CITATION REPORT List of articles citing

Density-functional exchange-energy approximation with correct asymptotic behavior

DOI: 10.1103/physreva.38.3098 Physical Review A, 1988, 38, 3098-3100.

Source: https://exaly.com/paper-pdf/19697918/citation-report.pdf

Version: 2024-04-28

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
2261	Electronic structure of copper-oxygen clusters in the high-Tc superconductor La2-xSrxCuO4. 1989 , 40, 8800-8808		13
2260	Exchange holes in inhomogeneous systems: A coordinate-space model. <i>Physical Review A</i> , 1989 , 39, 37	′61 <u>2</u> 3676	7 636
2259	Precise density-functional method for periodic structures. 1991 , 44, 7888-7903		391
2258	Exchange-energy density functional: Reparametrization of Becke's formula and derivation of second-order gradient correction. <i>Physical Review A</i> , 1991 , 44, 1536-1539	2.6	25
2257	Ground-state properties of Fe, Co, Ni, and their monoxides: Results of the generalized gradient approximation. 1991 , 44, 2923-2927		181
2256	The structure and stability of S2F10 and S2F11 and their anions. 1991 , 158, 33-39		6
2255	Theoretical investigation on the existence of the SiFB anion. 1991 , 184, 305-309		26
2254	Superhalogens among sp-elements: SF7. 1991 , 184, 93-98		14
2253	Bonding properties of IIA and IIB dimers in density functional theory with gradient corrections to the local density approximation. 1991 , 19, 169-171		13
2252	Gradient corrections to the Hartree-Fock-Slater exchange and their influence on bond energy calculations. 1991 , 81, 65-78		33
2251	Analytic energy derivatives in the numerical local-density-functional approach. 1991 , 94, 7245-7250		437
2250	Gradient-corrected density functionals: Full-potential calculations for iron. 1991 , 43, 11628-11634		157
2249	Self-consistent implementation of nonlocal exchange and correlation in a Gaussian density-functional method. 1991 , 43, 1399-1410		67
2248	Gradient-corrected density-functional studies of CaCuO2. 1991 , 44, 7715-7717		31
2247	Generalized gradient-expansion approximation for the exchange energy. 1991 , 44, 10921-10924		10
2246	Pseudopotentials for non-local-density functionals. 1991 , 43, 6376-6387		101
2245	Conjoint gradient correction to the Hartree-Fock kinetic- and exchange-energy density functionals. <i>Physical Review A</i> , 1991 , 44, 768-771	2.6	146

2244	Metastability of doubly charged transition-metal dimers in density-functional theory. 1991 , 44, 5881-5884	16
2243	Ab initio studies on high pressure phases of ice. 1992 , 69, 462-465	154
2242	Fermi surface and band structure of ferromagnetic cobalt. 1992 , 46, 3789-3797	16
2241	A theoretical investigation on the molecular and electronic structure of the SFn compounds n=1 B and their singly charged negative ions. 1992 , 96, 7623-7632	47
2240	Preliminary results on the performance of a family of density functional methods. 1992 , 97, 7846-7848	111
2239	Density-functional-theory calculations of static dipole polarizability of some ions of interest in MI Ssbauer spectroscopy. <i>Physical Review A</i> , 1992 , 45, 2076-2078	4
2238	Magnetism with generalized-gradient-approximation density functionals. 1992 , 46, 11570-11577	93
2237	Gradient-corrected pseudopotential calculations in semiconductors. 1992 , 45, 11328-11331	66
2236	Application of generalized gradient-corrected density functionals to iron. 1992 , 46, 1870-1873	65
2235	Comparison of kinetic-energy density functionals. <i>Physical Review A</i> , 1992 , 46, 6920-6924 2.6	90
2234	Singly ionized first-row dimers and hydrides calculated with the fully-numerical density-functional program numol. 1992 , 97, 9216-9221	89
2233	Metallic bonding in magnesium microclusters. 1992 , 45, 3838-3841	32
2232	Kinetic and Exchange Energy Densities of an Inhomogenous Electron Liquid Related in Hartreeflock Theory and Other Models. 1992 , 25, 43-50	2
2231	Stringlike Chemisorption and Rapid Dissociation of As4 and Sb4 on Si(100). 1992 , 280, 65	
2230	Application of Density Functional Theory to Al Distribution in Mordenite. 1992 , 291, 239	1
2229	Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. 1992 , 46, 6671-6687	17224
2228	Comparison of coupled-cluster results with a hybrid of Hartreeflock and density functional theory. 1992 , 97, 7528-7530	164
2227	Density-functional thermochemistry. I. The effect of the exchange-only gradient correction. 1992 , 96, 2155-2160	2025

2226	Density-functional thermochemistry. II. The effect of the PerdewWang generalized-gradient correlation correction. 1992 , 97, 9173-9177	1414
2225	Use of gradient-corrected functionals in total-energy calculations for solids. 1992 , 46, 9829-9832	114
2224	Hardware and quantum mechanical calculations. 1992 , 341, 361-371	
2223	An investigation of the performance of a hybrid of Hartree-Fock and density functional theory. 1992 , 44, 319-331	185
2222	First-order gradient correction for the exchange-energy density functional for atoms. 1992 , 84, 237-243	7
2221	Electronic polarizability of ionic crystals. 1992 , 81, 69-71	6
2220	A density functional investigation on the structure of the CFn compounds, n=15, and their singly charged anions. 1992 , 163, 59-67	26
2219	A theoretical investigation on the structure of the hypervalent carbon and silicon pentahalogenides as well as their singly charged anions. 1992 , 166, 57-68	20
2218	A theoretical investigation of the multiple states of the SFB anion. 1992, 115, 185-192	14
2217	The structure of the SF6 molecule and the SF B anion excited states. 1992 , 41, 504-510	2
2216	Application of density functional theory to infrared absorption intensity calculations on main group molecules. 1992 , 96, 9005-9012	212
2215	Density functional Gaussian-type-orbital approach to molecular geometries, vibrations, and reaction energies. 1992 , 96, 1280-1303	860
2214	Density functional calculations on cation-induced changes in the adsorption of sulphur on Ir4 clusters. 1992 , 190, 190-198	2
2213	Asymptotic properties of the exchange energy density and the exchange potential of finite systems: relevance for generalized gradient approximations. 1992 , 23, 7-14	100
2212	Chemisorption theory of ammonia on copper. 1992 , 188, 477-486	31
2211	KohnBham bond lengths and frequencies calculated with accurate quadrature and large basis sets. 1992 , 199, 551-556	117
221 0	KohnBham density-functional theory within a finite basis set. 1992 , 199, 557-560	364
2209	Water dimer properties in the gradient-corrected density functional theory. 1992 , 194, 172-174	95

2208	The performance of the Beckelleellanglarr (BllYP) density functional theory with various basis sets. 1992 , 197, 499-505	756
2207	The harmonic frequencies of benzene. 1992 , 197, 506-515	225
2206	The effect of a neon matrix on the hyperfine structure of CH+4. A model study. 1993 , 211, 88-93	20
2205	Fullerene derivatives. Comparative theoretical study of C60O and C60CH2. 1993 , 209, 223-228	74
2204	A standard grid for density functional calculations. 1993 , 209, 506-512	392
2203	Chemical applications of density functional theory: FB anion dissociation (FB -fF2 + F) 1993, 211, 265-271	20
2202	Calculations of NMR shielding constants by uncoupled density functional theory. 1993 , 204, 80-86	134
2201	Calculations of NMR shielding constants beyond uncoupled density functional theory. IGLO approach. 1993 , 204, 87-95	90
2200	Isomers of C20. Dramatic effect of gradient corrections in density functional theory. 1993 , 214, 357-361	135
2199	Density functionals without meshes and grids. 1993 , 214, 397-401	30
2198	A theoretical study of buckminsterfullerene reaction products: C60+C60. 1993 , 214, 576-582	157
2197	Structures of small water clusters using gradient-corrected density functional theory. 1993 , 207, 208-213	164
2196	Non-local exchange and local Coulomb correlation energy density functionals for finite many-electron systems. 1993 , 205, 348-353	19
2195	Density functional theory applied to proton-transfer systems. A numerical test. 1993 , 208, 364-368	86
2194	Proton transfer in ice. 1993 , 210, 279-284	20
2193	Structures and vibrational frequencies of FOOF and FONO using density functional theory. 1993 , 202, 489-494	31
2192	Analytic second derivatives of the gradient-corrected density functional energy. Effect of quadrature weight derivatives. 1993 , 216, 133-140	158
2191	An ab initio study of methanol adsorption in zeolites. 1993 , 216, 155-161	85

2190	Electronic structure calculations and dynamics of the chemisorption of methane on a Ni(111) surface. 1993 , 177, 407-420		35
2189	Nonlocal gradient corrections to the exchange free energy of an inhomogeneous many-fermion system at finite temperature. 1993 , 88, 81-85		9
2188	Nonlocal approximation to the exchange and kinetic energy functionals: Application to metallic clusters. 1993 , 45, 333-347		9
2187	Theoretical study of the geometric structures and energetic properties of anionic clusters. Ag ($n = 2$ to 6). 1993 , 48, 743-753		20
2186	The mercury-mercury bond in inorganic and organometallic compounds. A theoretical study. 1993 , 213, 233-246		54
2185	A theoretical investigation of the electronic and geometrical structure of silicon fluorides SiF n and their anions SiF n [h=1 B . 1993 , 42, 36-45		7
2184	Structure of carbon fluorochlorides CF n Cl m (n, m $\mathbb B$) and their singly charged negative ions. 1993 , 42, 996-1002		
2183	Density-functional thermochemistry. III. The role of exact exchange. 1993 , 98, 5648-5652		81103
2182	A new mixing of HartreeBock and local density-functional theories. 1993 , 98, 1372-1377		12266
2181	Small can be different. 1993 , 26, 119-125		6
	Small can be different. 1993 , 26, 119-125 Slab versus cluster approach for chemisorption studies. CO on Cu (100). 1993 , 177, 399-406		75
2180	Slab versus cluster approach for chemisorption studies. CO on Cu (100). 1993 , 177, 399-406		75
2180 2179	Slab versus cluster approach for chemisorption studies. CO on Cu (100). 1993 , 177, 399-406 Quadrature schemes for integrals of density functional theory. 1993 , 78, 997-1014 Born-Oppenheimer molecular-dynamics simulations of finite systems: Structure and dynamics of		75 309
2180 2179 2178	Slab versus cluster approach for chemisorption studies. CO on Cu (100). 1993 , 177, 399-406 Quadrature schemes for integrals of density functional theory. 1993 , 78, 997-1014 Born-Oppenheimer molecular-dynamics simulations of finite systems: Structure and dynamics of (H2O)2. 1993 , 48, 2081-2097		75 309 482
2180 2179 2178 2177	Slab versus cluster approach for chemisorption studies. CO on Cu (100). 1993, 177, 399-406 Quadrature schemes for integrals of density functional theory. 1993, 78, 997-1014 Born-Oppenheimer molecular-dynamics simulations of finite systems: Structure and dynamics of (H2O)2. 1993, 48, 2081-2097 Theoretical study of the monocarbonyls of first-row transition metal atoms. 1993, 99, 1801-1815 Dissociation of ammonia on a copper surface and the effect of oxygen coadsorption: a		75 309 482 105
2180 2179 2178 2177 2176	Slab versus cluster approach for chemisorption studies. CO on Cu (100). 1993, 177, 399-406 Quadrature schemes for integrals of density functional theory. 1993, 78, 997-1014 Born-Oppenheimer molecular-dynamics simulations of finite systems: Structure and dynamics of (H2O)2. 1993, 48, 2081-2097 Theoretical study of the monocarbonyls of first-row transition metal atoms. 1993, 99, 1801-1815 Dissociation of ammonia on a copper surface and the effect of oxygen coadsorption: a quantum-chemical study. 1993, 284, 361-371	2.6	75 309 482 105

2172	The physics of simple metal clusters: self-consistent jellium model and semiclassical approaches. 1993 , 65, 677-732	1411
2171	First-principles Molecular Dynamics. 1993 , 261-313	46
2170	Density functional calculations of isotropic hyperfine coupling constants of radical cations. 1993 , 9756-9763	73
2169	Tight bound and convexity constraint on the exchange-correlation-energy functional in the low-density limit, and other formal tests of generalized-gradient approximations. 1993 , 48, 11638-11645	143
2168	Examination of several exchange-correlation energy functionals by accurate self-consistent atomic calculations. 1993 , 98, 4814-4821	20
2167	Ab initio theoretical predictions of C28, C28H4, C28F4, (Ti@C28)H4, and M@C28 (M=Mg, Al, Si, S, Ca, Sc, Ti, Ge, Zr, and Sn). 1993 , 99, 352-359	149
2166	Nonlocal density functional calculations: Comparison of two implementation schemes. 1993 , 98, 2971-2974	18
2165	Kohn-Sham calculations on open-shell diatomic molecules. 1993 , 80, 1121-1134	61
2164	Density functional investigation on the electron affinity of the CFnClm series, n+m=3 and 4. 1993 , 98, 7072-7080	25
2163	A study of O3, S3, CH2, and Be2 using KohnBham theory with accurate quadrature and large basis sets. 1993 , 98, 7145-7151	97
2162	The performance of a family of density functional methods. 1993 , 98, 5612-5626	1659
2161	Energetics and electronic structure of the hypothetical cubic zincblende form of GeC. 1993 , 1, 741-754	45
2160	Nonlocal exchange- and kinetic-energy density functionals for electronic systems: Application to atoms and ions. <i>Physical Review A</i> , 1993 , 47, 1804-1810	13
2159	Full-potential calculations using the generalized gradient approximation: Structural properties of transition metals. 1993 , 48, 18304-18307	117
2158	A combined density functional and intrinsic reaction coordinate study on the ground state energy surface of H2CO. 1993 , 99, 3823-3835	103
2157	Pair interactions of rare-gas atoms as a test of exchange-energy-density functionals in regions of large density gradients. <i>Physical Review A</i> , 1993 , 47, 4681-4690	173
2156	Electronic structure of the CoO molecule. <i>Physical Review A</i> , 1993 , 48, 2679-2685 2.6	19
2155	Density functional pseudopotential studies of molecular geometries, vibrations, and binding energies. 1993 , 98, 8710-8717	79

