity Properties, Drug Likeness, and Bioactivity Scores of Seragamides A□ Anticancer Marine Peptides: Conceptual Density Functional Theory Viewpoint. *Computation*, **2019**, 7, 52	2.2	10
499	Screened hybrid meta-GGA exchange-correlation functionals for extended systems. **2019**, 21, 3002-3015		9
498	Photolytic properties of the biologically active forms of vitamin B12. **2019**, 385, 20-43		19
497	Non-linear optical response of meso substituted dipyrromethene boron difluoride dyes: Synthesis, photophysical, DFT and Z scan study. **2019**, 89, 164-172		5

496	Energetics of exciton binding and dissociation in polythiophenes: a tight binding approach. **2019**, 21, 11999-12011		5
495	Investigation of the chemical and optical properties of halogen-substituted N-methyl-4-piperidone curcumin analogs by density functional theory calculations. **2019**, 221, 117152		3
494	Structure of Electronically Reduced N-Donor Bidentate Ligands and Their Heteroleptic Four-Coordinate Zinc Complexes: A Survey of Density Functional Theory Results. *Inorganic Chemistry*, **2019**, 58, 7169-7179	5.1	5
493	Singling Out Dynamic and Nondynamic Correlation. **2019**, 10, 4032-4037		22
492	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. **2019**, 3, 846-855		6
491	Computational prediction of bioactivity scores and chemical reactivity properties of the Parasin I therapeutic peptide of marine origin through the calculation of global and local conceptual DFT descriptors. **2019**, 138, 1		9
490	Heteroatom substitution effect on electronic structures, photophysical properties, and excited-state intramolecular proton transfer processes of 3-hydroxyflavone and its analogues: A TD-DFT study. *Journal of Molecular Structure*, **2019**, 1195, 280-292	3.4	12
489	Range-separated hybrid density functionals made simple. *Journal of Chemical Physics*, **2019**, 150, 201102	3.9	40
488	Rational design of D-π-A organic dyes to prevent "trade off" effect in dye-sensitized solar cells. **2019**, 221, 117167		5
487	Comment on "Theoretical Investigations on Geometrical and Electronic Structures of Silver Clusters". *Journal of Computational Chemistry*, **2019**, 40, 1990-1993	3.5	3
486	Non-empirical, low-cost recovery of exact conditions with model-Hamiltonian inspired expressions in jmDFT. *Journal of Chemical Physics*, **2019**, 150, 154115	3.9	9
485	Effect of mono-halogen-substitution on the electron transporting properties of perylene diimides: A density functional theory study. *Journal of Molecular Liquids*, **2019**, 287, 110968	6	3
484	Can Density Functional Theory Be Trusted for High-Order Electric Properties? The Case of Hydrogen-Bonded Complexes. *Journal of Chemical Theory and Computation*, **2019**, 15, 3570-3579	6.4	11
483	Oxidation energies of shuttle molecules candidates in lithium-ion batteries from double-hybrid models. *International Journal of Quantum Chemistry*, **2019**, 119, e25950	2.1	5
482	Efficiently evaluating the Krieger-Li-Iafrate and common-energy-denominator approximations in the frequency-dependent Sternheimer scheme. **2019**, 99,		1
481	The Fragment Molecular Orbital Method Based on Long-Range Corrected Density-Functional Tight-Binding. *Journal of Chemical Theory and Computation*, **2019**, 15, 3008-3020	6.4	27
480	Insights into Direct Methods for Predictions of Ionization Potential and Electron Affinity in Density Functional Theory. **2019**, 10, 2692-2699		11
479	Quantum Chemistry for Studying Electronic Spectroscopy and Dynamics of Complex Molecular Systems. **2019**, 79-118		1

478	Theoretical and Experimental Molecular Spectroscopy of the Far-Ultraviolet Region. **2019**, 119-145		4
477	Characterization of Charge Transfer in Excited States of Extended Clusters of Stacked Donor and Acceptor Complexes in Lock-Arm Supramolecular Ordering. *Journal of Physical Chemistry A*, **2019**, 123, 4532-4542	2.8	5
476	Molecular Simulations with in-deMon2k QM/MM, a Tutorial-Review. *Molecules*, **2019**, 24,	4.8	16
475	Calculation of Charge-Transfer Electronic Coupling with Nonempirically Tuned Range-Separated Density Functional. **2019**, 123, 11351-11361		3
474	Local Density Approximation for the Short-Range Exchange Free Energy Functional. **2019**, 4, 7675-7683		9
473	Improving the electron transport performance by changing side chains in sulfur-containing azaacenes: a combined theoretical investigation on free molecules and an adsorption system. *New Journal of Chemistry*, **2019**, 43, 5414-5422	3.6	1
472	The correlation factor model for the exchange-correlation energy and its application to transition metal compounds. *Journal of Chemical Physics*, **2019**, 150, 084107	3.9	8
471	Absorption spectrum of magnesium and aluminum hydride nanoparticles. **2019**, 228, 244-253		2
470	Palladiumkatalysierte decarboxylierende Arylierung: Ein Zugang zu tetrasubstituierten chiralen Allenen. **2019**, 131, 6616-6620		6
469	First Principles Investigation of the Polarizability and First Hyperpolarizability of Anhydride Derivatives. **2019**, 2, 443-453		11
468	Palladium-Catalyzed Decarboxylative Arylation for the Synthesis of Tetrasubstituted Chiral Allenes. **2019**, 58, 6545-6548		20
467	A Density Functional Theory-Based Scheme to Compute the Redox Potential of a Transition Metal Complex: Applications to Heme Compound. *Molecules*, **2019**, 24,	4.8	1
466	Electronic Excitation Dynamics in DNA under Proton and Particle Irradiation. **2019**, 141, 5241-5251		11
465	Linear-Response and Real-Time, Time-Dependent Density Functional Theory for Predicting Optoelectronic Properties of Dye-Sensitized Solar Cells. **2019**, 171-201		1
464	TCA self-assembled fluorescence probe for Cu (II) ion based on the unique configuration of extra nuclear electrons of metal ions: A TDDFT study. **2019**, 1157, 1-10		
463	Reaction energy benchmarks of hydrocarbon combustion by Gaussian basis and plane wave basis approaches. *Journal of Computational Chemistry*, **2019**, 40, 1866-1873	3.5	1
462	Toward an Accurate Description of Thermally Activated Delayed Fluorescence: Equal Importance of Electronic and Geometric Factors. **2019**, 123, 13869-13876		8
461	Superalkalis as a source of diffuse excess electrons in newly designed inorganic electrides with remarkable nonlinear response and deep ultraviolet transparency: A DFT study. **2019**, 483, 1118-1128		56

460	NLOphoric benzyl substituted BODIPY and BOPHY: A comprehensive linear and nonlinear optical study by spectroscopic, DFT and Z-scan measurement. **2019**, 215, 122-129		8
459	Ionization and fragmentation of uracil upon microhydration. **2019**, 21, 4810-4821		10
458	Molecular Basis of the Chemiluminescence Mechanism of Luminol. **2019**, 25, 5202-5213		24
457	Benchmarking quantum chemistry methods for spin-state energetics of iron complexes against quantitative experimental data. **2019**, 21, 4854-4870		73
456	Recent Progresses in Ab Initio Electronic Structure Calculation toward Understandings of Functional Mechanisms of Biological Macromolecular Systems. **2019**,		
455	Improvement of functionals in density functional theory by the inverse Kohn□Sham method and density functional perturbation theory. **2019**, 52, 245003		8
454	On principal features of organic electrolyte molecules in lithium ion battery performance. **2019**, 21, 22990-22998		3
453	Systematic modification of the indium tin oxide work function via side-chain modulation of an amino-acid functionalization layer. **2019**, 21, 21875-21881		4
452	Synthesis, X-ray structure, photophysical properties, and theoretical studies of six-membered cyclometalated iridium(iii) complexes: revisiting Ir(pnbi)(acac). **2019**, 48, 15212-15219		1
451	Effects of □expansion, an additional hydroxyl group, and substitution on the excited state single and double proton transfer of 2-hydroxybenzaldehyde and its relative compounds: TD-DFT static and dynamic study. *New Journal of Chemistry*, **2019**, 43, 19107-19119	3.6	8
450	Beyond the Coulson-Fischer point: characterizing single excitation CI and TDDFT for excited states in single bond dissociations. **2019**, 21, 21761-21775		12
449	Non-Linear Optical Properties of Disperse Blue 354 and Disperse Blue183 by DFT and Z-Scan Technique. **2019**, 1-18		3
448	. **2019**,		8
447	Excess electron solvation in ammonia clusters. *Journal of Chemical Physics*, **2019**, 151, 204304	3.9	5
446	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. *Journal of Chemical Physics*, **2019**, 151, 214108	3.9	34
445	Many-Electron Treatments. **2019**, 195-253		
444	Modeling absorption spectra of molecules in solution. *International Journal of Quantum Chemistry*, **2019**, 119, e25719	2.1	38
443	The effects of dye aggregation on the performance of organic dyes in dye-sensitized solar cells: From static model to molecular dynamics simulation. **2019**, 205, 7-13		5