2154	Molecular gradients and hessians implemented in density functional theory. 1993 , 98, 1398-1421	195
2153	Exact exchange functional for the hydrogen atom. <i>Physical Review A</i> , 1993 , 47, 2383-2385 2.6	35
2152	Calculation of hyperfine coupling constants of radicals by density-functional theory. <i>Physical Review A</i> , 1993 , 48, 1691-1694	35
2151	Ab initio calculation of hyperfine parameters for nitrogen-pair defects in amorphous silicon nitride. 1993 , 48, 14653-14655	
2150	Basis-set-free local density-functional calculations of geometries of polyatomic molecules. 1993 , 99, 3898-3905	151
2149	Electronic spectroscopy of the niobium dimer molecule: Experimental and theoretical results. 1993 , 99, 8504-8518	72
2148	Application of gradient corrections to density-functional theory for atoms and solids. 1993 , 48, 14944-14952	78
2147	Augmented-plane-wave calculations on small molecules. 1993 , 48, 2046-2056	23
2146	Stability, bonding, and geometric structure of Ti8C12, Ti8N12, V8C12, and Zr8C12. 1993 , 71, 1732-1735	63
2145	Theoretical investigation of the insertion of nickel in the CH bond of CH4. Electronic structure calculations and dynamics. 1993 , 98, 8810-8818	38
2144	Hydration of sodium in water clusters. 1993 , 70, 1775-1778	130
2143	Density functionals and dimensional renormalization for an exactly solvable model. 1993 , 99, 417-425	144
2142	Theoretical study of linear and bent CrCO, NiCO, and CuCO. 1993 , 98, 8041-8050	79
2141	Role of nonlocal exchange correlation in activated adsorption. 1993 , 70, 3971-3974	155
2140	Weighted-density exchange and local-density Coulomb correlation energy functionals for finite systems: Application to atoms. <i>Physical Review A</i> , 1993 , 48, 4197-4212	39
2139	Ab initio studies on the structural and dynamical properties of ice. 1993 , 47, 4863-4872	149
2138	A general purpose exchange-correlation energy functional. 1993 , 99, 8765-8773	86
2137	Intrinsic Structures of [CuCl4]2目nd [CuBr4]2Lnions by Ab Initio Density Functional Calculations. 1993, 22, 1145-1148	5

2136	Density Functional Calculation of the Si-H Dissociation Energies on the Si(100) Surface. 1993 , 315, 273		1
2135	First Principles Study of Aluminum Deposition on Hydrogen-terminated Si(100) Surface. 1993 , 334, 289		
2134	Scaling properties of inhomogeneity kinetic energy in some diatomic molecules, in relation to dissociation energies. 1994 , 81, 1497-1500		1
2133	Recent constrained-search advances for approximating density functionals. 1994 , 69, 763-769		29
2132	Modelling the reaction OH- + CO2 -fHCO- 3 in the gas phase and in aqueous solution: a combined density functional continuum approach. 1994 , 83, 327-333		11
2131	Improved local density approximation to the exchange and kinetic energy functionals for atomic systems. 1994 , 27, 381-387		42
2130	Density functional study of symmetric proton transfers. 1994 , 101, 6658-6665		36
2129	Local density component of the LeeNangParr correlation energy functional. 1994 , 100, 9018-9024		26
2128	Characterization of the potential energy surface of the HO2 molecular system by a density functional approach. 1994 , 101, 10666-10676		87
2127	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. 1994 , 49, 5323-5328		81
2126	Automatic numerical integration techniques for polyatomic molecules. 1994 , 100, 6520-6534		91
2125	Hydrolysis at stepped MgO surfaces. 1994 , 73, 504-507		149
2124	Core-cancellation functions for evaluating exchange-correlation functionals in first-principles pseudopotential calculations. 1994 , 49, 2351-2361		13
2123	The determination of hyperpolarizabilities using density functional theory with nonlocal functionals. 1994 , 101, 9704-9709		72
2122	Theory of the crystal structures of selenium and tellurium: The effect of generalized-gradient corrections to the local-density approximation. 1994 , 50, 13181-13185		229
2121	Pairing of hydrogen atoms on the Si(100)-(2 \times 1) surface: The role of interactions among dimers. 1994 , 49, 11191-11195		48
2120	Obtaining a gradient-corrected kinetic-energy functional from the Perdew-Wang exchange functional. <i>Physical Review A</i> , 1994 , 50, 5328-5331	2.6	170
2119	Density-functional theory of macroscopic stress: Gradient-corrected calculations for crystalline Se. 1994 , 50, 4327-4331		61

2118	Gradient-free exchange-correlation functional beyond the local-spin-density approximation. Physical Review A, 1994, 50, 3766-3774	14
2117	Theoretical study of the mechanism of recombinative hydrogen desorption from the monohydride phase of Si(100): The role of defect migration. 1994 , 101, 8073-8081	82
2116	Complete active space self-consistent field and density functional study of FNO. 1994 , 100, 459-463	14
2115	Tests of nonlocal kinetic energy functionals. 1994 , 100, 4446-4452	67
2114	Comparison of exact and approximate density functionals for an exactly soluble model. 1994 , 100, 1290-1296	152
2113	Inclusion of Hartree B ock exchange in density functional methods. Hyperfine structure of second row atoms and hydrides. 1994 , 101, 6834-6838	139
2112	The effect of grid quality and weight derivatives in density functional calculations. 1994 , 101, 8894-8902	50
2111	Fourth-order gradient corrections to the exchange-only energy functional: Importance of. 1994 , 50, 10498-105	5 96
2110	Exchange energy from Gaussian-type basis sets. 1994 , 27, 423-427	5
2109	Density functional transition states of organic and organometallic reactions. 1994 , 100, 434-443	120
	Density functional transition states of organic and organometallic reactions. 1994 , 100, 434-443 Simple but efficient correlation functional from a model pair-correlation function. 1994 , 49, 7874-7886	120 40
2108	Simple but efficient correlation functional from a model pair-correlation function. 1994 , 49, 7874-7886 Electron correlation in extended systems: Fourth-order many-body perturbation theory and density-functional methods applied to an infinite chain of hydrogen atoms. 1994 , 50, 14791-14801	40
2108	Simple but efficient correlation functional from a model pair-correlation function. 1994 , 49, 7874-7886 Electron correlation in extended systems: Fourth-order many-body perturbation theory and density-functional methods applied to an infinite chain of hydrogen atoms. 1994 , 50, 14791-14801	40
2108 2107 2106	Simple but efficient correlation functional from a model pair-correlation function. 1994, 49, 7874-7886 Electron correlation in extended systems: Fourth-order many-body perturbation theory and density-functional methods applied to an infinite chain of hydrogen atoms. 1994, 50, 14791-14801 Simplified electronic-structure model for hydrogen-bonded systems: Water. 1994, 50, 10516-10530 Property evaluation using the HartreeHock-density-functional-theory method: An efficient formalism for first- and second-order properties. 1994, 101, 7788-7794	40 44 32
2108 2107 2106 2105	Simple but efficient correlation functional from a model pair-correlation function. 1994, 49, 7874-7886 Electron correlation in extended systems: Fourth-order many-body perturbation theory and density-functional methods applied to an infinite chain of hydrogen atoms. 1994, 50, 14791-14801 Simplified electronic-structure model for hydrogen-bonded systems: Water. 1994, 50, 10516-10530 Property evaluation using the HartreeBock-density-functional-theory method: An efficient formalism for first- and second-order properties. 1994, 101, 7788-7794	40 44 32 17
2108 2107 2106 2105 2104	Simple but efficient correlation functional from a model pair-correlation function. 1994, 49, 7874-7886 Electron correlation in extended systems: Fourth-order many-body perturbation theory and density-functional methods applied to an infinite chain of hydrogen atoms. 1994, 50, 14791-14801 Simplified electronic-structure model for hydrogen-bonded systems: Water. 1994, 50, 10516-10530 Property evaluation using the HartreeFlock-density-functional-theory method: An efficient formalism for first- and second-order properties. 1994, 101, 7788-7794 Stability of charged aluminum clusters. 1994, 49, 17464-17467 Accurate exchange-correlation potentials and total-energy components for the helium	40 44 32 17 21

2100 Density functional studies of representative pericyclic reactions. 1994 , 311, 325-330	3
Determination of the heat of formation of oxygen containing radicals using density functional theory. 1994 , 310, 13-16	
Electronic structure calculations of 1,3-dipolar cycloadditions using density functional and Hartree E ock methods. 1994 , 49, 511-526	33
Density functionals for exchange and correlation energies: Exact conditions and comparison of approximations. 1994 , 49, 539-548	53
2096 Density functional studies on hydrogen-bonded complexes. 1994 , 52, 465-478	38
Transition states and energy barriers from density functional studies: Representative isomerization reactions. 1994 , 52, 695-704	15
2094 An analysis of nonlocal density functionals in chemical bonding. 1994 , 52, 711-730	28
2093 The determination of intrinsic reaction coordinates by density functional theory. 1994 , 52, 731-765	86
Numerical grids for density functional calculations of molecular properties. 1994 , 52, 799-807	29
Predictive chemical kinetics: Density functional and hartreefock calculations on free-radial reaction transition states. 1994 , 52, 837-847	28
The effects of nonlocal gradient corrections in density functional calculations of hydrocarbon radical hyperfine structures. 1994 , 52, 879-901	46
Investigations of hydrogen-bonded systems: Local density approximation and gradient corrections. 1994 , 52, 957-961	20
2088 Bonding of acetylene to copper atom, dimer, and trimer. 1994 , 52, 973-985	22
Ionization potentials of atoms calculated with a nonlocal exchange and a local correlation functional. 1994 , 52, 993-1010	9
2086 Density functional treatment of waterdarbon dioxide van der waals complex. 1994 , 52, 1011-1015	19
2085 A density functional study of pseudotetrahedral metallitrosyl complexes. 1994 , 52, 1039-1049	8
2084 The chemisorption of hydrogen on Cu(111): A dynamical study. 1994 , 52, 1067-1080	16
2083 Systematic LSD investigation on cationic boron clusters: B(n ? 2🛮 4). 1994 , 52, 1081-1111	125

2082	A study of small systems containing H and O atoms using nonlocal functionals: comparisons with ab initio and experiment. 1994 , 52, 655-666	19
2081	Computational materials design: A perspective for atomistic approaches. 1994 , 1, 215-242	13
2080	A density functional theory study of the hyperfine structures of the atoms B to O and the species NH2 and NH+3. 1994 , 217, 24-30	32
2079	Statistical model for delocalized Donding in the C60 molecule. 1994 , 218, 229-233	1
2078	Theoretical calculation of the height of the barrier for OH rotation in phenol. 1994 , 218, 261-269	21
2077	An implementation of a KohnBham density functional program using a Gaussian-type basis set. Application to the equilibrium geometry of C60 and C70. 1994 , 219, 8-14	41
2076	Local density studies of diatomic AB molecules, A, B?C, N, O, F, Si, P, S, and Cl. 1994 , 220, 102-108	42
2075	Tautomeric equilibria in 2-hydroxypyridine and in cytosine. An assessment of density functional methods, including gradient corrections. 1994 , 220, 129-132	46
2074	Density functional LCAO calculation of periodic systems. A posteriori correction of the Hartree-Fock energy of covalent and ionic crystals. 1994 , 220, 145-153	87
2073	Isomers of C24. Density functional studies including gradient corrections. 1994 , 220, 385-390	79
2072	Equilibrium solvent effect in the framework of density functional theory. Application to the study of the thermodynamics of some organic and inorganic tautomeric equilibria. 1994 , 223, 54-60	20
2071	Properties of supercritical water: an ab initio simulation. 1994 , 223, 411-415	132
2070	Theoretical study of direct and water-assisted isomerization of formaldehyde radical cation. A comparison between density functional and post-Hartree-Fock approaches. 1994 , 224, 432-438	80
2069	Density functional methods and the spatial distribution of electronic charge. 1994 , 225, 285-292	17
2068	Inclusion of Hartree-Fock exchange in the density functional approach. Benchmark computations for diatomic molecules containing H, B, C, N, O, and F atoms. 1994 , 226, 392-398	76
2067	The effect of density-gradient corrections for a molecule-surface potential energy surface. Slab calculations on Cu(100)c(2x2)-CO. 1994 , 226, 583-588	74
2066	Theoretical study of metastable N2CO isomers. New candidates for high energy materials?. 1994 , 227, 312-320	35
2065	The performance of density functional methods for the description of weak interaction potentials. The torsional potential of butane. 1994 , 227, 390-395	21