442	Density functionals for nondynamical correlation constructed from an upper bound to the exact exchange energy density. **2019**, 117, 1226-1241		6
441	Complex Structures of Monoglucosylrutin with ent-Gallocatechin-3- O-gallate and Epigallocatechin-3- O-gallate in Aqueous Solutions and the Mechanism of Color Change Induced by Complexation. **2019**, 82, 2-8		3
440	Molecular and NLO Properties of Red Fluorescent Coumarins - DFT Computations Using Long-Range Separated and Conventional Functionals. **2019**, 29, 241-253		3
439	Alkylation of uracil and thymine in the gas phase through interaction with alkylmercury compounds. **2019**, 436, 153-165		3
438	Approximating Quasiparticle and Excitation Energies from Ground State Generalized Kohn-Sham Calculations. *Journal of Physical Chemistry A*, **2019**, 123, 666-673	2.8	23
437	Photophysics of OLED Materials with Emitters Exhibiting Thermally Activated Delayed Fluorescence and Used in Hole/Electron Transporting Layer from Optimally Tuned Range-Separated Density Functional Theory. **2019**, 123, 746-761		11
436	Quantum Chemistry on Quantum Computers: A Method for Preparation of Multiconfigurational Wave Functions on Quantum Computers without Performing Post-Hartree-Fock Calculations. **2019**, 5, 167-175		37
435	Gas-Phase Ozone Reactions with a Structurally Diverse Set of Molecules: Barrier Heights and Reaction Energies Evaluated by Coupled Cluster and Density Functional Theory Calculations. *Journal of Physical Chemistry A*, **2019**, 123, 517-536	2.8	11
434	Estimation of maximum absorption wavelength of polymethine dyes in visible and near-infrared region based on time-dependent density functional theory. **2019**, 518, 15-24		9
433	Accelerated long-range corrected exchange functional using a two-gaussian operator combined with one-parameter progressive correlation functional [LC-BOP(2Gau)]. *Journal of Computational Chemistry*, **2019**, 40, 105-112	3.5	4
432	Beyond Koopmans' theorem: electron binding energies in disordered materials. **2019**, 31, 043001		7
431	Triplet Tuning: A Novel Family of Non-Empirical Exchange-Correlation Functionals. *Journal of Chemical Theory and Computation*, **2019**, 15, 1226-1241	6.4	23
430	Effect of donor acceptor substitution position on the electrical responsive properties of azulene system: a computational study. **2019**, 117, 1781-1789		1
429	Non-linear optical response of meso hybrid BODIPY: Synthesis, photophysical, DFT and Z scan study. **2019**, 209, 126-140		8
428	Electronic processes in NO dimerization on Ag and Cu clusters: DFT and MRMP2 studies. *Journal of Computational Chemistry*, **2019**, 40, 181-190	3.5	6
427	Theoretical investigations on geometrical and electronic structures of silver clusters. *Journal of Computational Chemistry*, **2019**, 40, 206-211	3.5	17
426	Shedding Light on the Basis Set Dependence of the Minnesota Functionals: Differences Between Plane Waves, Slater Functions, and Gaussians. *Journal of Chemical Theory and Computation*, **2019**, 15, 557-571	6.4	5
425	Performance of DFT for C Isomerization Energies: A Noticeable Exception to Jacob's Ladder. *Journal of Physical Chemistry A*, **2019**, 123, 257-266	2.8	13

424	Unbiased Rotational Motions of an Ellipsoidal Guest in a Tight Yet Pliable Host. **2019**, 131, 2062-2066		11
423	Unbiased Rotational Motions of an Ellipsoidal Guest in a Tight Yet Pliable Host. **2019**, 58, 2040-2044		16
422	Star-Shaped Molecules as Dopant-Free Hole Transporting Materials for Efficient Perovskite Solar Cells: Multiscale Simulation. **2019**, 19, 938-946		7
421	The reHISS Three-Range Exchange Functional with an Optimal Variation of Hartree-Fock and Its Use in the reHISSB-D Density Functional Theory Method. *Journal of Computational Chemistry*, **2019**, 40, 29-38	3.5	5
420	UV-Visible spectroscopy and density functional study of solvent effect on halogen bonded charge-transfer complex of 2-Chloropyridine and iodine monochloride. **2019**, 12, 4522-4532		6
419	Influence of π-spacer of donor-acceptor-π-acceptor sensitizers on photovoltaic properties in dye-sensitized solar cells. **2020**, 76, 105429		4
418	A theoretical study of the absorption spectra of electron-deficient pentacene derivatives using DFT and TDDFT. **2020**, 225, 117480		3
417	New oxacalix[4]arene carboxylate detects viologen in protic media. **2020**, 32, 313-319		2
416	From a week to less than a day: Speedup and scaling of coordinate-scaled exact exchange calculations in plane waves. **2020**, 247, 106943		3
415	Performance of Range Separated Density Functional in Solvent Continuum: Tuning Long-range Hartree-Fock Exchange for Improved Orbital Energies. *Journal of Computational Chemistry*, **2020**, 41, 295-304	3.5	5
414	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. *Journal of Computational Chemistry*, **2020**, 41, 427-438	3.5	18
413	Linear-Response Time-Dependent Density Functional Theory with Stochastic Range-Separated Hybrids. *Journal of Chemical Theory and Computation*, **2020**, 16, 1064-1072	6.4	12
412	Solvatochromic dual luminescence of Eu-Au dyads decorated with chromophore phosphines. **2020**, 7, 140-149		10
411	Time-dependent DFT study of the K-edge spectra of vanadium and titanium complexes: effects of chloride ligands on pre-edge features. **2020**, 22, 674-682		9
410	Spectroscopic, DFT and Z-scan approach to study linear and nonlinear optical properties of Disperse Red 277. **2020**, 99, 109536		7
409	Spectroscopic investigation of some electron withdrawing groups substituted TTF donor. **2020**, 231, 117849		3
408	Mechanism of Copigmentation of Monoglucosylrutin with Caffeine. **2020**, 68, 323-331		1
407	Ab Initio Many-Body Perturbation Theory Calculations of the Electronic and Optical Properties of Cyclometalated Ir(III) Complexes. *Journal of Chemical Theory and Computation*, **2020**, 16, 1188-1199	6.4	5

406	Density Functional Theory as a Data Science. **2020**, 20, 618-639		5
405	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. *Journal of Chemical Theory and Computation*, **2020**, 16, 587-600	6.4	32
404	The influence of driving force on intramolecular electron transfer: A theoretical study of subphthalocyanine-AzaBODIPY-C60 supramolecular triad. *International Journal of Quantum Chemistry*, **2020**, 120, e26131	2.1	1
403	Kinetics and Thermodynamics of Reactions Involving Criegee Intermediates: An Assessment of Density Functional Theory and Ab Initio Methods Through Comparison with CCSDT(Q)/CBS Data. *Journal of Computational Chemistry*, **2020**, 41, 328-339	3.5	10
402	Carbazole-substituted NP-based derivative as hole transporting material for highly efficient perovskite solar cells. **2020**, 228, 117808		5
401	Recent developments in symmetry-adapted perturbation theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1452	7.9	47
400	Self-Consistent Implementation of Hybrid Functionals with Local Range Separation. *Journal of Chemical Theory and Computation*, **2020**, 16, 953-963	6.4	6
399	Self-interaction correction, electrostatic, and structural influences on time-dependent density functional theory excitations of bacteriochlorophylls from the light-harvesting complex 2. *Journal of Chemical Physics*, **2020**, 153, 144114	3.9	3
398	UV/Vis absorption spectrum calculations of benzo-1,2-dipyrene isomer using long-range corrected density functional theory. **2020**, 761, 138023		2
397	Acceptor plane expansion enhances horizontal orientation of thermally activated delayed fluorescence emitters. **2020**, 6,		47
396	Subsystem density-functional theory for interacting open-shell systems: spin densities and magnetic exchange couplings. **2020**, 224, 201-226		3
395	Tunneling matrix element and tunneling pathways of protein electron transfer calculated with a fragment molecular orbital method. *Journal of Chemical Physics*, **2020**, 153, 104104	3.9	1
394	Variational fitting of the Fock exchange potential with modified Cholesky decomposition. *Journal of Chemical Physics*, **2020**, 153, 134112	3.9	3
393	A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Left-Right Correlation. *Journal of Chemical Theory and Computation*, **2020**, 16, 5645-5657	6.4	18
392	Unmasking Static Correlation Error in Hybrid Kohn-Sham Density Functional Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 5432-5440	6.4	10
391	Structural Evolution and Stability Trend of Small-Sized Gold Clusters Au (= 20-30). *Journal of Physical Chemistry A*, **2020**, 124, 1289-1299	2.8	18
390	Density Functional Theories and Coordination Chemistry. **2020**,		2
389	Assessing the structure and first hyperpolarizability of Li@BH in solution: a sequential QM/MM study using the ASEC-FEG method. **2020**, 22, 17314-17324		3

388	A New Mixing of Nonlocal Exchange and Nonlocal Correlation with Multiconfiguration Pair-Density Functional Theory. **2020**, 11, 10158-10163		7
387	Towards a Holomorphic Density Functional Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 7400-7412	6.4	2
386	Self-Consistent Calculation of the Localized Orbital Scaling Correction for Correct Electron Densities and Energy-Level Alignments in Density Functional Theory. **2020**, 11, 10269-10277		8
385	Experimental and theoretical studies on circularly polarized phosphorescence of a [2.2]paracyclophane-based platinum(ii) complex. **2020**, 56, 15438-15441		12
384	The effect of N-heterocyclic carbene units on the absorption spectra of Fe(II) complexes: a challenge for theory. **2020**, 22, 27605-27616		5
383	A Review of Density Functional Models for the Description of Fe(II) Spin-Crossover Complexes. *Molecules*, **2020**, 25,	4.8	6
382	Electronic couplings for photo-induced processes from subsystem time-dependent density-functional theory: The role of the diabatization. *Journal of Chemical Physics*, **2020**, 153, 184113	3.9	5
381	Comprehensive Photophysical Properties of Thiophene/Phenylene Co-oligomers Investigated by Theoretical and Experimental Studies. **2020**, 124, 18946-18955		2
380	Kinetic prediction of reverse intersystem crossing in organic donor-acceptor molecules. **2020**, 11, 3909		30
379	A polarizable molecular dynamics method for electrode-electrolyte interfacial electron transfer under the constant chemical-potential-difference condition on the electrode electrons. *Journal of Chemical Physics*, **2020**, 153, 054126	3.9	5
378	A new ionone derivative from Boiss. (Solanaceae). **2020**, 1-8		2
377	Evaluation of Complexation Energies for Cyclodextrin-Drug Inclusion Complexes. **2020**, 5, 19371-19376		5
376	Theoretical Molecular Design of Phenanthrenes for Singlet Fission by Diazadibora-Substitution. *Journal of Physical Chemistry A*, **2020**, 124, 6778-6789	2.8	4
375	Accurate Prediction of Vertical Emission from Excited-State Tuning of Range-Separated Density Functional Theory. **2020**, 124, 17964-17970		4
374	Large-scale comparison of 3d and 4d transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics. **2020**, 22, 19326-19341		13
373	Reorganization energies and spectral densities for electron transfer problems in charge transport materials. **2020**, 22, 21630-21641		11
372	Models and corrections: Range separation for electronic interaction-Lessons from density functional theory. *Journal of Chemical Physics*, **2020**, 153, 160901	3.9	5
371	Fenton reaction mechanism generating no OH radicals in Nafion membrane decomposition. *Scientific Reports*, **2020**, 10, 18144	4.9	8