2064	Density functional theory studies of 4-Electron systems. 1994 , 228, 239-245	11
2063	Density functional studies of the carbonium ion species CH+5, C2H+7 and C3H+9. 1994 , 228, 246-251	37
2062	Theoretical study of the lanthanide fullerene CeC82. Comparison with ScC82, YC82 and LaC82. 1994 , 228, 106-110	81
2061	The performance of a variety of density functional and ab initio methods on the structural problem of beryllium borohydride. 1994 , 228, 252-258	13
2060	The molecular structure of cis-FONO. 1994 , 228, 583-588	23
2059	Can (semi)local density functional theory account for the London dispersion forces?. 1994 , 229, 175-180	888
2058	Density functional study of the equilibrium geometry and Si-O-Si potential energy curve of disiloxane. 1994 , 229, 191-197	27
2057	Structure and stability of C13 carbon clusters. 1994 , 229, 491-494	9
2056	Density-functional based determination of the CH3-CH4 hydrogen exchange reaction barrier. 1994 , 230, 54-60	19
2055	Photoelectron and theoretical investigations on bismuth and antimony pentamer anions. 1994 , 230, 99-102	27
2054	Role of Hartree-Fock exchange in density functional theory. 1994 , 230, 189-195	24
2053	A Kohn-Sham method involving the direct determination of the Coulomb potential on a numerical grid. 1994 , 230, 17-24	32
2052	Gradient corrections in density functional theory calculations for surfaces: Co on Pd{110}. 1994 , 230, 501-506	143
2051	Nonlocal correlation functional involving the Laplacian of the density. 1994 , 230, 419-428	61
2050	The chemical Hamiltonian approach in density functional theory. 1994 , 230, 485-490	21
2049	Effective exchange integrals for open-shell species by density functional methods. 1994 , 231, 25-33	285
2048	Proton transfer in model hydrogen-bonded systems by a density functional approach. 1994 , 231, 295-300	90
2047	Cr2 revisited. 1994 , 231, 277-282	98

2046	Theoretical study of the dimetallofullerene Sc2@C84. 1994 , 231, 319-324	78
2045	An evaluation of the performance of density functional theory, MP2, MP4, F4, G2(MP2) and G2 procedures in predicting gas-phase proton affinities. 1994 , 231, 345-351	124
2044	Calculation of spinBpin coupling constants using density functional theory. 1994 , 221, 91-99	176
2043	A density functional study of the simplest hydrogen abstraction reaction. Effect of self-interaction correction. 1994 , 221, 100-108	311
2042	Studies of solvent effects using density functional theory. Co-operative interactions in H3NHBr proton transfer. 1994 , 221, 109-116	33
2041	Analysis and assignment of the optical absorption transitions in CuCl2 with Gaussian density functional calculations. 1994 , 219, 228-236	33
2040	Density-functional-theory calculations of isotropic hyperfine coupling constants of radicals. 1994 , 225, 462-466	20
2039	Gas-Phase Generation and Characterization of Nitrileimine, HCNNH: A new, stable isomer of diazomethane. 1994 , 77, 2354-2362	22
2038	Structural and electronic property changes of the nucleic acid bases upon base pair formation. 1994 , 15, 981-996	49
2037	Potential energy surfaces for Rh?CO from DFT calculations. 1994 , 15, 1053-1063	3
<i>3,</i>	Potential energy surfaces for Rh?CO from DFT calculations. 1994 , 15, 1053-1063 s-Indacene: A Delocalized, Formally Antiaromatic 12 Œlectron System. 1994 , 33, 1192-1194	3
2036		
2036	s-Indacene: A Delocalized, Formally Antiaromatic 12 Œlectron System. 1994 , 33, 1192-1194	42
2036	s-Indacene: A Delocalized, Formally Antiaromatic 12 Œlectron System. 1994 , 33, 1192-1194 s-Indacen: ein delokalisiertes, formal antiaromatisches 12-Œlektronensystem. 1994 , 106, 1252-1254 A neutralizationæionization (NR) case study for cationic iron complexes with simple ligands: NR	42
2036 2035 2034	s-Indacene: A Delocalized, Formally Antiaromatic 12 Œlectron System. 1994 , 33, 1192-1194 s-Indacen: ein delokalisiertes, formal antiaromatisches 12-Œlektronensystem. 1994 , 106, 1252-1254 A neutralizationæionization (NR) case study for cationic iron complexes with simple ligands: NR mass spectra of Fe(C2H4)+ and Fe(CO)+. 1994 , 134, 239-248	42 20 18
2036 2035 2034 2033	s-Indacene: A Delocalized, Formally Antiaromatic 12 [Electron System. 1994, 33, 1192-1194] s-Indacen: ein delokalisiertes, formal antiaromatisches 12-Elektronensystem. 1994, 106, 1252-1254 A neutralization (NR) case study for cationic iron complexes with simple ligands: NR mass spectra of Fe(C2H4)+ and Fe(CO)+. 1994, 134, 239-248 X-ray absorption and dichroism of transition metals and their compounds. 1994, 67, 529-622 Comparison of molecular energy predictions for the neutral and ionic (C, Hn, O; n=0 4) system by ab initio Gaussian-2 and density functional methods. 1994, 179, 365-375	42 20 18 553
2036 2035 2034 2033 2032	s-Indacene: A Delocalized, Formally Antiaromatic 12 [Electron System. 1994, 33, 1192-1194] s-Indacen: ein delokalisiertes, formal antiaromatisches 12-Elektronensystem. 1994, 106, 1252-1254 A neutralization eionization (NR) case study for cationic iron complexes with simple ligands: NR mass spectra of Fe(C2H4)+ and Fe(CO)+. 1994, 134, 239-248 X-ray absorption and dichroism of transition metals and their compounds. 1994, 67, 529-622 Comparison of molecular energy predictions for the neutral and ionic (C, Hn, O; n=0 and density functional methods. 1994, 179, 365-375	42 20 18 553

2028 Ab initio path-integral molecular dynamics. 1994 , 95, 143-144	196
2027 Relativistic density functional calculation of the total energy and Fermi surface of gold. 1994 , 95, 145-	-150 3
Combined Hartree-Fock and density functional theory: a distributed memory parallel implementation. 1994 , 315, 97-107	3
2025 Density functional studies of representative pericyclic reactions. 1994 , 311, 325-330	53
Determination of the heat of formation of oxygen containing radicals using density functional theory. 1994 , 310, 13-16	1
2023 Ab initio simulations of water and water ions. 1994 , 6, A93-A100	56
New pseudospectral algorithms for electronic structure calculations: Length scale separation and analytical two-electron integral corrections. 1994 , 101, 4028-4041	117
2021 Ab Initio Calculations of NMR Chemical Shielding. 1994 , 29, 71-122	50
Electronic structure calculations and dynamics of methane activation on nickel and cobalt. 1994 , 101, 11012-11020	74
2019 Non-local energy density functional for atoms and metal clusters. 1994 , 2, 441-449	26
Binding energies, molecular structures, and vibrational frequencies of transition metal carbonyls using density functional theory with gradient corrections. 1994 , 100, 5785-5791	229
2017 Exchange-correlation potential with correct asymptotic behavior. <i>Physical Review A</i> , 1994 , 49, 2421-24	43 2.6 1247
2016 Relativistic total energy using regular approximations. 1994 , 101, 9783-9792	2379
Generalized-gradient-approximation description of band splittings in transition-metal oxides and fluorides. 1994 , 49, 10170-10175	123
Automatic numerical integration techniques for polyatomic molecules. Backward trimming. 1994 , 101, 1738-1740	11
2013 Applications of Engel and Vosko's generalized gradient approximation in solids. 1994 , 50, 7279-7283	321
2012 A density functional study of small alkali halide systems. 1994 , 101, 8903-8907	12
2011 Density functional study of nitrogen oxides. 1994 , 100, 2910-2923	160

Implementation of gradient-corrected exchange-correlations. 1994 , 50, 4954-4957	tion potentials in Car-Parrinello	834
2009 Density functional calculations on first-row transition me	etals. 1994 , 101, 7729-7737	226
A systematic comparison of molecular properties obtained Hartree Bock density-functional-theory, and coupled-clus	ed using Hartree F lock, a hybrid ter methods. 1994 , 100, 6550-6561	188
Application of density functional methods for the study by hydrogen fluoride dimer. 1994 , 101, 9793-9799	of hydrogen-bonded systems: The	132
Density functional study of phosphorus and arsenic clust functionals. 1994 , 100, 4941-4946	ers using local and nonlocal energy	96
2005 The molecular structure of C6: A theoretical investigatio	n. 1994 , 101, 2213-2216	37
An implementation of analytic second derivatives of the energy. 1994 , 100, 7429-7442	gradient-corrected density functional	194
2003 The hyperfine structures of small radicals from density fo	unctional calculations. 1994 , 100, 5066-5075	118
Assessment of Kohn-Sham density-functional orbitals as calculation of electron-momentum-spectroscopy scatter 50, 4707-4728		240
All-electron local-density and generalized-gradient calcu semiconductors. 1994 , 50, 14947-14951	lations of the structural properties of	146
2000 Does fulminic acid have a bent equilibrium structure?. 19	994 , 69, 755-762	16
Erratum: The performance of a family of density function (1993)]. 1994 , 101, 9202-9202	nal methods [J. Chem. Phys. 98, 5612	5
1998 Ab initio molecular dynamics simulations of molecular cr	ystals. 1995 , 408, 477	2
1997 Computational Determination of Heats of Formation of I	Energetic Compounds. 1995 , 418, 55	11
1996 Modeling of adsorption properties of zeolites. 1995 , 109	D-116	5
1995 Chapter 19 Annealing to a moving target: first-principles	molecular dynamics. 1995, 15, 417-444	
Experimentelle und quantenchemische Untersuchungen Dimethyltrithiocarbonats. 1995 , 191, 159-177	zum Schwingungsspektrum des	5
Matrix isolation IR detection of Fex(NO)y (x, y = 1, 2) com FeNO and CuNo. 1995 , 372, 113-125	plexes. Density functional calculations of	

(1995-1995)

1992	Das lipophil umhil lite Polyionen-Aggregat {[Ba6Li3O2]11+[DC(CH3)3]11(OC4H8)3}; ein flii dhenverknii pftes (Oktaeder + Prisman)- Ba6Li3O2-Polyeder in einem Kohlenwasserstoff-Ellipsoid: Darstellung, Einkristallstrukturbestimmung und Dichtefunktionalberechnungen. 1995 , 107, 1439-1441	16
1991		55
1990	Structures and stabilities of XCCY2+ dications (X, Y = O, S and NH), doubly charged isoelectronic analogues of cyanogen. 1995 , 30, 1144-1148	2
1989	NUO+, a New Species Isoelectronic to the Uranyl Dication UO. 1995 , 1, 7-11	67
1988	Structural and energetic studies on double salts of M(II)Mg2Cl6•12H2O (M ? Ca, Mn, Cd) by X-ray diffraction and density functional methods. 1995 , 238, 121-127	1
1987	Further evidence of the conjoint correction to the local kinetic and exchange energy density functionals. 1995 , 232, 31-34	18
1986	Energetics, structure and excess electrons in small sodium-chloride clusters. 1995 , 232, 79-89	25
1985	Accurate calculation of core-electron binding energies by the density-functional method. 1995 , 232, 486-490	99
1984	A density-functional study of van der Waals forces: rare gas diatomics. 1995 , 233, 134-137	459
1983	Validation of self-consistent hybrid approaches for the study of transition metal complexes. NiCO and CuCO as case studies. 1995 , 233, 129-133	55
1982	Electron correlation and the structure of 1- and 2-hydrotrioxy. An ab initio and density functional approach. 1995 , 233, 111-114	16
1981	A comparative study of ab initio SCF-CI and DFT. Example of small boron clusters. 1995 , 233, 273-278	68
1980	Ab initio helium NMR chemical shifts of endohedral fullerene compounds He@Cn (n = 32f180). 1995 , 233, 585-589	45
1979	Structure and bonding in cisplatin and other Pt(II) complexes. 1995 , 234, 50-56	82
1978	Density functional and post Hartree-Fock equilibrium geometries, potential energy surface and vibrational frequencies for methylamine. 1995 , 233, 611-618	17
1977	Critical assessment of density functional methods for study of proton transfer processes. (FHF)[] 1995 , 234, 159-164	77
1976	Density functional calculations of Fermi contact hyperfine coupling parameters. 1995 , 234, 405-412	29
1975	Adsorption energies of NH3 and NH4+ in zeolites. An embedded cluster model including electron correlation. 1995 , 234, 367-372	31