370	Introductory lecture: when the density of the noninteracting reference system is not the density of the physical system in density functional theory. **2020**, 224, 9-26		3
369	Charge-Transfer Excitation Energies Expressed as Orbital Energies of Kohn-Sham Density Functional Theory with Long-Range Corrected Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 8079-8087	2.8	7
368	Molecular excitations from meta-generalized gradient approximations in the Kohn-Sham scheme. *Journal of Chemical Physics*, **2020**, 153, 114106	3.9	2
367	Virtual Screening of Marine Natural Compounds by Means of Chemoinformatics and CDFT-Based Computational Peptidology. **2020**, 18,		14
366	Conceptual DFT-Based Computational Peptidology of Marine Natural Compounds: Discodermins A-H. *Molecules*, **2020**, 25,	4.8	14
365	Transition-Metal Capping to Suppress Back-Donation to Enhance Donor Ability. **2020**, 39, 4191-4194		5
364	Predicting Excitation Energies of Twisted Intramolecular Charge-Transfer States with the Time-Dependent Density Functional Theory: Comparison with Experimental Measurements in the Gas Phase and Solvents Ranging from Hexanes to Acetonitrile. *Journal of Chemical Theory and Computation*, **2020**, 16, 6244-6255	6.4	10
363	Insight and performance of LC-DFT vs DFT in the NMR shielding and chemical shift calculations: Case of CHCl?CH?CF3. *International Journal of Quantum Chemistry*, **2020**, 120, e26408	2.1	
362	Theoretical Chemistry for Experimental Chemists. **2020**,		
361	Assessing the Tamm-Dancoff approximation, singlet-singlet, and singlet-triplet excitations with the latest long-range corrected double-hybrid density functionals.. *Journal of Chemical Physics*, **2020**, 153, 064106	3.9	29
360	Superhalogen doping: a new and effective approach to design materials with excellent static and dynamic NLO responses. *New Journal of Chemistry*, **2020**, 44, 16358-16369	3.6	17
359	In Silico Modeling of New "Y-Series"-Based Near-Infrared Sensitive Non-Fullerene Acceptors for Efficient Organic Solar Cells. **2020**, 5, 24125-24137		48
358	Designing Star-Shaped Subphthalocyanine-Based Acceptor Materials with Promising Photovoltaic Parameters for Non-fullerene Solar Cells. **2020**, 5, 23039-23052		21
357	Theoretical analysis of the influence of C□H(cdots)O bonds on the NMR constants of uracil in DMSO. **2020**, 139, 1		2
356	Core-Level Excitation Energies of Nucleic Acid Bases Expressed as Orbital Energies of the Kohn-Sham Density Functional Theory with Long-Range Corrected Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 10482-10494	2.8	4
355	Artificial neural networks for predicting charge transfer coupling. *Journal of Chemical Physics*, **2020**, 153, 214113	3.9	13
354	Halogen Bond of Halonium Ions: Benchmarking DFT Methods for the Description of NMR Chemical Shifts. *Journal of Chemical Theory and Computation*, **2020**, 16, 7690-7701	6.4	4
353	An X-shaped cyano□arbonyl interaction on the polar surface of (cyanoacetyl)hydrazones. **2020**, 22, 3274-3278		

352	An efficient hybrid scheme for time dependent density functional theory. *Journal of Chemical Physics*, **2020**, 152, 184104	3.9	5
351	Nonlinear optical activity of imino-dyes with furan, thiophene or thiazole moieties as π-conjugated bridge: a computational investigation. **2020**, 118, e1761471		3
350	Molecular Design Principle for Efficient Singlet Fission Based on Diradical Characters and Exchange Integrals: Multiple Heteroatom Substitution Effect on Anthracenes. **2020**, 124, 11800-11809		10
349	Electron Spin Densities and Density Functional Approximations: Open-Shell Polycyclic Aromatic Hydrocarbons as Case Study. *Journal of Chemical Theory and Computation*, **2020**, 16, 3567-3577	6.4	6
348	A new tuned range-separated density functional for the accurate calculation of second hyperpolarizabilities. **2020**, 22, 11871-11880		11
347	Fully numerical calculations on atoms with fractional occupations and range-separated exchange functionals. **2020**, 101,		8
346	Covalent interactions depend on the distances between metals and fullerenes for thermodynamically stable M@C78 (M = La, Ce, and Sm). **2020**, 7, 2538-2547		3
345	Selected molecules based on (-1-cyanovinyl)benzonitrile as new materials for NLO applications – Experimental and computational studies. *Journal of Molecular Liquids*, **2020**, 314, 113622	6	4
344	Unveiling the Physics Behind Hybrid Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 5606-5614	2.8	13
343	Diindenoanthracene Diradicaloids Enable Rational, Incremental Tuning of Their Singlet-Triplet Energy Gaps. **2020**, 6, 1353-1368		19
342	Application of accelerated long-range corrected exchange functional [LC-DFT(2Gau)] to periodic boundary condition systems: CO adsorption on Cu(111) surface. *Journal of Chemical Physics*, **2020**, 152, 104105	3.9	1
341	The Quest for Highly Accurate Excitation Energies: A Computational Perspective. **2020**, 11, 2374-2383		58
340	Band Alignment in Two-Dimensional Halide Perovskite Heterostructures: Type I or Type II?. **2020**, 11, 2910-2916		25
339	4-(4-Chloro-2-oxo-3(1H-phenanthro[9,10-d]imidazol-2-yl)-2H-chromen-6-yl) benzaldehyde as a fluorescent probe for medical imaging: linear and nonlinear optical properties. **2020**, 19, 473-484		
338	Characterization of the structural, spectroscopic, nonlinear optical, electronic properties and antioxidant activity of the N-{4[(E)-3-(Fluorophenyl)-1-(phenyl)-prop-2-en-1-one]}-acetamide. *Journal of Molecular Structure*, **2020**, 1220, 128765	3.4	13
337	Theoretical study on aromatic and open-shell characteristics of carbon nanobelts composed of indeno[1,2-]fluorene units: dependence on the number of units and charge states.. *RSC Advances*, **2020**, 10, 25736-25745	3.7	2
336	Range-separated hybrid and double-hybrid density functionals: A quest for the determination of the range-separation parameter. *Journal of Chemical Physics*, **2020**, 152, 244124	3.9	13
335	Performance of DFT functionals for calculating the second-order nonlinear optical properties of dipolar merocyanines. **2020**, 22, 16579-16594		26

334	Dopant levels in large nanocrystals using stochastic optimally tuned range-separated hybrid density functional theory. **2020**, 102,		3
333	A molecular perspective on Tully models for nonadiabatic dynamics. **2020**, 22, 15183-15196		32
332	Theoretical study of new push□pull molecules based on transition metals for NLO applications and determination of ICT mechanisms by DFT calculations. **2020**, 19, 2050026		4
331	Wavelength-decomposition-based embedded cluster density approximation for systems with nonlocal electron correlation. *International Journal of Quantum Chemistry*, **2020**, 120, e26347	2.1	1
330	Competing excited-state deactivation processes in bacteriophytochromes. **2020**, 243-268		1
329	High first-hyperpolarizabilities of thiobarbituric acid derivative-based donor-□acceptor nonlinear optical-phores: Multiple theoretical investigations of substituents and conjugated bridges effect. *International Journal of Quantum Chemistry*, **2020**, 120, e26176	2.1	2
328	Role of □electron conjugation in determining the electrical responsive properties of polychlorinated biphenyls: a DFT based computational study. **2020**, 2, 1		0
327	Excitation energies expressed as orbital energies of Kohn-Sham density functional theory with long-range corrected functionals. *Journal of Computational Chemistry*, **2020**, 41, 1368-1383	3.5	9
326	Benchmark of Simplified Time-Dependent Density Functional Theory for UV□Vis Spectral Properties of Porphyrinoids. **2020**, 3, 1900192		4
325	Initial-state preparation effects in time-resolved electron paramagnetic resonance experiments. *Journal of Chemical Physics*, **2020**, 152, 044304	3.9	0
324	Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states. *Journal of Computational Chemistry*, **2020**, 41, 1242-1251	3.5	26
323	Pigments of the Moss : Isolation and Structure Elucidation of Prenyl-Substituted 8,8'-Linked 9,10-Phenanthrenequinone Dimers. **2020**, 83, 268-276		1
322	Theoretical study on the effect of spacer groups on the nonlinear optical properties of polyvinyl carbazole molecular fragments. **2020**, 31, 1471-1479		1
321	Theoretical investigation on the ESIPT mechanism and fluorescent sensing mechanism of 2-(2'-hydroxyphenyl) thiazole-4-carboxaldeyde in methanol. **2020**, 233, 118214		11
320	Vibrational Spectra of the Ruthenium-Tris-Bipyridine Dication and Its Reduced Form in Vacuo. *Journal of Physical Chemistry A*, **2020**, 124, 2449-2459	2.8	2
319	Extensive Quantum Chemistry Study of Neutral and Charged C4N Chains: An Attempt To Aid Astronomical Observations. **2020**, 4, 434-448		4
318	A solvent-catalyzed four-molecular two-path solvolysis mechanism of t-butyl chloride or bromide in water or alcohol derived by density functional theory calculation and confirmed by high-resolution electrospray ionization-mass spectrometry. **2020**, 129, 583-612		2
317	Large-scale excited-state calculation using dynamical polarizability evaluated by divide-and-conquer based coupled cluster linear response method. *Journal of Chemical Physics*, **2020**, 152, 024102	3.9	7

316	Excitonic Coupling on a Heliobacterial Symmetrical Type-I Reaction Center: Comparison with Photosystem I. **2020**, 124, 389-403		6
315	Preserving Symmetry and Degeneracy in the Localized Orbital Scaling Correction Approach. **2020**, 11, 1528-1535		14
314	Investigation of Thermally Activated Delayed Fluorescence from a Donor-Acceptor Compound with Time-Resolved Fluorescence and Density Functional Theory Applying an Optimally Tuned Range-Separated Hybrid Functional. *Journal of Physical Chemistry A*, **2020**, 124, 1535-1553	2.8	12
313	Meta-Stable Molecular Configuration Enables Thermally Stable and Solution Processable Organic Charge Transporting Materials. **2020**, 30, 2000729		2
312	Bayesian Optimization for Calibrating and Selecting Hybrid-Density Functional Models. *Journal of Physical Chemistry A*, **2020**, 124, 4053-4061	2.8	39
311	Elucidating the binding mechanism of thione-containing mercaptopurine and thioguanine drugs to small gold clusters. *Journal of Computational Chemistry*, **2020**, 41, 1748-1758	3.5	5
310	Modulating ESIPT behavior and fluorescent sensing mechanism of 2-(2?-hydroxyphenol)thiazole-4-carbonxaldeyde derivatives: A theoretical study. **2020**, 747, 137342		3
309	Range-Separated Density-Functional Theory in Combination with the Random Phase Approximation: An Accuracy Benchmark. *Journal of Chemical Theory and Computation*, **2020**, 16, 2985-2994	6.4	8
308	Regular Two-Dimensional Arrays of Surface-Mounted Molecular Switches: Switching Monitored by UV-vis and NMR Spectroscopy. **2020**, 142, 9337-9351		8
307	How accurate are TD-DFT excited-state geometries compared to DFT ground-state geometries?. *Journal of Computational Chemistry*, **2020**, 41, 1718-1729	3.5	25
306	Hybrid functionals with system-dependent parameters: Conceptual foundations and methodological developments. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1476	7.9	6
305	Approximate versus Exact Embedding for Chiroptical Properties: Reconsidering Failures in Potential and Response. *Journal of Chemical Theory and Computation*, **2020**, 16, 3104-3120	6.4	11
304	Nonadiabatic Dynamics of Charge-Transfer States Using the Anthracene-Tetracyanoethylene Complex as a Prototype. *Journal of Physical Chemistry A*, **2020**, 124, 3347-3357	2.8	8
303	The Trip to the Density Functional Theory Zoo Continues: Making a Case for Time-Dependent Double Hybrids for Excited-State Problems. **2021**, 74, 3		23
302	Improving the optoelectronic efficiency of novel meta-azo dye-sensitized TiO semiconductor for DSSCs. **2021**, 247, 119143		3
301	Production of copper nanoparticles exhibiting various morphologies via pulsed laser ablation in different solvents and their catalytic activity for reduction of toxic nitroaromatic compounds. **2021**, 409, 124412		20
300	Reversible Silylium Transfer between P-H and Si-H Donors. **2021**, 60, 2379-2384		1
299	First principle study of lithium and phosphorus co-doped graphitic carbon nitride as a nonlinear optical material. **2021**, 26, 101911		2

298	A Stable Triplet-Ground-State Conjugated Diradical Based on a Diindenopyrazine Skeleton. **2021**, 60, 4594-4598		13
297	Efficient Hybrid Density Functional Calculations for Large Periodic Systems Using Numerical Atomic Orbitals. *Journal of Chemical Theory and Computation*, **2021**, 17, 222-239	6.4	1
296	A Stable Triplet-Ground-State Conjugated Diradical Based on a Diindenopyrazine Skeleton. **2021**, 133, 4644-4648		1
295	Theoretical investigation of aromaticity and charge transfer in emission process of triarylmethyl radicals as OLED materials. *International Journal of Quantum Chemistry*, **2021**, 121, e26522	2.1	3
294	Reversible Silylium Transfer between P-H and Si-H Donors. **2021**, 133, 2409-2414		0
293	Time-Dependent Density Functional Theory Study of Copper(II) Oxo Active Sites for Methane-to-Methanol Conversion in Zeolites. *Inorganic Chemistry*, **2021**, 60, 1149-1159	5.1	6
292	Shedding light on ultrafast ring-twisting pathways of halogenated GFP chromophores from the excited to ground state. **2021**, 23, 14636-14648		4
291	Quantum computational investigations and molecular docking studies on amentoflavone. **2021**, 7, e06079		8
290	Global double hybrids do not work for charge transfer: A comment on "Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states". *Journal of Computational Chemistry*, **2021**, 42, 528-533	3.5	9
289	Theoretical Investigation of Intermolecular Dihydrogen Bonds in C2H2⋯HM and C2H4⋯HM (M = Li, Na and K) Complexes: A DFT and ab initio Study. **2021**, 33, 1811-1818		
288	Advances, challenges and perspectives of quantum chemical approaches in molecular spectroscopy of the condensed phase. **2021**, 50, 10917-10954		14
287	Excitation energies through Becke□ exciton model within a Cartesian-grid KS DFT. **2021**, 140, 1		3
286	A Simple Range-Separated Double-Hybrid Density Functional Theory for Excited States. *Journal of Chemical Theory and Computation*, **2021**, 17, 927-942	6.4	19
285	Delving Charge-Transfer Excitations in Hybrid Organic□norganic Hetero Junction of Dye-Sensitized Solar Cell: Assessment of Excitonic Optical Properties Using the GW and Bethe□alpeter Green□ Function Formalisms. **2021**, 99-126		
284	Unravelling the nature of a toluene-fumaronitrile complex. **2021**, 23, 16128-16141		2
283	Unveiling the catalytic potential of the Fe(IV)oxo species for the oxidation of hydrocarbons in the solid state. **2021**, 11, 4560-4569		1
282	Evaluating the nature of the vertical excited states of fused-ring electron acceptors using TD-DFT and density-based charge transfer. **2021**, 23, 15282-15291		3
281	The Role of Range-Separated Correlation in Long-Range Corrected Hybrid Functionals. **2021**, 12, 1207-1213		4

280	Comment on 'Structural characterization, reactivity and vibrational properties of silver clusters: a new global minimum for Ag' by P. L. Rodr□guez-Kessler, A. R. Rodr□guez-Dom□nguez, D. MacLeod Carey and A. Mu□oz-Castro, Phys. Chem. Chem. Phys., 2020, 22, 27255, DOI: D0CP04018E. **2021**, 23, 12900-12903		2
279	Gold nanoclusters as prospective carriers and detectors of pramipexole.. *RSC Advances*, **2021**, 11, 16619-16632	3.9	5
278	Predicting the structure and NMR coupling constant J(Xe-F) of XeF using quantum mechanics methods. **2021**, 23, 7240-7246		1
277	Assessment of the performance of DFT functionals in the fulfillment of off-diagonal hypervirial relationships. **2021**, 23, 15268-15274		8
276	The significance of long-range correction to the hydroperoxyl radical-scavenging reaction of trans-resveratrol and gnetin C. **2021**, 8, 201127		1
275	Electron-Nuclear Dynamics Accompanying Proton-Coupled Electron Transfer. **2021**, 143, 3104-3112		14
274	Spin-projected QM/MM Free Energy Simulations for Oxidation Reaction of Guanine in B-DNA by Singlet Oxygen. *ChemPhysChem*, **2021**, 22, 561-568	3.2	2
273	Superalkali-doped borazine and lithiated borazine complexes: diffuse excess electron and large first-hyperpolarizability. *Journal of Molecular Modeling*, **2021**, 27, 74	2	1
272	Theoretical investigation of a novel xylene-based light-driven unidirectional molecular motor. *Journal of Chemical Physics*, **2021**, 154, 064111	3.9	4
271	Describing polymer polarizability with localized orbital scaling correction in density functional theory. *Journal of Chemical Physics*, **2021**, 154, 054302	3.9	3
270	Effect of varying the TD-lc-DFTB range-separation parameter on charge and energy transfer in a model pentacene/buckminsterfullerene heterojunction. *Journal of Chemical Physics*, **2021**, 154, 054102	3.9	5
269	Thermal equilibration between singlet and triplet excited states in organic fluorophore for submicrosecond delayed fluorescence. **2021**, 7,		33
268	The Devil's Triangle of Kohn-Sham density functional theory and excited states. *Journal of Chemical Physics*, **2021**, 154, 074106	3.9	6
267	Symmetry-adapted density fitting in auxiliary density functional theory. **2021**, 140, 1		
266	Non long-range corrected density functionals incorrectly describe the intensity of the C?H stretching band in polycyclic aromatic hydrocarbons. *Journal of Computational Chemistry*, **2021**, 42, 1018-1027	3.5	1
265	Applicability of DFT functionals for evaluating the first hyperpolarizability of phenol blue in solution. *Journal of Chemical Physics*, **2021**, 154, 094501	3.9	4
264	Theoretical Study on the Nonlinear Optical Property of Boron Nitride Nanoclusters Functionalized by Electron Donating and Electron Accepting Groups. *Journal of Physical Chemistry A*, **2021**, 125, 2436-2445	2.8	3
263	New Syntheses, Analytic Spin Hamiltonians, Structural and Computational Characterization for a Series of Tri-, Hexa- and Hepta-Nuclear Copper (II) Complexes with Prototypic Patterns. **2021**, 3, 411-439		0