1974	Molecular polarisabilities - a comparison of density functional theory with standard ab initio methods. 1995 , 235, 1-4	119
1973	Calculation of ligand NMR chemical shifts in transition-metal complexes using ab initio effective-core potentials and density functional theory. 1995 , 235, 382-388	79
1972	Density functional study of H2 desorption from monohydride and dihydride Si(100) surfaces. 1995 , 235, 334-340	69
1971	Density functional theory calculations of isotropic hyperfine coupling constants of atoms and monohydrides. 1995 , 235, 614-616	12
1970	Theoretical investigation of cis-nitric oxide dimer with hybrid density functional theory methods. 1995 , 236, 206-210	88
1969	The metal-ligand bond strengths in cationic gold(I) complexes. Application of approximate density functional theory. 1995 , 236, 194-200	72
1968	All-quantum simulations: H3O+ and H5O2+. 1995 , 237, 161-170	74
1967	OH + H2 -fH2O + H. The importance of <code>Bxact</code> exchangelin density functional theory. 1995 , 237, 53-60	126
1966	Kohn-Sham orbitals for many-body perturbation theory and CI. 1995 , 237, 256-263	19
1965	Structure and EPR parameters of CuC2H2 from a density functional approach. 1995 , 237, 189-194	18
1964	Density-functional theory using an optimized exchange-correlation potential. 1995 , 240, 141-150	137
1963	Structure and stability of small boron clusters. A density functional theoretical study. 1995 , 240, 135-140	115
1962	Theoretical studies of spin density populations on nitroxide and nitronylnitroxide derivatives. 1995 , 240, 268-277	16
1961	The performance of density functional/Hartree-Fock hybrid methods: the bonding in cationic first-row transition metal methylene complexes. 1995 , 240, 245-252	111
1960	Acidic properties of [Al], [Ga] and [Fe] isomorphously substituted zeolites. Density functional model cluster study of the complexes with a probe CO molecule. 1995 , 240, 547-552	46
1959	Coupled density functional/molecular mechanics Monte Carlo simulations of ions in water. The bromide ion. 1995 , 241, 450-456	50
1958	Density functional study of small aqueous Be2+ clusters. 1995 , 241, 457-462	42
1957	Bonding in (IG-C6H6) M and (IG-C6H6) M+, M? Ti, Cr, Ni, and Cu. A local spin density study. 1995 , 243, 269-274	19

1956	Density functional conformational analysis of 1,2-ethanediol. 1995 , 243, 419-428	45
1955	Direct approach to density functional theory: iterative treatment using a polynomial representation of the Heaviside step function operator. 1995 , 243, 367-377	10
1954	Use of molecular stoichiometry to estimate vibrational energy. 1995 , 244, 295-298	24
1953	Cr2 in density-functional theory: approximate spin projection. 1995 , 244, 427-432	70
1952	Ab initio and DFT investigations of intramolecular hydrogen bonding in 1,2-ethanediol. 1995 , 245, 129-135	26
1951	Gas-phase acidities: a comparison of density functional, MP2, MP4, F4, G2(MP2, SVP), G2(MP2) and G2 procedures. 1995 , 245, 123-128	64
1950	A theoretical study of C80 and La2@C80. 1995 , 245, 230-236	124
1949	Density functional theory: excited states and spin annihilation. 1995 , 245, 165-170	82
1948	Aspects of density functional theory in ab initio quantum chemistry: external correlation for free. 1995 , 245, 171-177	33
1947	The FO2 radical: a new success of density functional theory. 1995 , 245, 488-497	49
1946	On the electronic and geometric structure of bimetallic clusters. A comparison of the novel cluster Na6Pb to Na6Mg. 1995 , 245, 671-678	18
1945	Methyl addition to acetylene and ethylene from a density functional approach. 1995 , 246, 45-52	24
1944	Conformational analysis of n-alkanes using density functional theory. Comparison with ab initio calculations. 1995 , 246, 9-12	26
1943	A comparison of the accuracy of different functionals. 1995 , 246, 40-44	368
1942	Carboplatin versus cisplatin: density functional approach to their molecular properties. 1995 , 246, 469-474	25
1941	Transition metal monocarbonyls in the first excited electronic state. A hybrid density functional study. 1995 , 246, 463-468	15
1940	Investigations using the Becke-Roussel exchange functional. 1995 , 246, 381-386	26
1939	The mechanism of alkane activation over zeolite Br listed acid sites. A density-functional study. 1995 , 246, 555-561	33

1938	Adsorption of CO molecules on a MgO(001) surface. Model cluster density functional study employing a gradient-corrected potential. 1995 , 246, 546-554	75
1937	The prediction of Raman spectra by density functional theory. Preliminary findings. 1995 , 247, 120-125	52
1936	Computational evidence for a new C84 isomer. 1995 , 247, 63-68	84
1935	The sensitivity of B3LYP atomization energies to the basis set and a comparison of basis set requirements for CCSD(T) and B3LYP. 1995 , 240, 533-540	246
1934	An examination of a density functional/molecular mechanical coupled potential. 1995 , 16, 113-128	87
1933	On the accuracy of density functionals and their basis set dependence: An extensive study on the main group homonuclear diatomic molecules Li2 to Br2. 1995 , 16, 576-585	90
1932	Nonlocal density functional calculation of gas phase heats of formation. 1995 , 16, 654-658	48
1931	A comparative quantum mechanical study of bond separation energies as a measure of cyclic conjugation. 1995 , 16, 1227-1237	18
1930	Density functional theory and molecular clusters. 1995 , 16, 1315-1325	473
1929	Calculation of molecular geometries, relative conformational energies, dipole moments, and molecular electrostatic potential fitted charges of small organic molecules of biochemical interest by density functional theory. 1995 , 16, 1483-1506	90
1928	Density functional calculations of excitation energies and oscillator strengths for and excitations and ionization potentials in carbonyl containing molecules. 1995 , 191, 141-154	51
1927	An unscaled quantum mechanical harmonic force field for p-benzoquinone. 1995 , 199, 19-32	47
1926	Step structure in the atomic Kohn-Sham potential. 1995 , 33, 229-238	54
1925	Ab initio study of MgSiO3 C2/c enstatite. 1995 , 22, 453	24
1924	Nature of the highest occupied molecular orbitals of trans- and cis-bicyclo[4.1.0]hept-3-enes. 1995 , 8, 149-158	3
1923	Effective core potentials and the structures of metallocenes. 1995 , 53, 309-319	2
1922	Ab initio MO and approximate density functional theory studies on the lowest singlet and triplet states of s and as-indacene. 1995 , 54, 147-159	15
1921	Theoretical investigation of cis- and trans-nitric oxide dimers with ab initio and density functional Gaussian-type orbital approach. 1995 , 54, 161-166	92

(1995-1995)

1920	Theoretical investigation of the conrotatory ring opening of cyclobutene and 1, 2-dihydro-1, 2-diazacyclobutadienes with ab initio and density functional Gaussian-type-orbital approach. 1995 , 56, 115-123	36
1919	Real-space analysis of the exchange-correlation energy. 1995 , 56, 199-210	31
1918	Spin-unrestricted character of Kohn-Sham orbitals for open-shell systems. 1995 , 56, 303-305	183
1917	On the test of different atomic exchange functionals. 1995 , 56, 307-316	3
1916	The implementation of analytical energy gradients based on a quasi-relativistic density functional method: The application to metal carbonyls. 1995 , 56, 477-488	41
1915	Theoretical studies of organonickel compounds. I. A density functional and ab initio HF study. 1995 , 56, 575-587	7
1914	Solvent effects in density functional calculations of uracil and cytosine tautomerism. 1995 , 56, 615-625	72
1913	Stationary point structure and energetics: Density functional study including solvent effects on the tautomerization of formamide and 2-pyridone. 1995 , 56, 645-653	11
1912	A DFT study of the ground state of the N3 radical. 1995 , 56, 655-661	7
1911	Spectroscopic constants of SiH2, GeH2, SnH2, and their cations and anions from density functional computations. 1995 , 56, 669-675	13
1910	Density functional calculation of quinone electrode potentials. 1995 , 56, 677-687	25
1909	Proton transfer in small model systems: A density functional study. 1995 , 56, 697-705	25
1908	A density functional study of chemical reactions. 1995 , 56, 733-746	27
1907	Comparison of the performance of various gradient-corrected exchange and correlation functionals in density functional theory: Case studies of CO and N2O molecules. 1995 , 56, 753-762	12
1906	Density functional calculations of structures and ionization energies for heavy group V cluster anions. 1995 , 56, 771-777	12
1905	Exchange and correlation in density functional theory. 1995 , 56, 49-59	10
1904	Determining and extending the domain of exchange and correlation functionals. 1995 , 56, 61-78	75
1903	Kohn-Sham theory for orbital dependent exchange-correlation energy functionals: Application to the calculation of ionization potentials and electron affinities. 1995 , 56, 79-92	16

1902	Density functional study of the static longitudinal polarizability of model polymeric chains. 1995 , 56, 117-130	12
1901	Molecular dynamics simulation of liquid nitromethane shocked to 143 kbar. 1995 , 56, 621-625	9
1900	Potential energy surfaces and vibrational spectra of H5O and larger hydrated proton complexes. 1995 , 56, 657-668	82
1899	Structural quantum effects and three-centre two-electron bonding in CH+5. 1995 , 375, 216-218	172
1898	Evidence from molecular dynamics simulations for non-metallic behaviour of solid hydrogen above 160 GPa. 1995 , 378, 595-597	36
1897	An adiabatic model of chemisorbed molecules: electron spectroscopy and excited-state potential-energy surfaces. 1995 , 72, 9-18	6
1896	Valence electron momentum distributions of ethylene; comparison of EMS measurements with near Hartree-Fock limit, configuration interaction and density functional theory calculations. 1995 , 196, 13-35	48
1895	Momentum profiles for open shell molecules: studies of the HOMOs of NO, O2 and NO2 by electron momentum spectroscopy and SCF, post-Hartree-Fock and DFT calculations. 1995 , 201, 1-21	27
1894	On the molecular spin density and the electrostatic potential as determinants of the relaxivity of metalloporphyrins. 1995 , 13, 807-17	4
1893	A density functional study on the shape of C180 and C240 fullerenes. 1995 , 247, 491-493	15
1892	Bond energies in organofluorine systems: applications to Teflon and fullerenes. 1995 , 72, 209-214	17
1891	A deficiency of local density functionals for the calculation of self-consistent field atomic data in plasmas. 1995 , 54, 857-878	15
1890	Density functional approach on ground state RgH+ and RgHRg+ (Rg = Ar, Kr, Xe) ions. 1995 , 355, 291-297	40
1889	Matrix isolation IR detection of Fex(NO)y (x,y = 1,2) complexes. Density functional calculations on FeNO and CuNO. 1995 , 372, 113-125	7
1888	A density functional study on the insertion mechanism and chain termination in Kaminsky-type catalysts; comparison of frontside and backside attack. 1995 , 497, 91-104	84
1887	Theoretical calculations of heavy-atom isotope effects. 1995 , 19, 11-20	5
1886	Preliminary density functional calculations on the formic acid dimer. 1995 , 19, 181-187	12
1885	Applications of the adiabatic connection method to conformational equilibria and reactions involving formic acid. 1995 , 19, 145-154	7

1884	Theoretical calculations of heavy-atom isotope effects. 1995 , 19, 231-40	20
1883	On the proposed existence of a ketene derived from carbon monoxide and 1,3-di-1-adamantylimidazol-2-ylidene. 1995 , 36, 645-648	48
1882	Chemisorbed-molecule potential energy surfaces and DIET processes. 1995 , 101, 22-30	20
1881	Tautomerism in uracil, cytosine and guanine: a comparison of electron correlation predicted by ab initio and density functional theory methods. 1995 , 331, 147-154	112
1880	Comparative computational analysis of some nitramine and difluoramine structures, dissociation energies and heats of formation. 1995 , 338, 249-256	29
1879	Relativistic effects of p-block molecules. 1995 , 338, 347-362	21
1878	Charge analysis along the intrinsic reaction coordinate for the insertion reactions CFX + HY ($X = H$, F; $Y = H$, CH3). A comparison of MP2 and density functional theory. 1995 , 357, 75-86	5
1877	Structures and energetic properties of B-DNA nucleotides. 1995 , 357, 161-170	16
1876	Comparison of local density functional and RHF methods for geometry optimizations of Eallyl nickel complexes. 1995 , 357, 263-273	7
1875	Study of ring opening of 1,2-diformyl-1,2-diazacyclobutene by ab initio and density functional Gaussian-type-orbital approach. 1995 , 357, 243-253	27
1874	Structures, energetics and vibrational frequencies of zeolitic catalysts: a comparison between density functional and post-Hartree-Fock approaches. 1995 , 358, 179-193	13
1873	Hg?Hg bonding in mercurous Hg(I)2L2 compounds: the influence of ligand electronegativity. 1995 , 358, 195-203	10
1872	Heats of formation, structures and relative stabilities of some tetraazapentalene-related molecules. 1995 , 358, 63-69	15
1871	Theoretical investigation of F2NNO and F2NNO2 with density functional theory methods. 1995 , 358, 145-150	61
1870	Equilibrium reactions between molecular and ionic species in pure molten LiCl and in LiCl + MCl (M = Na, K, Rb) melts investigated by computational chemistry. 1995 , 358, 39-50	16
1869	Molecular structure and vibrational IR spectrum of ketene. Comparison of conventional ab initio post-HartreeBock and density functional theory calculations. 1995 , 342, 43-49	14
1868	2,5-Dioxybicyclo[2.2.2]octane-3,6-diones. A conformational study by ab initio molecular orbital methods and molecular mechanics calculations. 1995 , 342, 93-101	4
1867	An ab initio study of the structure, vibrational frequencies and force field for the symmetric form of N2O3. 1995 , 342, 103-108	5