262	Investigating Primary Charge Separation in the Reaction Center of. **2021**, 125, 3468-3475		1
261	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. **2021**, 22, 100924		23
260	Triggering Electron Transfer in Co(I) Dimers: Computational Evidences for a Reversible Disproportionation Mechanism. *ChemPhysChem*, **2021**, 22, 788-795	3.2	
259	Explaining and Fixing DFT Failures for Torsional Barriers. **2021**, 12, 2796-2804		10
258	Tetraphenylethene-based fluorescent probe with aggregation-induced emission behavior for Hg detection and its application. **2021**, 1148, 238178		15
257	Koopmans'-Type Theorem in Kohn-Sham Theory with Optimally Tuned Long-Range-Corrected (LC) Functionals. *Journal of Physical Chemistry A*, **2021**, 125, 3489-3502	2.8	5
256	Atomistic Modeling of PEDOT:PSS Complexes I: DFT Benchmarking. **2021**, 54, 3634-3646		3
255	A TD-DFT molecular screening for fluorescence probe based on excited-state intramolecular proton transfer of 2□hydroxychalcone derivatives. **2021**, 410, 113165		6
254	Theoretical Study of the Binding of the Thiol-Containing Cysteine Amino Acid to the Silver Surface Using a Cluster Model. *Journal of Physical Chemistry A*, **2021**, 125, 3244-3256	2.8	5
253	Fermi-L□□wdin-orbital self-interaction correction using the optimized-effective-potential method within the Krieger-Li-Iafrate approximation. **2021**, 103,		6
252	Accurate prediction of the properties of materials using the CAM-B3LYP density functional. *Journal of Computational Chemistry*, **2021**, 42, 1486-1497	3.5	11
251	Theoretical study by DFT of organometallic complexes based on metallocenes active in NLO. *Journal of Molecular Modeling*, **2021**, 27, 179	2	3
250	Modeling UV-Vis spectra of low dimensional materials using electrostatic embedding: The case of CdSe. *Journal of Computational Chemistry*, **2021**, 42, 1212-1224	3.5	0
249	Reference Energies for Intramolecular Charge-Transfer Excitations. *Journal of Chemical Theory and Computation*, **2021**, 17, 3666-3686	6.4	14
248	Exploring Avenues beyond Revised DSD Functionals: I. Range Separation, with DSD as a Special Case. *Journal of Physical Chemistry A*, **2021**, 125, 4614-4627	2.8	15
247	Analysis of Recent BLYP- and PBE-Based Range-Separated Double-Hybrid Density Functional Approximations for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. *Journal of Physical Chemistry A*, **2021**, 125, 4026-4035	2.8	8
246	On the relation between oxidation states and d-electron populations of the 1st row transition metal complexes I. Tetrachloro complexes. **2021**, 201, 115172		0
245	Effect of the Chloro-Substitution on Electrochemical and Optical Properties of New Carbazole Dyes. **2021**, 14,		1

244	Band gaps of liquid water and hexagonal ice through advanced electronic-structure calculations. *Physical Review Research*, **2021**, 3,	3.9	3
243	Spin-Opposite-Scaled Range-Separated Exchange Double-Hybrid Models (SOS-RSX-DHs): Marriage Between DH and RSX/SOS-RSX Is Not Always a Happy Match. *Journal of Chemical Theory and Computation*, **2021**, 17, 4077-4091	6.4	2
242	Assessing locally range-separated hybrid functionals from a gradient expansion of the exchange energy density. *Journal of Chemical Physics*, **2021**, 154, 214101	3.9	2
241	Spin-Scaled Range-Separated Double-Hybrid Density Functional Theory for Excited States. *Journal of Chemical Theory and Computation*, **2021**, 17, 4211-4224	6.4	9
240	Difluorodithieno[3,2-a:2?,3?-c]phenazine as a strong acceptor for materials displaying thermally activated delayed fluorescence or room temperature phosphorescence. **2021**, 190, 109301		2
239	DFT calculation of the interplay effects between cation and intramolecular hydrogen bond interactions of mesalazine drug with selected transition metal ions (Mn+, Fe2+, Co+, Ni2+, Cu+, Zn2+). **2021**, 140, 1		2
238	Investigating functional performance and substituent effect in modelling molecular structure, UV-visible spectra, and optical properties of D- A conjugated organic dye molecules: a DFT and TD-DFT study. *Journal of Molecular Modeling*, **2021**, 27, 229	2	1
237	An improved Slater's transition state approximation. *Journal of Chemical Physics*, **2021**, 155, 034101	3.9	3
236	Highly efficient implementation of the analytical gradients of pseudospectral time-dependent density functional theory. *Journal of Chemical Physics*, **2021**, 155, 024115	3.9	
235	Electron spin resonance resolves intermediate triplet states in delayed fluorescence. **2021**, 12, 4532		9
234	Novel W-Shaped Oxygen Heterocycle-Fused Fluorene-Based Non-Fullerene Acceptors: First Theoretical Framework for Designing Environment-Friendly Organic Solar Cells. **2021**, 35, 12436-12450		24
233	Time-Dependent Long-Range-Corrected Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling: A Comprehensive Analysis of Singlet-Singlet and Singlet-Triplet Excitation Energies. *Journal of Chemical Theory and Computation*, **2021**, 17, 5165-5186	6.4	17
232	Porphyrin dimer as efficient optical thermometer: Experimental and computational evaluation of the barrier to torsional rotation. **2021**, 235, 117986		1
231	Future directions of chemical theory and computation. **2021**,		1
230	Benchmarking of Density Functionals for -Azoarene Half-Lives via Automated Transition State Search. *Journal of Physical Chemistry A*, **2021**, 125, 6474-6485	2.8	1
229	Exact Second-Order Corrections and Accurate Quasiparticle Energy Calculations in Density Functional Theory. **2021**, 12, 7236-7244		4
228	Examination of How Well Long-Range-Corrected Density Functionals Satisfy the Ionization Energy Theorem. *Journal of Chemical Theory and Computation*, **2021**, 17, 4823-4830	6.4	5
227	Self-interaction-corrected Kohn-Sham effective potentials using the density-consistent effective potential method. *Journal of Chemical Physics*, **2021**, 155, 064109	3.9	3

226	Another look at energetically quasi-degenerate structures of the gold cluster Au with q´=´1, 0, -1. *Journal of Computational Chemistry*, **2021**, 42, 2145-2153	3.5	3
225	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
224	Range-separated multiconfigurational density functional theory methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, e1566	7.9	5
223	Pseudospectral implementations of long-range corrected density functional theory. *Journal of Computational Chemistry*, **2021**, 42, 2089-2102	3.5	0
222	Assessment of the Accuracy of DFT-Predicted Li-Nucleic Acid Binding Energies. *Journal of Chemical Theory and Computation*, **2021**, 17, 5392-5408	6.4	1
221	A Novel Dialkylamino GFP Chromophore as an Environment-Polarity Sensor Reveals the Role of Twisted Intramolecular Charge Transfer. **2021**, 9, 234		3
220	In Silico Pharmacokinetics, ADMET Study and Conceptual DFT Analysis of Two Plant Cyclopeptides Isolated From Rosaceae as a Computational Peptidology Approach. **2021**, 9, 708364		1
219	A hybrid molecular peapod of sp- and sp-nanocarbons enabling ultrafast terahertz rotations. **2021**, 12, 5062		3
218	Stacked Ensemble Machine Learning for Range-Separation Parameters. **2021**, 12, 9516-9524		1
217	Properties of a furan ring-opening reaction in aqueous micellar solutions for selective sensing of mesalazine. **2021**, 258, 119846		0
216	A self-consistent systematic optimisation of range-separated hybrid functionals from first principles.		1
215	A CDFT-Based Computational Peptidology (CDFT-CP) Study of the Chemical Reactivity and Bioactivity of the Marine-Derived Alternaramide Cyclopentadepsipeptide. **2021**, 2021, 1-11		2
214	Tight distance-dependent estimators for screening two-center and three-center short-range Coulomb integrals over Gaussian basis functions. *Journal of Chemical Physics*, **2021**, 155, 124106	3.9	1
213	Theoretical exploration of optoelectronic performance of PM6:Y6 series-based organic solar cells. **2021**, 26, 101385		4
212	Research Progress of Intramolecular Stacked Small Molecules for Device Applications. **2021**, e2104125		21
211	Tunable keto emission of 2-(2?-hydroxyphenyl)benzothiazole derivatives with expansion, substitution and additional proton transfer site for excited-state proton transfer-based fluorescent probes: Theoretical insights. **2021**, 419, 113450		4
210	Theoretical study of thieno[3,4-b]pyrazine derivatives with enhanced NLO response. **2021**, 781, 138976		3
209	Perfluoro effect on the electronic excited states of -benzoquinone revealed by experiment and theory. **2021**, 23, 2141-2153		1