1866	Potentially stable carbenes: a theoretical study of pyrazol-ylidenes. 1995 , 342, 115-120	9
1865	Density functional study of molecular properties of hydrazoic acid and methyl azide. 1995 , 343, 31-41	14
1864	Theoretical study of the vibrational spectra of the transition metal carbonyls M(CO)6 [M=Cr, Mo, W], M(CO)5 [M=Fe, Ru, Os], and M(CO)4 [M=Ni, Pd, Pt]. 1995 , 102, 8474-8484	375
1863	N2 and CO molecules as probes of zeolite acidity: an infrared spectroscopy and density functional investigation. 1995 , 31, 273-285	95
1862	On the accuracy of gradient corrected density functional methods for transition metal complexes. 1995 , 102, 872-878	69
1861	Thermochemistry of disulfur decafluoride, S2F10. 1995 , 103, 10162-10168	3
1860	Potential symmetry breaking, structure and definite vibrational assignment for azulene: Multiconfigurational and density functional results. 1995 , 103, 5650-5661	77
1859	Validation of self-consistent hybrid density functionals for the study of structural and electronic characteristics of organic [radicals. 1995 , 102, 384-393	133
1858	Fourier transform infrared study and ab initio calculation of ClNO complex with HCl. 1995 , 103, 6930-6940	6
1857	Binding sites, migration paths, and barriers for hydrogen on Si(111)-(7 x 7). 1995 , 75, 4756-4759	70
1856	Thermal and photodesorption from a molecular surface: Ammonia on Ag2. 1995 , 74, 2070-2073	29
1855	Density functional based studies of transition states and barriers for hydrogen exchange and abstraction reactions. 1995 , 102, 9345-9349	63
1854	A study of some organic reactions using density functional theory. 1995 , 102, 2063-2079	209
1853	Calculated phase diagram for the gamma. 1995 , 74, 2335-2338	110
1852	Electronic structure calculations and dynamics of CC coupling on nickel and cobalt. 1995 , 103, 6562-6570	12
1851	Use of the generalized gradient approximation in pseudopotential calculations of solids. 1995 , 51, 9521-9525	58
1850	Exchange energy in Kohn-Sham density-functional theory. <i>Physical Review A</i> , 1995 , 51, 3571-3575 2.6	34
1849	All-electron study of gradient corrections to the local-density functional in metallic systems. 1995 , 51, 4105-4109	193

	1848	One-electron properties of several small molecules calculated using the local density approximation within density functional theory. 1995 , 102, 3312-3321	29
·	1847	The adsorption of acetylene on Ni(110): An experimental and theoretical study. 1995 , 102, 9709-9724	33
	1846	Thermal and vibrational-state selected rates of the CH4+Cl<-HCl+CH3 reaction. 1995 , 103, 9642-9652	148
	1845	FeCnland FeCnH[(n=3,4): A photoelectron spectroscopic and density functional study. 1995 , 102, 2701-2707	49
;	1844	Soft X-ray photoabsorption of the NO dimer. 1995 , 85, 619-633	16
:	1843	Energy band gaps of silicon-carbon alloys. 1995 , 51, 7295-7298	22
	1842	Energy expressions in density-functional theory using line integrals. <i>Physical Review A</i> , 1995 , 51, 170-17&.6	54
	1841	A hybrid density functional study of the first-row transition-metal monocarbonyls. 1995 , 103, 10605-10613	96
	1840	A density functional/molecular dynamics study of the structure of liquid nitromethane. 1995 , 102, 8281-8282	52
	1839	Gradient-corrected exchange potential with the correct asymptotic behavior and the corresponding exchange-energy functional obtained from the virial theorem. <i>Physical Review A</i> , 2.6 1995 , 52, 3704-3710	44
·	1838	Energy differences between Kohn-Sham and Hartree-Fock wave functions yielding the same electron density. <i>Physical Review A</i> , 1995 , 51, 4501-4513	119
	1837	Conformational behavior of gaseous glycine by a density functional approach. 1995 , 102, 364-370	162
	1836	Local and nonlocal relativistic exchange-correlation energy functionals: Comparison to relativistic optimized-potential-model results. <i>Physical Review A</i> , 1995 , 52, 2750-2764	82
	1835	The performance of density-functional/Hartreeflock hybrid methods: Cationic transition-metal methyl complexes MCH+3 (M=Scau,La,Hfau). 1995 , 102, 4931-4941	141
	1834	Effect of solvent on semiconductor surface electronic states: A first-principles study. 1995 , 103, 7569-7575	12
	1833	H2O photodissociation dynamics based on potential energy surfaces from density functional calculations. 1995 , 103, 2538-2547	12
	1832	How can (semi)local density functional theory account for the ground-state total energy of highly ionized atoms of the first three periods in the periodic table?. 1995 , 102, 278-284	9
	1831	Molecular Kohn-Sham exchange-correlation potential from the correlated ab initio electron density. <i>Physical Review A</i> , 1995 , 52, 1870-1874	98

1830	Dissociation of H2 on Cu(100): Dynamics on a new two-dimensional potential energy surface. 1995 , 102, 3873-3883	63
1829	Theoretical study of the Cu(H2O) and Cu(NH3) complexes and their photolysis products. 1995 , 103, 1860-1870	0 33
1828	Theoretical study of the bonding of ammonia, carbon monoxide, and ethylene, to copper atom, dimer, and trimer. 1995 , 102, 5396-5407	41
1827	Fourier transform infrared observation of the 🛭 stretching mode of linear C9 in Ar at 10 K. 1995 , 103, 6841-6850	35
1826	Structural and electronic properties of trans-polysilene (SiH)x: Many-body perturbation theory versus density-functional methods. 1995 , 52, 1674-1677	13
1825	Theoretical study of the bonding of NO2 to Cu and Ag. 1995 , 103, 9738-9743	20
1824	Si adatom binding and diffusion on the Si(100) surface: Comparison of ab initio, semiempirical and empirical potential results. 1995 , 102, 1044-1056	69
1823	Electron correlation and dimerization in trans-polyacetylene: Many-body perturbation theory versus density-functional methods. 1995 , 51, 16553-16567	82
1822	Theoretical study on the high-pressure phase transformation in ZnSe. 1995 , 52, 4658-4661	46
1821	Cusp relations for local strongly decaying properties in electronic systems. <i>Physical Review A</i> , 1995 , 52, 2645-2651	36
1820	All-electron local and gradient-corrected density-functional calculations of Nan dipole polarizabilities for n=1-6. 1995 , 52, 2184-2200	71
1819	Mu @ C70: A theoretical study. 1995 , 72, 259-266	1
1818	Theoretical Studies of Spin Populations on Nitronyl Nitroxide, Phenyl Nitronyl Nitroxide and P-NPNN. 1995 , 271, 19-28	2
1817	Non-additive forces in atomic clusters. 1995 , 84, 105-114	40
1816	Ab Initio Computation of the Spin Population of Substituted ENitronyl Nitroxide Radicals. 1995 , 271, 79-90	16
1815	Muon-nuclear quadrupolar level crossing resonance in solid nitrogen Evidence for [N2MuN2]+ complex formation?. 1995 , 72, 251-257	
1814	MuCO: Elusive isotopomer of HCO. 1995 , 72, 267-273	3
1813	Semilocal density functionals for exchange and correlation: Theory and applications. 1995 , 2, 29-74	12

1812	Development, implementation and applications of efficient methodologies for density functional calculations. 1995 , 2, 169-219	3
1811	Symmetry and density-functional exchange and correlation. 1995 , 151-167	2
1810	Towards a practical algorithm for large molecule calculations. 1995 , 2, 125-150	1
1809	Theoretical study of the arsenic-hydrogen complex in silicon. 1995 , 72, 193-199	1
1808	High Performance Computational Chemistry; NWChem and Fully Distributed Parallel Applications. 1995 , 10, 395-427	1
1807	Refined embedded-cluster calculations for trapped hole bipolarons in BaTiO3. 1995 , 7, L689-L694	2
1806	A dynamical study of the chemisorption of molecular hydrogen on the Cu(111) surface. 1995 , 7, 7195-7207	32
1805	Coordinate Scaling Requirements for Approximating Exchange and Correlation. 1995, 11-31	9
1804	Ab initio studies of cyclic water clusters (H2O)n, n=18. III. Comparison of density functional with MP2 results. 1995 , 102, 4505-4517	351
1803	DMol, a standard tool for density functional calculations: Review and advances. 1995 , 221-254	79
1802	Density functional theory predictions of the nonlinear optical properties of molecules. 1995 , 71, 1667-1670	6
1801		
	Reactions of silica strained rings: an experimental and ab-initio study. 1995 , 323, 151-162	52
1800	Reactions of silica strained rings: an experimental and ab-initio study. 1995 , 323, 151-162 Methane activation and dehydrogenation on nickel and cobalt: a computational study. 1995 , 324, 345-356	52 110
1800 1799		
	Methane activation and dehydrogenation on nickel and cobalt: a computational study. 1995 , 324, 345-356 The photoelectron spectrum of ethylene oxide adsorbed at metal surfaces: a density functional	110
1799	Methane activation and dehydrogenation on nickel and cobalt: a computational study. 1995 , 324, 345-356 The photoelectron spectrum of ethylene oxide adsorbed at metal surfaces: a density functional model cluster study of. 1995 , 326, 53-58 Correlation energy density from ab initio first- and second-order density matrices: A benchmark for	110
1799 1798 1797	Methane activation and dehydrogenation on nickel and cobalt: a computational study. 1995, 324, 345-356 The photoelectron spectrum of ethylene oxide adsorbed at metal surfaces: a density functional model cluster study of. 1995, 326, 53-58 Correlation energy density from ab initio first- and second-order density matrices: A benchmark for approximate functionals. 1995, 103, 10085-10094	110 5 31

1794	Quantum chemical studies of the pyrrole-water and pyridine-water complexes. 1995 , 85, 573-585	32
1793	Relativistic effects in the electronic structure of the monoxides and monocarbonyls of Ni, Pd, and Pt: Local and gradient-corrected density functional calculations. 1995 , 102, 3695-3702	93
1792	An introduction to density functional theory in chemistry. 1995 , 1-27	39
1791	Ab initio molecular dynamics simulation of the solvation and transport of hydronium and hydroxyl ions in water. 1995 , 103, 150-161	699
1790	Concepts in Theoretical Heterogeneous Catalytic Reactivity. 1995 , 37, 557-698	250
1789	Application of gradient-corrected density functional theory to the structures and thermochemistries of ScF3, TiF4, VF5, and CrF6. 1995 , 102, 8023-8028	75
1788	BeckeWigner: a simple but powerful density functional. 1995 , 91, 4337-4341	15
1787	Structure, epr parameters, and reactivity of organic free radicals from a density functional approach. 1995 , 91, 113-128	83
1786	A relativistic KohnBham density functional procedure by means of direct perturbation theory. 1995 , 103, 3589-3599	46
1785	Constrained optimization procedure for finding transition states and reaction pathways in the framework of gaussian based density functional method: the case of isomerization reactions. 1995 , 2, 255-272	3
1784	Imaging the Electron Density in the Highest Occupied Molecular Orbital of Glycine. 1995 , 270, 786-788	91
1783	The calculation of NMR and ESR spectroscopy parameters using density functional theory. 1995 , 2, 273-347	117
1782	A comparison of density functional theory withab initio approaches for systems involving first transition row metals. 1995 , 92, 123-131	11
1781	Association and insertion complexes of nickel with water and methanol studied using Kohn-Sham theory. 1995 , 91, 129-146	8
1780	Density functional calculations of the structures and bond energies of Cr(CO)6 and (E6-C6H6) Cr(CO)2(CX) (X=O, S) complexes. 1995 , 91, 157-167	1
1779	Transition state localization by a density functional method. Applications to isomerization and symmetry-forbidden reactions. 1995 , 91, 179-186	7
1778	Solvent effects on isomerization equilibria: An energetic analysis in the framework of density functional theory. 1995 , 91, 199-214	5
1777	Density-functional investigation of the excited state properties and the Jahn-Teller effect in [CrX6]3[[X=Cl[]Br]] 1995, 91, 215-224	5

1776	Computation of oscillator strengths from Kohn-Sham wave functions: the example of small lithium clusters. 1995 , 91, 249-266	15
1775	Calculated properties of P2, P4, and of closed-shell clusters up to P18. 1995 , 102, 3703-3711	85
1774	Incorporation of solvent effects into density functional calculations of molecular energies and geometries. 1995 , 103, 9312-9320	682
1773	Some identities in density-functional theory. <i>Physical Review A</i> , 1995 , 52, 969-976 2.6	51
1772	Density-functional calculation of core-electron binding energies of C, N, O, and F. 1995 , 103, 1842-1845	126
1771	Density-functional methods give accurate vibrational frequencies and spin densities for phenoxyl radical. 1995 , 102, 1689-1698	116
1770	A density functional study on olefin insertion and hydrogen transfer in the reaction between Cl2Ti+Bthyl and ethylene. Possible implications for the stereochemistry and chain termination in olefin polymerization. 1995 , 73, 989-998	28
1769	Theoretical investigation of the electronic structures of the mixed-ring sandwich molecules [M(☑-C7H7)(☑-C5H5)](M = Ti, V, Nb or Ta). 1995 , 3727-3730	17
1768	Theoretical and experimental studies on the novel thiazylfluoroformate, FC(O)SN. 1995, 91, 231-235	6
1767	The nature of the platinumphosphine bond. An ab initio HartreeBock and density functional study. 1995 , 4121-4126	18
1766	The influence of generalized gradient corrections to the LDA on predictions of structural phase stability: the Peierls distortion in As and Sb. 1995 , 7, 3683-3692	28
1765	The density functional calculation of nuclear shielding constants using London atomic orbitals. 1995 , 103, 10095-10109	169
1764	A density functional theory study of the alkali metal atomBarbon monoxide interactions: Singularity of the Li atom. 1995 , 102, 5719-5724	16
1763	Vibrational spectrum and structure of the K2O2 complex in solid argon: A far infrared and density functional theory study. 1995 , 103, 1284-1291	8
1762	Self-consistent approximation to the Kohn-Sham exchange potential. <i>Physical Review A</i> , 1995 , 51, 1944-1 96 4	209
1761	Comparison of AM1 and density functional theory generated transition state structures and activation energies for cyanoalkenes addition to cyclopentadiene. 1995 , 358, 139-143	53
1760	Application of generalized gradient approximations: The diamond- beta -tin phase transition in Si and Ge. 1995 , 52, 2550-2556	121
1759	Structure and spectroscopy of phosphorus cluster anions: Theory (simulated annealing) and experiment (photoelectron detachment). 1995 , 103, 9549-9562	74

1758	Efficient molecular numerical integration schemes. 1995 , 102, 346-354	2078
1757	Ab initio calculations of structural and electronic properties of gallium solid-state phases. 1995 , 52, 9988-9998	3133
1756	Basis Set Effects in Density Functional Calculations on the Metalligand and MetallMetal Bonds of Cr(CO)5IIO and (CO)5MnIMn(CO)5. 1996 , 100, 5690-5696	115
1755	Improved density functional theory results for frequency-dependent polarizabilities, by the use of an exchange-correlation potential with correct asymptotic behavior. 1996 , 105, 3142-3151	184
1754	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. 1996 , 53, 1180-1185	204
1753	The Osmium(VIII) Oxofluoro Cations OsO(2)F(3)(+) and F(cis-OsO(2)F(3))(2)(+): Syntheses, Characterization by (19)F NMR Spectroscopy and Raman Spectroscopy, X-ray Crystal Structure of F(cis-OsO(2)F(3))(2)(+)Sb(2)F(11)(-), and Density Functional Theory Calculations of OsO(2)F(3)(+),	51
1752	Molecular electrostatic potentials as indicators of covalent radii. 1996 , 104, 5109-5111	30
1751	Linkage Isomerism in Complexes of o-Xylylene: Density Functional Study of the Structure and Bonding in endo- and exo-Ru(PH3)3(o-xylylene). 1996 , 15, 3109-3114	15
1750	A relativistic KohnBham density functional procedure by means of direct perturbation theory. II. Application to the molecular structure and bond dissociation energies of transition metal carbonyls and related complexes. 1996 , 105, 5485-5493	37
1749	A comparison of models for calculating nuclear magnetic resonance shielding tensors. 1996 , 104, 5497-5509	1842
1749 1748	A comparison of models for calculating nuclear magnetic resonance shielding tensors. 1996 , 104, 5497-5509 Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. 1996 , 105, 11060-11067	1842 182
1748	Development and validation of reliable quantum mechanical approaches for the study of free	
1748	Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. 1996 , 105, 11060-11067	182
1748	Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. 1996 , 105, 11060-11067 Density Functional Studies on N-Methylacetamide Water Complexes. 1996 , 100, 3942-3949	182
1748 1747 1746	Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. 1996, 105, 11060-11067 Density Functional Studies on N-Methylacetamide Water Complexes. 1996, 100, 3942-3949 Density Functional Calculations on WH6 and WF6. 1996, 100, 19818-19823 The Structure of Hexamethyltungsten, W(CH3)6: Distorted Trigonal Prismatic with C3 Symmetry.	182 96 32
1748 1747 1746 1745	Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. 1996, 105, 11060-11067 Density Functional Studies on N-Methylacetamidel Water Complexes. 1996, 100, 3942-3949 Density Functional Calculations on WH6 and WF6. 1996, 100, 19818-19823 The Structure of Hexamethyltungsten, W(CH3)6: Distorted Trigonal Prismatic with C3 Symmetry. 1996, 118, 3018-3024 Theoretical study of the addition of alkyl and halogenoalkyl radicals to the ethylene double bond: a	182 96 32 72 21
1748 1747 1746 1745	Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. 1996, 105, 11060-11067 Density Functional Studies on N-MethylacetamidelWater Complexes. 1996, 100, 3942-3949 Density Functional Calculations on WH6 and WF6. 1996, 100, 19818-19823 The Structure of Hexamethyltungsten, W(CH3)6: Distorted Trigonal Prismatic with C3 Symmetry. 1996, 118, 3018-3024 Theoretical study of the addition of alkyl and halogenoalkyl radicals to the ethylene double bond: a comparison between HartreeBock, perturbation theory and density functional theory. 1996, 2041-2047	182 96 32 72 21

1740	methods. 1996 , 104, 6628-6630	48
1739	Ab initio molecular dynamics simulation of liquid water: Comparison of three gradient-corrected density functionals. 1996 , 105, 1142-1152	562
1738	Distinguishing Features of Indolyl Radical and Radical Cation: Implications for Tryptophan Radical Studies1. 1996 , 100, 1530-1535	74
1737	Interactions Between Adsorbate Particles. 1996 , 577-650	17
1736	CH3IIs Planar Due to HIII Steric Repulsion. Theoretical Study of MH3Iand MH3Cl (M = C, Si, Ge, Sn). 1996 , 15, 1477-1487	62
1735	A theoretical study of ethylene oligomerization by organometallic nickel catalysts. 1996 , 100, 507-514	6
1734	Theoretical Study of 13C and 17O NMR Shielding Tensors in Transition Metal Carbonyls Based on Density Functional Theory and Gauge-Including Atomic Orbitals. 1996 , 100, 3359-3367	62
1733	Solvent effects on the relative stability of the PdCl2(H2O)n and PdHCl(H2O)n cis and trans isomers. 1996 , 89, 279-296	12
1732	Theoretical Study of Ethylene Oligomerization by an Organometallic Nickel Catalyst. 1996 , 35, 4003-4006	48
1731	Geometric structure of Ar?NO+: Revisited. A failure of density functional theory. 1996 , 105, 7579-7582	40
1730	Theoretical Infrared Spectra for Polycyclic Aromatic Hydrocarbon Neutrals, Cations, and Anions. 1996 , 100, 2819-2841	403
1729	Comparison ofab Initioand Density Functional Theory for Alkali Peroxynitrite: A Highly Correlated System with Hartree Bock Instability. 1996 , 100, 6942-6949	20
1728	Density Functional Study of Ethylene Adsorption on Palladium Clusters. 1996 , 100, 5676-5680	64
1727	Local, Gradient-Corrected, and Hybrid Density Functional Calculations on PdnClusters forn= 1 B . 1996 , 100, 10827-10830	66
1726	Systematic Model Chemistries Based on Density Functional Theory: Comparison with traditional Models and with Experiment. 1996 , 4, 679-707	37
1725	Intramolecular Hydrogen Bonding in 2-Hydroxybenzoyl Compounds: Infrared Spectra and Quantum Chemical Calculations. 1996 , 100, 7418-7425	96
1724	Treatment of the outlying charge in continuum solvation models. 1996 , 105, 9972-9981	691
1723	Solvent and Substituent Effects in the Periselectivity of the Staudinger Reaction between Ketenes and alpha,beta-Unsaturated Imines. A Theoretical and Experimental Study. 1996 , 61, 3070-3079	35

1722	Reactions of Laser-Ablated Iron Atoms with Nitrogen Atoms and Molecules. Matrix Infrared Spectra and Density Functional Calculations of Novel Iron Nitride Molecules. 1996 , 100, 14609-14617	68
1721	Density-Functional-Derived Structures, Spin Properties, and Vibrations for Phenol Radical Cation. 1996 , 100, 10554-10563	47
1720	The Mechanism of Dimethyl Ether Formation from Methanol Catalyzed by Zeolitic Protons. 1996 , 118, 5152-5153	170
1719	Ab initio molecular dynamics study of proton transfer in a polyglycine analog of the ion channel gramicidin A. 1996 , 71, 1172-8	95
1718	How Does Helium Get into Buckminsterfullerene?. 1996 , 118, 7164-7172	76
1717	Stationary points on the lowest doublet and quartet hypersurfaces of the N3 radical: A comparison of molecular orbital and density functional approaches. 1996 , 105, 10969-10982	34
1716	How Does Fe+ Activate Ct and C⊞ Bonds in Ethane? A Theoretical Investigation Using Density Functional Theory 1996, 100, 6236-6242	157
1715	The electron affinities of the silicon fluorides SiFn (n=18). 1996 , 105, 6880-6886	71
1714	Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. 1996 , 100, 5274-5280	20
1713	Density Functional Theory of Molecular Solids: Local versus Periodic Effects in the Two-Dimensional Infinite Hydrogen-Bonded Sheet of Formamide. 1996 , 100, 3950-3958	36
1712	A density-functional study of the intermolecular interactions of benzene. 1996 , 105, 8684-8689	224
1711	Comparative Study of Ethane and Propane Cation Radicals by B3LYP Density Functional and High-Level ab Initio Methods. 1996 , 100, 15774-15784	54
1710	Activation of CEI and CEI Bonds by an Acidic Zeolite: A Density Functional Study. 1996, 100, 3463-3472	144
1709	Energetics of Reactions Involving Transition Metal Complexes: Calculation of Relative Electrode Potentials for Cobalt Complexes at Various Ionic Strengths Using Density Functional and Poisson B oltzmann Methods. 1996 , 118, 10545-10550	4
1708	Ecyanoethyl Anion: Lusus Naturae. 1996 , 118, 4462-4468	10
1707	Ab Initio Study of the Mechanism of the Binding of Triplet O2 to Hemocyanin. 1996 , 35, 5207-5212	43
1706	Properties of Closed-Shell, Octahedral, Multiply-Charged Hexafluorometallates MF63-, M = Sc, Y, La, ZrF62-, and TaF6 1996 , 118, 1173-1180	55
1705	Binuclear Platinum(II) Triazolopyrimidine Bridged Complexes. Preparation, Crystal Structure, NMR Spectroscopy, and ab Initio MO Investigation on the Bonding Nature of the Pt(II) #Pt(II) Interaction in the Model Compound {Pt2[NHCHN(C(CH2)(CH3))]4}. 1996, 35, 7829-7835	52

1704	A Dynamical Density Functional Study on the Reaction of Ethylene with Cp2Zr(C2H5)+. 1996 , 118, 4434-4441	117
1703	Cluster Models of Cu Binding and CO and NO Adsorption in Cu-Exchanged Zeolites. 1996 , 100, 6032-6046	83
1702	Relative Stabilities and Hydride Affinities of Silatropylium and Silabenzyl Cations and Their Isomers. Comparison with the Carbon Analogues Tropylium and Benzyl Cations. 1996 , 118, 10561-10570	32
1701	Theoretical Bond and Strain Energies of Molecules Derived from Properties of the Charge Density at Bond Critical Points. 1996 , 118, 1529-1534	82
1700	Octacarbonyl Diiron. A Density Functional Study. 1996 , 118, 4631-4635	75
1699	Migratory CO Insertion and Aldehyde Formation in Carbonylation of Methane by the Rh(PH3)2Cl Catalyst. A Dynamical Density Functional Study. 1996 , 118, 5412-5419	40
1698	Electronic Structure of the Perturbed Blue Copper Site in Nitrite Reductase: Spectroscopic Properties, Bonding, and Implications for the Entatic/Rack State. 1996 , 118, 7755-7768	178
1697	Nonempirical Calculations of a Hydrated RNA Duplex. 1996 , 118, 8710-8712	40
1696	Addition of Aryl and Fluoroalkyl Radicals to Fullerene C70: ESR Detection of Five Regioisomeric Adducts and Density Functional Calculations 1996, 118, 7608-7617	30
1695	Intermediates and Transition Structures of the Benzannulation of Heteroatom-Stabilized Chromium Carbene Complexes with Ethyne: A Density Functional Study. 1996 , 118, 10551-10560	72
1694	Communication between Porphyrin Rings in the Butadiyne-Bridged Dimer Ni(OEP)(EC4)Ni(OEP): A Density Functional Study. 1996 , 35, 7791-7797	36
1693	Density Functional Study of the Photodissociation of Mn2(CO)10. 1996 , 35, 2886-2897	51
1692	Intrinsic Aptitude of Cationic Methyl- and Ethylpalladium To Associate Ethylene and To Further Undergo Subsequent Migratory Insertion. A Theoretical Study. 1996 , 15, 5542-5550	35
1691	HD SpinBpin Coupling in Stretched Molecular Hydrogen Complexes of Osmium(II): Density Functional Studies of JHD. 1996 , 118, 3753-3756	38
1690	Recent Developments in the Theory of Supralattices. 1996 , 8, 1793-1806	12
1689	Ab Initio Studies of the Exocyclic Hydroxymethyl Rotational Surface in ⊞-Glucopyranose. 1996 , 118, 1190-1193	51
1688	Bonding Properties of a Novel Inorganometallic Complex, Ru(SnPh(3))(2)(CO)(2)(iPr-DAB) (iPr-DAB = N,N'-Diisopropyl-1,4-diaza-1,3-butadiene), and its Stable Radical-Anion, Studied by UV-Vis, IR, and EPR Spectroscopy, (Spectro-) Electrochemistry, and Density Functional Calculations. 1996 , 35, 5468-5477	49
1687	Racemization Barriers of Helicenes: A Computational Study1. 1996 , 118, 6031-6035	169