208	Forecasting System of Computational Time of DFT/TDDFT Calculations under the Multiverse Ansatz via Machine Learning and Cheminformatics. **2021**, 6, 2001-2024		3
207	Unravelling the nature of the β-keratin EPR signal: an ab initio study. **2021**, 23, 6815-6822		1
206	Evaluation of charge-transfer rates in fullerene-based donor-acceptor dyads with different density functional approximations. **2021**, 23, 5376-5384		3
205	Theoretical study on adiabatic electron affinity of fatty acids. *New Journal of Chemistry*, **2021**, 45, 16892-16905		3
204	Exploring the Franck-Condon region of a photoexcited charge transfer complex in solution to interpret femtosecond stimulated Raman spectroscopy: excited state electronic structure methods to unveil non-radiative pathways. **2021**, 12, 8058-8072		6
203	A Comparative Investigation of the Role of the Anchoring Group on Perylene Monoimide Dyes in NiO-Based Dye-Sensitized Solar Cells. **2020**, 13, 1844-1855		6
202	Hohenberg-Kohn-Sham Density Functional Theory. **2007**, 153-201		1
201	TDDFT and Quantum-Classical Dynamics: A Universal Tool Describing the Dynamics of Matter. **2020**, 75-121		2
200	Electronic Structure and Transition in the Far-Ultraviolet Region. **2015**, 29-54		1
199	Calculation of Magnetic Properties and Spectroscopic Parameters of Manganese Clusters with Density Functional Theory. **2012**, 449-460		0
198	Two Photon Absorption in Biological Molecules. **2015**, 1-19		1
197	Optical Properties of Noble Metal Clusters from the Ab Initio Perspective. **2018**, 546-558		1
196	Exceptionally high NLO response and deep ultraviolet transparency of superalkali doped macrocyclic oligofuran rings. *New Journal of Chemistry*, **2020**, 44, 2609-2618	3.6	41
195	Density-functional theory models of Fe(iv)O reactivity in metal-organic frameworks: self-interaction error, spin delocalisation and the role of hybrid exchange. **2020**, 22, 12821-12830		5
194	Screening methods for linear-scaling short-range hybrid calculations on CPU and GPU architectures. *Journal of Chemical Physics*, **2017**, 146, 144108	3.9	5
193	Unveiling the role of short-range exact-like exchange in the optimally tuned range-separated hybrids for fluorescence lifetime modeling. *Journal of Chemical Physics*, **2020**, 152, 204301	3.9	3
192	Coulomb explosion imaging for gas-phase molecular structure determination: An ab initio trajectory simulation study. *Journal of Chemical Physics*, **2020**, 153, 184201	3.9	7
191	Nonempirical dielectric-dependent hybrid functional with range separation for semiconductors and insulators. **2018**, 2,		93

190	Optical properties of CsCu2X3 (X=Cl, Br, and I): A comparative study between hybrid time-dependent density-functional theory and the Bethe-Salpeter equation. **2020**, 4,		7
189	CTM4DOC: electronic structure analysis from X-ray spectroscopy. **2016**, 23, 1264-71		19
188	A comprehensive analysis of the history of DFT based on the bibliometric method RPYS. **2019**, 11, 72		15
187	The Fragment Molecular Orbital-Based Time-Dependent Density Functional Theory for Excited States in Large Systems. **2009**, 91-118		3
186	Time-resolved high-harmonic spectroscopy of ultrafast photoisomerization dynamics. **2018**, 26, 31039-31054		8
185	On Occupied-orbital Dependent Exchange-correlation Functionals: From Local Hybrids to Beckes B05 Model. **2010**, 255-277		1
184	Periodic-Boundary-Condition Calculation using Heyd-Scuseria-Ernzerhof Screened Coulomb Hybrid Functional: Electronic Structure of Anatase and Rutile TiO2. **2006**, 5, 7-18		22
183	Geometric Isotope Effect on Low Barrier Hydrogen-Bonding Systems of Acetic Acid Dimer, Formic Acid Dimer, and Their Anionic Clusters by Using the Multi-Component Molecular Orbital Method. **2010**, 9, 21-28		4
182	Application of Long-range-corrected Density Functional in Metallated Porphyrin Analogues for Dye-sensitized Solar Cells. **2011**, 32, 705-708		15
181	Influence of Exchange-Correlation Functional in the Calculations of Vertical Excitation Energies of Halogenated Copper Phthalocyanines using Time-Dependent Density Functional Theory (TD-DFT). **2013**, 34, 2276-2280		6
180	One-to-One Correspondence between Reaction Pathways and Reactive Orbitals. *Journal of Chemical Theory and Computation*, **2021**, 17, 6901-6909	6.4	1
179	Local hybrid functionals augmented by a strong-correlation model. *Journal of Chemical Physics*, **2021**, 155, 144101	3.9	0
178	Performance of new exchange□correlation functionals in providing vertical excitation energies of metal complexes. **2021**, 140, 1		0
177	Do Double-Hybrid Exchange-Correlation Functionals Provide Accurate Chemical Shifts? A Benchmark Assessment for Proton NMR. *Journal of Chemical Theory and Computation*, **2021**, 17, 6876-6885	6.4	9
176	Modeling Spectral Tuning in Red Fluorescent Proteins Using the Dipole Moment Variation upon Excitation. **2021**, 61, 5125-5132		0
175	Efficient improvement of W05-based dyes by inserting auxiliary electron acceptors for dye-sensitized solar cells: A theoretical investigation. e4290		
174	A new hybrid DFT functional- Accurate description of response properties and van der Waals interactions. **2006**, 155-164		
173	Conceptual Density Functional Theory. **2009**,		

172	Coupling of Short-range Density-functional with Long-range Post-Hartree-Fock Methods. **2010**, 191-201		
171	An Additive Long-range Potential to Correct for the Charge-transfer Failure of Time-dependent Density Functional Theory. **2010**, 21-34		
170	Theoretical Studies on Metal-Containing Artificial DNA Bases. **2012**, 433-460		
169	Density Functional Study of Manganese Complexes: Protonation Effects on Geometry and Magnetism. **2012**, 461-473		1
168	Electronic structure theory: present and future challenges. **2012**, 99-102		
167	Alkyl mercury compounds: an assessment of DFT methods. **2014**, 111-118		
166	Stacking on Density Functional Theory: A Review. **2014**, 245-270		0
165	Quantum Chemistry. **2014**, 1-33		1
164	Corrections for Functionals. **2014**, 125-160		
163	Photoactive Semiconducting Oxides for Energy and Environment: Experimental and Theoretical Insights. **2015**, 1-48		
162	Development of the Divide-and-Conquer Based Single Reference Theory for Static Correlation Systems with Finite Temperature Scheme. **2018**, 17, 212-214		
161	Encyclopedia of Geochemistry. **2018**, 347-352		
160	Self-Consistent Auxiliary Density Perturbation Theory. *Journal of Chemical Theory and Computation*, **2021**, 17, 6934-6946	6.4	1
159	Excited-State Dynamics of a meta-Dimethylamino Locked GFP Chromophore as a Fluorescence Turn-on Water Sensor. **2021**,		1
158	Electronic second hyperpolarizability of alkaline earth metal chains end capped with NH2 and CN. **2021**, 100234		0
157	First-Principles Investigations of Electronically Excited States in Organic Semiconductors. **2021**, 155-193		
156	Assessing the Performance of DFT Functionals for Excited-State Properties of Pyridine-Thiophene Oligomers. *Journal of Physical Chemistry A*, **2021**, 125, 115-125	2.8	5
155	Assessment of long-range corrected density functional theory on the absorption and vibrationally resolved fluorescence spectrum of carbon nanobelts. *Journal of Computational Chemistry*, **2021**, 42, 505-515	3.5	0

154	Synthesis, electrochemical, optical and biological properties of new carbazole derivatives. **2021**, 267, 120497		0
153	Experimental and theoretical approach on third-order optical nonlinearity of a highly efficient anthracene-based chalcone derivative for optical power limiting. *Journal of Molecular Structure*, **2022**, 1250, 131704	3.4	0
152	Natural reaction orbitals for characterizing electron transfer responsive to nuclear coordinate displacement. **2021**,		0
151	Fundamentals of the Analysis Tools. **2020**, 101-153		
150	Singlet fission relevant energetics from optimally tuned range-separated hybrids. **2020**, 22, 27060-27076		2
149	Constructing and representing exchange-correlation holes through artificial neural networks. *Journal of Chemical Physics*, **2021**, 155, 174121	3.9	5
148	Exploration of promising optical and electronic properties of (non-polymer) small donor molecules for organic solar cells. *Scientific Reports*, **2021**, 11, 21540	4.9	6
147	Density Functional Theory Calculations of Redox Potentials of Neptunium Complexes in Ionic Liquid. **2020**, 167, 136503		2
146	Benchmarking isotropic hyperfine coupling constants using (QTP) DFT functionals and coupled cluster theory.. *Journal of Chemical Physics*, **2022**, 156, 094107	3.9	0
145	Combining Metal Nanoparticles with an Ir(III) Photosensitizer. **2021**, 125, 25765-25773		
144	Charge-Separation and Charge-Recombination Rate Constants in a Donor-Acceptor Buckybowl-Based Supramolecular Complex: Multistate and Solvent Effects. *Journal of Physical Chemistry A*, **2021**, 125, 9982-9994	2.8	
143	Hydration, Prediction of the p , and Infrared Spectroscopic Study of Sulfonated Polybenzophenone (SPK) Block-Copolymer Hydrocarbon Membranes and Comparisons with Nafion.. **2021**, 6, 32739-32748		0
142	Prompt and Long-Lived Anti-Kasha Emission from Organic Dyes. *Molecules*, **2021**, 26,	4.8	4
141	A global analysis of excited states: the global transition contribution grids. **2021**, 140, 1		0
140	Just Add the Gold: Aggregation-Induced-Emission Properties of Alkynylphosphinegold(I) Complexes Functionalized with Phenylene-Terpyridine Subunits. *Inorganic Chemistry*, **2021**,	5.1	1
139	N-Arylation of Protected and Unprotected 5-Bromo-2-aminobenzimidazole as Organic Material: Non-Linear Optical (NLO) Properties and Structural Feature Determination through Computational Approach. *Molecules*, **2021**, 26,	4.8	0
138	Unity of Kohn-Sham density-functional theory and reduced-density-matrix-functional theory. **2021**, 104,		5
137	Charge delocalization and hyperpolarizability in ionic liquids. *Journal of Molecular Liquids*, **2021**, 118153	6	0