1686	Structures and Conformations of (Trifluoromethyl)thioacetic Acid, CF3C(O)SH, and Derivatives CF3C(O)SCH3 and CF3C(O)SCl. 1996 , 35, 6152-6157	29
1685	Structural Distortion of the TpCo-L Fragment (Tp = tris(pyrazolyl)borate). Analysis by X-ray Diffraction and Density Functional Theory. 1996 , 118, 1703-1712	76
1684	Theoretical Study on Acetaldehyde and Ethanol Elimination from the Hydrogenation of CH3(O)CCo(CO)3. 1996 , 15, 2611-2618	48
1683	Electronic Structure, Heisenberg Coupling Constants, and Metal M etal Bond in Dimeric Iron(II) Organometallics with the Metal Centers at Variable Distances: A Density Functional Approach. 1996, 35, 7776-7785	13
1682	Changes in the Interaction Mode of Bridging [12]Units According to Transition Metal Parameters: A Theoretical Approach. 1996 , 15, 4264-4273	24
1681	Second Coordination Shell Water Exchange Rate and Mechanism: Experiments and Modeling on Hexaaquachromium(III). 1996 , 118, 12777-12787	75
1680	A Nonlocal Density Functional Study of the Pd(II)-Assisted Copolymerization of Ethylene and CO. 1996 , 118, 7337-7344	103
1679	A Density Functional Study of Substituent Effects on the O-H and O-CH(3) Bond Dissociation Energies in Phenol and Anisole. 1996 , 61, 7904-7910	114
1678	Contrasting Stabilities of Classical and Bridged Pyramidal Si3H3X Molecules (X = BH-, CH, N, NH+, NO, SiH, P, PH+, and PO). 1996 , 118, 3738-3742	13
1677	Interconversions of Phenylcarbene, Cycloheptatetraene, Fulvenallene, and Benzocyclopropene. A Theoretical Study of the C(7)H(6) Energy Surface. 1996 , 61, 7022-7029	116
1676	Unconventional Bonding of Azafullerenes: Theory and Experiment. 1996 , 118, 11335-11336	103
1675	CH3+ Is the Most Trivial Carbocation, but Are Its Heavier Congeners Just Lookalikes?. 1996 , 118, 12154-12158	37
1674	Synthesis and Chemistry of Bicyclo[4.1.0]hept-1,6-ene. 1996 , 61, 764-770	19
1673	(Cyanovinyl)ketenes From Azafulvenones. An Apparent Retro-Wolff Rearrangement. 1996 , 118, 3852-3861	31
1672	The C7H6 Potential Energy Surface Revisited: Relative Energies and IR Assignment. 1996 , 118, 1535-1542	142
1671	Zirconium-91 Chemical Shifts and Line Widths as Indicators of Coordination Geometry Distortions in Zirconocene Complexes 1996, 15, 778-785	49
1670	Theoretical Study of the [{Fe(CO)2Cp}3(B-C3)]+ Tricarbido Cation. 1996 , 15, 5330-5334	5
1669	Mechanism of the Participation of Water in the Decomposition of Hydrogen Trioxide (HOOOH). A Theoretical Study. 1996 , 118, 2470-2472	40

1668	Unusual 31P Chemical Shielding Tensors in Terminal Phosphido Complexes Containing a Phosphorus Metal Triple Bond. 1996 , 118, 10654-10655	76
1667	13C Dipolar NMR Spectrum of Matrix-Isolated o-Benzyne-1,2-13C2. 1996 , 118, 846-852	54
1666	Study of the Electronic Structure of Ni(eta(5)-C(5)H(5))(NO) by Variable-Photon-Energy Photoelectron Spectroscopy and Density Functional Calculations. 1996 , 35, 2504-2514	18
1665	A new gradient-corrected exchange functional. 1996 , 89, 433-445	178
1664	Substituent Effects in the Hetero-DielsAlder Reaction of Thiocarbonyl Compounds with Butadiene. 1996 , 61, 5121-5129	13
1663	Electronic Structure and Properties of the Transactinides and Their Compounds. 1996 , 96, 1977-2010	141
1662	Electronic Structure and Properties of Trihalogen Cations $X(3)(+)$ and $XY(2)(+)$ (X, Y = F, Cl, Br, I). 1996 , 35, 100-109	13
1661	Structure and Bonding in Pentacyano(L)ferrate(II) and Pentacyano(L)ruthenate(II) Complexes (L = Pyridine, Pyrazine, and N-Methylpyrazinium): A Density Functional Study. 1996 , 35, 6832-6837	22
1660	Spin-Density Maps for an Oxamido-Bridged Mn(II)Cu(II) Binuclear Compound. Polarized Neutron Diffraction and Theoretical Studies. 1996 , 118, 11822-11830	56
1659	The Structure of XeF6 and of Compounds Isoelectronic with It. A Challenge to Computational Chemistry and to the Qualitative Theory of the Chemical Bond. 1996 , 118, 11939-11950	62
1658	Nanocrystal [Ti14C13] to Metallocarbohedrene [Ti8C13]: Structural Principles and Mechanism. 1996 , 118, 2699-2707	25
1657	Conformational and electronic properties of the two cis (5S,6R) and (5R,6S) diastereoisomers of 5,6-dihydroxy-5,6-dihydrothymidine: X-ray and theoretical studies. 1996 , 9, 298-305	10
1656	Molecular Structure of Dimethyldichlorotitanium(IV) by Gas-Phase Electron Diffraction, IR and NMR Spectroscopies, and Density Functional Theory Calculations. Unexpected Distortion from Tetrahedral Coordination Geometry. 1996 , 35, 4713-4718	25
1655	Combined Static and Dynamic Density Functional Study of the Ti(IV) Constrained Geometry Catalyst (CpSiH2NH)TiR+. 1. Resting States and Chain Propagation. 1996 , 118, 13021-13030	144
1654	The CeO(2)(+) Cation: Gas-Phase Reactivity and Electronic Structure. 1996 , 35, 2463-2475	74
1653	Fe B Bonding in (Dibromoboryl)ferrocene: A Structural and Theoretical Investigation. 1996 , 15, 1188-1194	82
1652	Experimental and Theoretical Investigations of the Formation of the Diazene PhSN=C(H)N=NC(H)=NSPh from HCN(2)(SPh)(3) by a Thiyl-Radical-Catalyzed Mechanism: Identification of the HC(NSPh)(2)(*) Radical and X-ray Structures of HCN(2)(SPh)(3) and	13
1651	PhSN=C(H)N=NC(H)=NSPh. 1996 , 35, 3839-3847 Difluorodioxirane: An Unusual Cyclic Peroxide. 1996 , 118, 10595-10608	51

1650	Intramolecular Chalcogen Nitrogen Interactions: Molecular and Electronic Structures of Geometrical Isomers of the Diazenes RSNC(R)NNC(R)NSR. 1996 , 35, 5836-5842	17
1649	Influence of gradient corrections on the bulk and surface properties of TiO2 and SnO2. 1996 , 53, 957-960	154
1648	Theoretical Studies of the [N]Phenylenes. 1996 , 118, 8470-8474	58
1647	Photoelectron Spectra and Structures of Proazaphosphatranes. 1996 , 35, 6102-6107	16
1646	Electronic Structure of Rh(2)(&mgr-CO)(CO)(2)(H(2)PCH(2)PH(2))(2). An Example of a Non-A-Frame Structure. 1996 , 35, 3298-3306	13
1645	Response Function Basis Sets: Application to Density Functional Calculations. 1996 , 100, 6231-6235	27
1644	Electronic and Vibrational Circular Dichroism of Model	23
1643	Modeling the Solvent Sphere: Mechanism of the Shilov Reaction. 1996 , 118, 4442-4450	126
1642	New high-pressure phase of ice. 1996 , 76, 2934-2936	141
1641	The torsional potential of perfluoro n-alkanes: A density functional study. 1996 , 104, 3692-3700	48
1640	On the adsorption site of ethylene at the Ni(110) surface: a combined experimental and theoretical study involving the unoccupied band structure. 1996 , 345, 331-346	17
1639	Bond selectivity in the dissociative adsorption of c-CH2N2 on single crystals: a comparative DFT-LSD investigation for Pd(110) and Cu(110). 1996 , 347, 11-24	8
1638	The adsorption of H2O on TiO2 and SnO2(110) studied by first-principles calculations. 1996 , 350, 145-158	230
1637	Comparison of the nature of the hydrogen-metal bond on Pd(111) and Ni(111) by a periodic density functional method. 1996 , 356, L403-L409	44
1636	Density-functional periodic study of the adsorption of hydrogen on a palladium (111) surface. 1996 , 53, 8015-8027	112
1635	Infrared intensities and Raman-scattering activities within density-functional theory. 1996 , 54, 7830-7836	479
1634	Radical Ions of Acetylene in ZSM5 Zeolites: An EPR and Theoretical Study (1996, 100, 8408-8417)	32
1633	A Systematic Appraisal of Density Functional Methodologies for Hydrogen Bonding in Binary Ionic Complexes. 1996 , 100, 4781-4789	86

1632	Comparison between Optimized Geometries and Vibrational Frequencies Calculated by the DFT Methods. 1996 , 100, 15056-15063	173
1631	DFT and MO calculations of atomic and molecular chemisorption energies on surface cluster models. 1996 , 94, 297-310	19
1630	Density Functional for van der Waals Forces at Surfaces. 1996 , 77, 2029-2032	106
1629	The energetics of adsorption of HCOOH on the MgO(100) surface. 1996 , 367, 135-148	32
1628	Density functional and infrared spectroscopy studies of bonding and vibrations of NH species adsorbed on the Ru(001) surface: a reassignment of the bending mode band. 1996 , 369, 300-312	26
1627	Spin and charge distribution in hexaperylene hexafluorophosphate, (C20H12)6PF6. 1996 , 82, 53-58	5
1626	Reactivity of Carbenes and Ketenes in Low-Temperature Matrices. Carbene CO Trapping, Wolff Rearrangement, and Ketene Pyridine Ylide (Zwitterion) Observation. 1996 , 118, 12598-12602	53
1625	Density Functional Theory and Perturbation Calculations on Some Lewis Acid B ase Complexes. A Systematic Study of Substitution Effects. 1996 , 100, 15079-15082	48
1624	The zero-order regular approximation for relativistic effects: The effect of spinBrbit coupling in closed shell molecules. 1996 , 105, 6505-6516	1273
1623	Hybrid DFT-MD simulations of geometry and hyperfine structure of the CCH radical in argon matrices at low temperatures. 1996 , 105, 8195-8203	17
1622	Structural and vibrational analysis of indole by density functional and hybrid HartreeHock/density functional methods. 1996 , 2653-2662	28
1621	Electron Correlation Effects in Molecules. 1996 , 100, 12960-12973	173
1620	Mechanism of Atmospheric Photooxidation of Aromatics: A Theoretical Study. 1996 , 100, 10967-10980	141
1619	Theoretical study of the vibrational spectra of the transition-metal carbonyl hydrides HM(CO)5 (M=Mn, Re), H2M(CO)4 (M=Fe, Ru, Os), and HM(CO)4 (M=Co, Rh, Ir). 1996 , 105, 3636-3648	79
1618	Relativistic density functional theory. 1996 , 1-80	36
1617	Synthesis and Characterization of the First Corannulene Cyclophane. 1996 , 118, 2754-2755	118
1616	On Transition Structures for Hydride Transfer Step in Enzyme Catalysis. A Comparative Study on Models of Glutathione Reductase Derived from Semiempirical, HF, and DFT Methods. 1996 , 61, 7777-7783	20
1615	Molecular Structure and Infrared Spectra of Adenine. Experimental Matrix Isolation and Density Functional Theory Study of Adenine 15N Isotopomers. 1996 , 100, 3527-3534	171

1614	Interaction of CO Molecules with Electron-Deficient Pt Atoms in Zeolites: A Density Functional Model Cluster Study. 1996 , 100, 3482-3487	21
1613	A First Principles Investigation of the Structure of a Bacteriochlorophyll Crystal. 1996 , 118, 7847-7848	20
1612	Structure of the Transition States and Intermediates Formed in the Water-Exchange of Metal Hexaaqua Ions of the First Transition Series. 1996 , 118, 6760-6766	124
1611	Nuclear magnetic resonance spin pin coupling constants from density functional theory: Problems and results. 1996 , 105, 8793-8800	136
1610	NMR SpinBpin Coupling Constants from Density Functional Theory with Slater-Type Basis Functions. 1996 , 100, 5286-5290	83
1609	Separable dual-space Gaussian pseudopotentials. 1996 , 54, 1703-1710	4104
1608	Cohesive energy of 3d transition metals: Density functional theory atomic and bulk calculations. 1996 , 54, 5326-5333	175
1607	Structural, Spectroscopic, and Theoretical Characterization of Bis(Ebxo)dicopper Complexes, Novel Intermediates in Copper-Mediated Dioxygen Activation. 1996 , 118, 11555-11574	224
1606	Theoretical and Experimental Study of Medium Effects on the Structure and Spectroscopy of the [Fe(CN)(5)NO](2)(-) Ion. 1996 , 35, 3897-3903	53
1605	Density Functional, Hartree E ock, and MP2 Studies on the Vibrational Spectrum of Phenol. 1996 , 100, 17786-17790	184
1604	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. 1996 , 54, 16533-16539	4634
1603	On the Enhanced Stability of the Guaninetytosine Base-Pair Radical Cation. 1996 , 118, 7574-7577	178
1602	A theoretical study of the valence- and dipole-bound states of the nitromethane anion. 1996 , 105, 8785-8792	112
1601	Comparative Study of Nonlocal Density Functional Theory and ab Initio Methods: The Potential Energy Surface of sym-Triazine Reactions. 1996 , 100, 15368-15382	15
1600	Prediction of Nitrogen and Oxygen NMR Chemical Shifts in Organic Compounds by Density Functional Theory. 1996 , 100, 16881-16891	44
1599	Formation, Spectroscopy, Photochemistry, and Quantum Chemistry of the (S2)(O2) Complex in Solid Argon. 1996 , 118, 5469-5473	14
1598	Ab Initio Molecular Dynamics Simulations. 1996 , 100, 12878-12887	149
1597	Quantum Chemistry and Molecular Processes. 1996 , 100, 13213-13225	21 0