136	Reply to the 'Comment on "Theoretical investigations on hydrogen peroxide decomposition in aquo"' by W. H. Koppenol, , 2021, , DOI: 10.1039/D1CP03545B. **2021**, 23, 26006-26008		0
135	Computational peptidology approach to the study of the chemical reactivity and bioactivity properties of Aspergillipeptide D, a cyclopentapeptide of marine origin.. *Scientific Reports*, **2022**, 12, 506	4.9	0
134	Linear fractional charge behavior in density functional theory through dielectric tuning of conductor-like polarizable continuum model.. *Journal of Chemical Physics*, **2022**, 156, 014106	3.9	1
133	Axial-ligand-cleavable silicon phthalocyanines triggered by near-infrared light toward design of photosensitizers for photoimmunotherapy. **2022**, 426, 113749		1
132	Physical mechanisms of photoinduced charge transfer in neutral and charged donor-acceptor systems.. *RSC Advances*, **2021**, 11, 38302-38306	3.7	0
131	An assessment of long-range corrected density functional approximations in the calculation of the reduction potentials of Ni(S 2 C 2 H 2) 2 , Ni(Se 2 C 2 H 2) 2 , Ni(S 2. *International Journal of Quantum Chemistry*,	2.1	
130	Reliability of computed molecular structures.. *Journal of Computational Chemistry*, **2022**,	3.5	0
129	Non-covalent interactions between molecular dimers (S66) in electric fields. **2022**, 4, 014005		
128	Novel Star-Shaped Benzotriindole-Based Nonfullerene Donor Materials: Toward the Development of Promising Photovoltaic Compounds for High-Performance Organic Solar Cells. 2100751		6
127	LibSC: Library for Scaling Correction Methods in Density Functional Theory.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	2
126	Conceptual DFT-Based Computational Peptidology, Pharmacokinetics Study and ADMET Report of the Veraguamides A-G Family of Marine Natural Drugs.. **2022**, 20,		1
125	Lack of the ESIPT band of aromatic -aminoaldehyde derivatives triggered by N-H vibration.. **2022**,		
124	Accurate Spectral Properties within Double-Hybrid Density Functional Theory: A Spin-Scaled Range-Separated Second-Order Algebraic-Diagrammatic Construction-Based Approach.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	2
123	Choosing Bad versus Worse: Predictions of Two-Photon-Absorption Strengths Based on Popular Density Functional Approximations.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	4
122	Water-oxidation mechanism of cobalt phosphate co-catalyst in artificial photosynthesis: a theoretical study.. **2022**,		1
121	Unraveling the Symmetry Effects on the Second-Order Nonlinear Optical Responses of Molecular Switches: The Case of Ruthenium Complexes.. *Inorganic Chemistry*, **2022**,	5.1	1
120	The lowest-energy structure of the gold cluster Au: planar nonplanar?. **2021**, 24, 42-47		1
119	Density functionals with asymptotic-potential corrections are required for the simulation of spectroscopic properties of materials.. **2022**, 13, 1492-1503		0

118	Structural characteristics and chemical reactivity of gold-based clusters Au (n = 16, 17) toward lone pairs.. *Journal of Molecular Modeling*, **2022**, 28, 54	2	0
117	Free Energy Profiles of Proton Transfer Reactions: Density Functional Benchmark from Biased Ab Initio Dynamics.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	1
116	Do any types of double-hybrid models render the correct order of excited state energies in inverted singlet-triplet emitters?. *Journal of Chemical Physics*, **2022**, 156, 064302	3.9	1
115	Unravelling the ultrafast dynamics of a N-BODIPY compound. **2022**, 200, 110181		0
114	On the Photostability of Cyanuric Acid and Its Candidature as a Prebiotic Nucleobase.. *Molecules*, **2022**, 27,	4.8	
113	Improving Density Functional Prediction of Molecular Thermochemical Properties with a Machine-Learning-Corrected Generalized Gradient Approximation.. *Journal of Physical Chemistry A*, **2022**,	2.8	2
112	Trend in light-induced excited-state spin trapping in Fe(II)-based spin crossover systems.. **2022**,		1
111	Excited-state properties of organic semiconductor dyes as electrically pumped lasing candidates from new optimally tuned range-separated models.. **2022**,		1
110	Structures and electronic states of trimer radical cations of coronene: DFT-ESR simulation study.. **2022**,		1
109	A theoretical study on the proton affinity of sulfur ylides. *New Journal of Chemistry*,	3.6	1
108	Charge-Transfer Excitations within Density Functional Theory: How Accurate Are the Most Recommended Approaches?. *Journal of Chemical Theory and Computation*, **2022**,	6.4	1
107	Charge-Transfer Excitation within a Hybrid-(G)KS Framework through Cartesian Grid DFT.. *Journal of Physical Chemistry A*, **2022**, 126, 1448-1457	2.8	1
106	Functional-Based Description of Electronic Dynamic and Strong Correlation: Old Issues and New Insights.. **2022**, 1744-1751		0
105	Approximate functionals in hypercomplex Kohn–Sham theory. **2022**, 4, 014011		0
104	Theoretical insights into the nonlinear optical properties of cyclotriphosphazene (P3N3Cl6), tris(4-hydroxyphenyl) ethane and their various inorganic–organic hybrid derivatives. **2022**, 57, 6971-6987		0
103	Hybrid functionals with local range separation: Accurate atomization energies and reaction barrier heights.. *Journal of Chemical Physics*, **2022**, 156, 104109	3.9	1
102	Comprehensive Basis-Set Testing of Extended Symmetry-Adapted Perturbation Theory and Assessment of Mixed-Basis Combinations to Reduce Cost.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	3
101	Vertical Ionization Potential Benchmarks from Koopmans Prediction of Kohn-Sham Theory with Long-Range Corrected (LC) Functional.. **2022**,		0

100	All-hydrocarbon, all-conjugated cycloparaphenylene-polycyclic aromatic hydrocarbon host-guest complexes stabilized by CH□interactions. 1		1
99	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. **2022**, 8, 36		0
98	Determining the Energy Gap between the S and T States of Thermally Activated Delayed Fluorescence Molecular Systems Using Transient Fluorescence Spectroscopy.. **2022**, 2507-2515		1
97	Natural range separation of the Coulomb hole.. *Journal of Chemical Physics*, **2022**, 156, 184106	3.9	1
96	Deep dive into machine learning density functional theory for materials science and chemistry. **2022**, 6,		5
95	Aggregation induced emission (AIE)-active ferrocene conjugated linear □extended multi donor□cceptor (D-D?-□A) chromophores: Synthesis, structural, theoretical, linear and nonlinear optical studies. **2022**, 201, 110193		3
94	Density functional theory investigation of the second hyperpolarizability of the phenol blue in solution. **2022**, 796, 139549		0
93	Is charge-transfer excitation through a polyalkane single-bond chain an intramolecular charge-transfer?: EOM-CCSD and LC-BOP study. **2022**, 796, 139563		
92	Attochemistry of hydrogen bonded amide and thioamide model complexes in protein following vertical ionization. **2022**, 559, 111508		1
91	The Density Functional Theory Account of Interplaying Long-Range Exchange and Dispersion Effects in Supramolecular Assemblies of Aromatic Hydrocarbons with Spin.. *Molecules*, **2021**, 27,	4.8	1
90	Electronic Energy and Local Property Errors at QTAIM Critical Points while Climbing Perdew's Ladder of Density-Functional Approximations.. *Journal of Chemical Theory and Computation*, **2021**,	6.4	3
89	Double and Charge-Transfer Excitations in Time-Dependent Density Functional Theory.. *Annual Review of Physical Chemistry*, **2021**,	15.7	7
88	Novel quad-rotor-shaped photovoltaic materials: first example of fused-ring non-fullerene acceptors with proficient photovoltaic properties for high-performance solar cells.. *Journal of Molecular Modeling*, **2021**, 28, 18	2	1
87	Extraction of a One-Particle Reduced Density Matrix from a Quantum Monte Carlo Electronic Density: A New Tool for Studying Nondynamic Correlation. *Computation*, **2021**, 9, 135	2.2	
86	Benchmarking Density Functional Approximations for Excited-State Properties of Fluorescent Dyes.. *Molecules*, **2021**, 26,	4.8	2
85	Quinoline based thiosemicarbazones as colorimetric chemosensors for fluoride and cyanide ions and DFT studies.. *Scientific Reports*, **2022**, 12, 4927	4.9	3
84	Theoretical Protocol Based on Long-Range Corrected Density Functional Theory and Tuning of Range-Split Parameter for Two-Electron Two-Proton Reduction of Phenylazocarboxylates.. *Journal of Physical Chemistry A*, **2022**,	2.8	
83	Data_Sheet_1.PDF. **2019**,		

82	Automated Generation of Optimized Auxiliary Basis Sets for Long-Range-Corrected TDDFT Using the Cholesky Decomposition.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	1
81	Noncovalently bound excited-state dimers: a perspective on current time-dependent density functional theory approaches applied to aromatic excimer models.. *RSC Advances*, **2022**, 12, 13014-13034	3.7	4
80	TAO-DFT fictitious temperature made simple.. *RSC Advances*, **2022**, 12, 12193-12210	3.7	0
79	First steps towards achieving both ultranonlocality and a reliable description of electronic binding in a meta-generalized gradient approximation. *Physical Review Research*, **2022**, 4,	3.9	0
78	Examining fundamental and excitation gaps at the thermodynamic limit: a combined (QTP) DFT and Coupled Cluster study on trans-polyacetylene and polyacene. *Journal of Chemical Physics*,	3.9	1
77	Comparative Study of Vibrational Raman Optical Activity with Different Time-Dependent Density Functional Approximations: The VROA36 Database.. *Journal of Physical Chemistry A*, **2022**, 126, 2909-2927	2.8	1
76	Ferrocene appended Y-shaped imidazole aldehyde chromophores: Synthesis, the effect of alkyl chain in the second order nonlinear optical properties and theoretical studies. *Journal of Molecular Structure*, **2022**, 1264, 133137	3.4	1
75	Theoretical investigation of electronic structures, second-order NLO responses of cyclometalated Ir(III) and Rh(III) counterpart complexes: effect of metal center. *New Journal of Chemistry*,	3.6	1
74	High harmonic spectra computed using time-dependent Kohn-Sham theory with Gaussian orbitals and a complex absorbing potential. *Journal of Chemical Physics*,	3.9	1
73	Synthesis and characterization of a computationally predicted redox and radiation stable Deep Eutectic Solvent. *Journal of Molecular Liquids*, **2022**, 119377	6	0
72	Assessing Recent Time-Dependent Double-Hybrid Density Functionals on Doublet–Doublet Excitations. *ACS Physical Chemistry Au*,		1
71	A Theoretical Study of the Sensing Mechanism of a Schiff-Based Sensor for Fluoride. *Sensors*, **2022**, 22, 3958	3.8	
70	Understanding the Deactivating/Activating Mechanisms in Three Optical Chemosensors Based in Crown Ether with Na+/K+ Selectivity Using Quantum Chemical Tools. *ChemPhysChem*,	3.2	
69	From Small Metal Clusters to Molecular Nanoarchitectures with a Core–Shell Structure: The Synthesis, Redox Fingerprint, Theoretical Analysis, and Solid-State Structure of [Co38As12(CO)50]4− *Inorganic Chemistry*,	5.1	0
68	On-Surface Synthesis of C144 Hexagonal Coronoid with Zigzag Edges. *ACS Nano*,	16.7	0
67	Efficiently Computing NMR 1H and 13C Chemical Shifts of Saccharides in Aqueous Environment. *Journal of Chemical Theory and Computation*,	6.4	2
66	Acriflavine in aqueous solution: excitation and hydration. *Journal of Molecular Modeling*, **2022**, 28,	2	
65	Following the density evolution using real time density functional theory and density based indexes: Application to model push–pull molecules. *Journal of Computational Chemistry*, **2022**, 43, 1464-1473	3.5	0

64	Modeling the spectral properties of poly(x-phenylenediamine) conducting polymers using a combined TD-DFT and electrostatic embedding approach. *Journal of Computational Chemistry*,	3.5	
63	Delocalization error: The greatest outstanding challenge in density-functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,	7.9	6
62	Ultra-fast spectroscopy for high-throughput and interactive quantum chemistry. *International Journal of Quantum Chemistry*,	2.1	0
61	Molecular Electrides: An In Silico Perspective. *ChemPhysChem*,	3.2	1
60	Localized orbital scaling correction for periodic systems. **2022**, 106,		
59	Recent Advances in Cartesian-Grid DFT in Atoms and Molecules. 10,		
58	Intramolecular force field for carboxylate Pt(II)-complexes. **2022**, 141,		
57	Evaluating Zn-Porphyrin-Based Near-IR-Sensitive Non-Fullerene Acceptors for Efficient Panchromatic Organic Solar Cells. **2022**, 11,		
56	Benchmarking time-dependent density functional theory for singlet excited states of thermally activated delayed fluorescence chromophores. **2022**, 4,		1
55	Benefits of Range-Separated Hybrid and Double-Hybrid Functionals for a Large and Diverse Data Set of Reaction Energies and Barrier Heights. **2022**, 126, 5492-5505		1
54	The Au12 Gold Cluster: Preference for a Non-Planar Structure. **2022**, 14, 1665		
53	Self-adaptive real-time time-dependent density functional theory for x-ray absorptions. **2022**, 157, 074106		2
52	IR, UV-Visible, NMR Spectra and Aromaticity of the Covalent Organic Tetraoxa[8]Circulene Frameworks.		0
51	Redox-switchable host–guest complexes of metallocenes and [8]cycloparaphenylene. **2022**, 14, 14276-14285		0
50	Toward highly efficient hyperfluorescence-based emitters through excited-states alignment using novel optimally tuned range-separated models. **2022**, 24, 23718-23736		0
49	Local Hybrid Functional Applicable to Weakly and Strongly Correlated Systems.		0
48	A computational study on acetaminophen drug complexed with Mn+, Fe2+, Co+, Ni2+, and Cu+ ions: structural analysis, electronic properties, and solvent effects. **2022**, 28,		0
47	IR, UV-Visible, NMR Spectra And Aromaticity Of The Covalent Organic TetraoxaCirculene Frameworks. **2022**, 113900		0

46	DFT calculations, structural analysis, solvent effects, and non-covalent interaction study on the para-aminosalicylic acid complex as a tuberculosis drug: AIM, NBO, and NMR analyses. **2022**, 28,	0
45	Computational Design of Crescent Shaped Promising Nonfullerene Acceptors with 1,4-Dihydro-2,3-quinoxalinedione Core and Different Electron-withdrawing Terminal Units for Photovoltaic Applications.	0
44	Reactive orbital energy theory serving a theoretical foundation for the electronic theory of organic chemistry.	0
43	Which DFT factors influence the accuracy of 1H, 13C and 195Pt NMR chemical shift predictions in organopolymetallic square-planar complexes? New scaling parameters for homo- and hetero-multimetallic compounds and their direct applications.	0
42	Polarity-Dependent Twisted Intramolecular Charge Transfer in Diethylamino Coumarin Revealed by Ultrafast Spectroscopy. **2022**, 10, 411	3
41	Molecular electrides: An overview of their structure, bonding, and reactivity. **2023**, 275-295	0
40	Structural evolution, stability, and spectra of small silver and gold clusters: A view from the electron shell model. **2023**, 99-121	0
39	Singlet fission initiating triplet generations of BODIPY derivatives through $$pi $$-stacking: a theoretical study. **2022**, 12,	0
38	Computationally rational design of metal-involving halogen bonds with □covalency: Structures and bonding analysis.	0
37	Tunning the optical properties of a Photocatalytic Metal-Organic Framework by means of molecular modelling.	0
36	A comprehensive benchmark investigation of quantum chemical methods for carbocations.	0
35	Either Accurate Singlet□Triplet Gaps or Excited-State Structures: Testing and Understanding the Performance of TD-DFT for TADF Emitters. **2022**, 18, 7702-7713	0
34	Modeling the electronic structure of organic materials: a solid-state physicist□ perspective. **2023**, 6, 012001	0
33	In Search of Hosts for Blue OLEDs: Computational Design and Experimental Validation.	0
32	Accelerated constant-voltage quantum mechanical/molecular mechanical method for molecular systems at electrochemical interfaces. **2022**, 157, 234107	0
31	Building on the Strengths of a Double-Hybrid Density Functional for Excitation Energies and Inverted Singlet-Triplet Energy Gaps.	0
30	The subsystem quantum chemistry program Serenity.	0
29	Characterization of Excited States in Time-Dependent Density FunctionalTheory Using Localized Molecular Orbitals.	0

28	Can range-separated functionals be optimally tuned to predict spectra and excited state dynamics in photoactive iron complexes?.	1
27	Understanding the Role of Intramolecular Ion-Pair Interactions in Conformational Stability Using an Ab Initio Thermodynamic Cycle.	0
26	Understanding Density-Driven Errors for Reaction Barrier Heights.	1
25	Full Implementation, Optimization, and Evaluation of a Range-Separated Local Hybrid Functional with Wide Accuracy for Ground and Excited States.	0
24	The mechanism insight for improved photocatalysis and interfacial charges transfer of surface-dispersed Ag0 modified layered graphite-phase carbon nitride nanosheets. **2023**, 34, 103936	0
23	Structural analysis and electronic properties of transition metal ions (Ni2+, Fe2+, Mn+ and Co+) with psoralen biomolecule as an anticancer drug. **2023**, 986, 122606	0
22	Electronic, Elastic, and Thermoelectric Properties of Half-Heusler Topological Semi-Metal HfIrAs from First-Principles Calculations. **2023**, 13, 37	0
21	Ab-initio and molecular dynamics simulation of a discotic liquid crystal in ionic solution. 1-10	0
20	New kind of electride sandwich complexes based on the cyclooctatetraene ligand M12(η8-C8H8)2M22 (M1 = Na, K and M2 = Ca, Mg): a theoretical study. **2023**, 25, 4710-4723	0
19	The core ionization energies calculated by delta SCF and Slater's transition state theory.	0
18	Modeling the Photo-Absorption Properties of Noble Metal Nanoclusters: A Challenge for Density-Functional Theory.	0
17	Revisiting the hydrogen atom transfer reactions through a simple and accurate theoretical model: Role of hydrogen bond energy in polyphenolic antioxidants. **2023**, 1223, 114097	0
16	Projected Hybrid Density Functionals: Method and Application to Core Electron Ionization. **2023**, 19, 837-847	0
15	Non-empirical Mixing Coefficient for Hybrid XC Functionals from Analysis of the XC Kernel. **2023**, 14, 1326-1333	1
14	Analytic Gradient for Time-Dependent Density Functional Theory Combined with the Fragment Molecular Orbital Method. **2023**, 19, 1276-1285	0
13	Conformational Dependence of the First Hyperpolarizability of the Li@B10H14 in Solution. **2023**, 3, 159-167	0
12	Mechanistic understanding of geopolymerization at the initial stage: Ab initio molecular dynamics simulations.	0
11	Molecular Orbitals. **2023**,	0

10	Performance of Density Functionals and Semiempirical 3c Methods for Small Gold Thiolate Clusters. **2023**, 127, 2242-2257	0
9	Solvation Effects on Polarizability of Aromatic Fluids. **2023**, 127, 2237-2249	0
8	Design of BPEA-based derivatives with high singlet fission performance: a theoretical perspective. **2023**, 25, 10071-10081	0
7	Density Functional Study on the Photopolymerization of Styrene Using Dinuclear RuPd and IrPd Complexes with Naphthyl-Substituted Ligands. **2023**, 127, 2810-2818	0
6	Understanding Primary Charge Separation in the Heliobacterial Reaction Center. **2023**, 14, 3092-3102	0
5	Multiple resonance induced thermally activated delayed fluorescence: effect of chemical modification. **2023**, 5, 014010	0
4	Theoretical investigation of copper clusters using the electron propagator theory. **2023**, 135,	0
3	Cost-Effective Simulations of Vibrationally-Resolved Absorption Spectra of Fluorophores with Machine-Learning-Based Inhomogeneous Broadening.	0
2	Competing excitation paths in luminescent heterobimetallic Ln-Al complexes: Unraveling interactions via experimental and theoretical investigations. **2023**, 26, 106614	0
1	Chemical and photophysical studies on the interaction of reactive oxygen species with carbonylated diazo derivatives: Their chromogenic, fluorescent detection and mechanistic investigation. **2023**, 216, 111317	0