1596 Origin of the Hydridic 1H NMR Chemical Shift in Low-Valent Transition-Metal Hydrides. 1996, 15, 3920-3923 81 1595 Conformers of Gaseous FAlanine. **1996**, 100, 3541-3551 176 Harmonic Vibrational Frequencies and Force Constants of M(CO)5CX (M = Cr, Mo, W; X = O, S, Se). The Performance of Density Functional Theory and the Influence of Relativistic Effects. **1996**, 100, 16538-1654 $\overset{?}{4}^{6}$ 1594 Theoretical Study of Structural and Thermodynamic Properties of Yttrium Carbides, YCn(n= 2B). 1593 20 1996, 100, 8254-8259 Linear and Cyclic Clusters of Hydrogen Cyanide and Cyanoacetylene: A Comparative ab Initio and 1592 47 Density Functional Study on Cooperative Hydrogen Bonding. 1996, 100, 13474-13486 Mechanistic Studies of the 1,4-Cis Polymerization of Butadiene According to the FAllyl Insertion Mechanism. 1. Density Functional Study of the Cla Bond Formation Reaction in Cationic 41 (B-Allyl)(№-/H-butadiene)nickel(II) Complexes [Ni(C3H5)(C4H6)]+ and [Ni(C3H5)(C4H6)(C2H4)]+. Density Functional Theory as a Tool for the Prediction of the Properties in Molecules with 1590 10 Biological and Pharmacological Significance. 1996, 743-772 Density-Functional Theory Concepts and Techniques for Studying Molecular Charge Distributions 1589 27 and Related Properties. 1996, 773-809 Kinetics of the Proton Transfer in $X^{(4)}(H2O)4$ Clusters (X = H2O, NH3, H2S, and HCl): Evidence of a 1588 64 Concerted Mechanism. 1996, 100, 16495-16501 A theoretical evaluation of steric and electronic effects on the structure of [OSO4 (NR3)] (NR3 = 1587 bulky chiral alkaloid derivative) complexes. 1996, 94, 67-73 1586 Exchange functionals and potentials. 1996, 87, 1-36 208 Electronic and Geometric Structure of Bimetallic Clusters: Density Functional Calculations on 1585 [M(4){Fe(CO)(4)}(4)](4-) (M = Cu, Ag, Au) and [Ag(13){Fe(CO)(4)}(8)](n)(-) (n = 0-5). **1996**, 35, 7370-7376 Electronic Structure of Transition Metal Clusters from Density Functional Theory. 1. Transition 1584 63 Metal Dimers. 1996, 100, 565-572 1583 The Carbon Lithium Electron Pair Bond in (CH3Li)n (n = 1, 2, 4). 1996, 15, 2923-2931 249 Density Functional Theory (DFT) Study of Enthalpy of Formation. 1. Consistency of DFT Energies 1582 67 and Atom Equivalents for Converting DFT Energies into Enthalpies of Formation. 1996, 100, 14665-14671 Molecular Structure and Vibrational IR Spectra of Cytosine and Its Thio and Seleno Analogues by 1581 116 Density Functional Theory and Conventional ab Initio Calculations. 1996, 100, 941-953 1580 Density functional theory studies of zeolite acidity and reactivity. 1996, 101, 1263-1271 2 1579 Novel intermolecular CH ? It interactions: an ab initio and density functional theory study. 1996, 563-568 33

1578	Determination of Arrhenius Parameters for Propagation in Free-Radical Polymerizations: An Assessment of ab Initio Procedures. 1996 , 100, 18997-19006	90
1577	Computational Analysis of Substituent Effects in Para-Substituted Phenoxide Ions. 1996 , 100, 10116-10120	29
1576	Complexes of [Ph2P(O)NP(E)Ph2](E = S or Se): disparate ring conformations within a new palladacycle. 1996 , 3659-3665	32
1575	Study of electron densities of methyl acetate, N-methylacetamide and N,N?-dimethylurea by quantum mechanical investigations. Part 1. Gas phase. 1996 , 1397-1401	7
1574	Reliability of Small Cluster Models for Cu-Exchanged Zeolites. 1996 , 100, 9292-9301	43
1573	Glycine Valence Orbital Electron Densities: Comparison of Electron Momentum Spectroscopy Experiments with Hartree Bock and Density Functional Theories. 1996 , 118, 10533-10544	78
1572	The use of density matrix expansions for calculating molecular exchange energies. 1996 , 87, 835-843	28
1571	Analysis of the Thermochemistry of NOx Decomposition over CuZSM-5 Based on Quantum Chemical and Statistical Mechanical Calculations. 1996 , 100, 17582-17592	113
1570	H2XO and (CH3)2XO Compounds (X = C, Si, Ge, Sn, Pb): Double Bonds vs Carbene-Like StructuresCan the Metal Compounds Exist at All?. 1996 , 118, 5745-5751	106
1569	Density Functional Study of Cℍ and Oℍ Bond Activation by Transition Metal dotoxo Complexes: 1. Thermodynamic Considerations. 1996 , 15, 3011-3021	46
1568	Methane Elimination from Ionized Propane through an IonNeutral Complex: An ab Initio Study. 1996 , 118, 9368-9376	17
1567	Palladium(II)-Assisted Copolymerization of Ethylene and CO: Influence of the Chain End on the Regularity of the Polymer. 1996 , 15, 5519-5523	70
1566	Bond Fixation in a [14]Annulene: Synthesis, Characterization, and ab Initio Computations of Furan Adducts of Dimethyldihydropyrene. 1996 , 118, 2907-2911	27
1565	A density functional study of the bonding in tertiary phosphine chalcogenides and related molecules. 1996 , 74, 2363-2371	33
1564	Density-functional calculation of core-electron binding energies of glycine conformers. 1996 , 74, 1005-1007	26
1563	Raman intensities from KohnBham calculations. 1996 , 104, 1254-1262	45
1562	The calculation of 77Se chemical shifts using gauge including atomic orbitals and density functional theory. 1996 , 104, 8605-8612	59
1561	Photoelectron investigations and density functional calculations of anionic Sbntand Bintelusters. 1996, 104, 9719-9728	64

1560	The structure and binding energy of K+#ther complexes: A comparison of MP2, RI-MP2, and density functional methods. 1996 , 105, 1940-1950	55
1559	A comparative analysis by means of quantum molecular similarity measures of density distributions derived from conventional ab initio and density functional methods. 1996 , 104, 636-647	43
1558	Density functional study of strong hydrogen-bonded systems: The hydrogen diformiate complex. 1996 , 104, 8524-8534	28
1557	Calculation of Proton Affinities Using Density Functional Procedures: A Critical Study. 1996 , 100, 11596-1159	951
1556	A systematic density functional study of fluorination in methane, ethane and ethylene. 1996 , 89, 211-237	34
1555	On the dissociation energy of Ti(OH2)+. An MCSCF, CCSD(T), and DFT study. 1996 , 74, 1824-1829	17
1554	On the accuracy of density functional theory for ionfinolecule clusters. A case study of PLn+clusters of the first and second row hydrides. 1996 , 74, 1032-1048	3
1553	Time-Dependent Density Functional Response Theory of Molecular Systems: Theory, Computational Methods, and Functionals. 1996 , 391-439	231
1552	The electronic structure of linearlhickel oxides. 1996 , 4555-4562	13
1551	Atomic and Electronic Properties of Small Hydrogenated Silicon Clusters: Si. 1996 , 452, 51	2
1550	Theory of Reactive Adsorption on Si(100). 1996 , 448, 45	3
1540		
1549	Generalized gradient approximations to density functional theory: comparison with exact results. 1996 , 295-326	30
1549		30
	1996, 295-326 Density functional study of isomerization of fluoro- and chloroformaldehyde radical cations. 1996,	
1548	1996, 295-326 Density functional study of isomerization of fluoro- and chloroformaldehyde radical cations. 1996, 17, 1309-17 A Simple Method of Removing Spin Contamination From Unrestricted Kohn-Sham Density	10
1548 1547	Density functional study of isomerization of fluoro- and chloroformaldehyde radical cations. 1996, 17, 1309-17 A Simple Method of Removing Spin Contamination From Unrestricted Kohn-Sham Density Functional Calculations. 1996, 4, 359-388 Theoretical Study of the Properties of InMH6 and MBH6 (M = B, Al, Ga, and In) EHydrido-Bridged	10
1548 1547 1546	Density functional study of isomerization of fluoro- and chloroformaldehyde radical cations. 1996, 17, 1309-17 A Simple Method of Removing Spin Contamination From Unrestricted Kohn-Sham Density Functional Calculations. 1996, 4, 359-388 Theoretical Study of the Properties of InMH6 and MBH6 (M = B, Al, Ga, and In) EHydrido-Bridged Compounds. 1996, 100, 9308-9313	10

1542	Adsorption complexes on oxides: Density functional model cluster studies. 1996 , 569-619	23
1541	Density Functional Calculations of Heats of Reaction. 1996 , 811-824	2
1540	Chemisorption and decomposition of C1 and C2 hydrocarbons on a Pd(111) surface: a periodic density functional study. 1996 , 101, 1253-1261	7
1539	Computation of the Infrared Spectrum of an Acidic Zeolite Proton Interacting with Acetonitrile. 1996 , 100, 9282-9291	28
1538	Azidotris(trifluoromethyl)germane, (CF(3))(3)GeN(3): Spectroscopic Characterization and Density Functional Computations. 1996 , 35, 4995-4998	8
1537	Density Functional Study of Water and Ammonia Activation by Platinum. 1996 , 197, 203-217	36
1536	Recent Developments in Configuration Interaction and Density Functional Theory Calculations of Radical Hyperfine Structure 1996 , 27, 297-369	77
1535	Endohedral Metallofullerenes: New Spherical Cage Molecules with Interesting Properties. 1996 , 69, 2131-214	2144
1534	Vibrational Analysis of the Radical Anion and Cation of Biphenyl Based on Density Functional Calculations. 1996 , 25, 913-914	13
1533	Ab initio and density functional theory study of structures and energies for dimethoxymethane as a model for the anomeric effect. 1996 , 17, 757-766	51
1532	Ab Initio and NMR Study of Peroxynitrite and Peroxynitrous Acid: Important Biological Oxidants. 1996 , 100, 15087-15095	78
1531	Generalized Gradient Approximation Made Simple. 1996 , 77, 3865-3868	121073
1530	Harmonic Vibrational Frequencies: An Evaluation of HartreeBock, M\[\textstyle \textstyl	3 ⁶¹⁵⁴
1529	Electron Affinities of Substituted p-Benzoquinones from Hybrid HartreeHock/Density-Functional Calculations. 1996 , 100, 10083-10087	72
1528	Substituent Effects on the C-H Bond Dissociation Energy of Toluene. A Density Functional Study. 1996 , 61, 746-750	100
1527	Density Functional Theory of Electronic Structure. 1996 , 100, 12974-12980	2208
1526	Small Clusters of Water Molecules Using Density Functional Theory. 1996 , 100, 8701-8711	176
1525	Rationale for mixing exact exchange with density functional approximations. 1996 , 105, 9982-9985	3907

1524	The monochlorine fluorides (ClFn) and their anions (ClFn-) $n = 1-7$: structures and energetics. 1996 , 89, 607-631	60
1523	Electron-Deficient Palladium Clusters in Zeolites and Their Complexes with Probe CO Molecules. A Density Functional Model Cluster Study. 1996 , 100, 413-417	11
1522	A Density Functional Study of Acidic Hydroxyl Groups in Zeolites and Their Interaction with Carbon Monoxide. 1996 , 100, 1814-1819	28
1521	Solvent Effects. 5. Influence of Cavity Shape, Truncation of Electrostatics, and Electron Correlation on ab Initio Reaction Field Calculations. 1996 , 100, 16098-16104	1127
1520	Density functionals: Where do they come from, why do they work?. 1996 , 1-30	38
1519	A density functional study of molecular adsorption in zeolites. 1996 , 3, 169-194	28
1518	Structures and harmonic force fields of 1,4-naphthoquinone and naphthalene: A density functional study. 1996 , 362, 7-21	21
1517	Prediction of geometrical parameters for silatranes: an ab initio molecular orbital and density functional theory study. 1996 , 362, 199-208	24
1516	An assessment of density functional theory on evaluating activation barriers for small organic gas-phase rearrangement reactions. 1996 , 362, 163-173	25
1515	Performance of Becke's exchange functional fitted for Gaussian basis sets. 1996 , 363, 279-290	6
1514	Computation of structures of phosphorus fluorides with ab initio and density functional methods. 1996 , 365, 47-54	48
1513	On the ⊞f values of tetrahedrane and cubane: density functional theory calculations. 1996 , 364, 183-188	22
1512	Performance of pure and hybrid DFT methods in calculations of ethylene iodonium and methyl iodide. 1996 , 365, 111-117	1
1511	SOS-DFPT-IGLO calculations of 59Co NMR shielding parameters of hexacoordinated diamagnetic Co(III) complexes. 1996 , 365, 125-130	13
1510	Energetics of HF elimination and N?F bond cleavage in some difluoramines and gem-nitro/difluoramines. 1996 , 365, 89-92	8
1509	Study of trichloromethyl radical proton abstraction reaction with ab initio and density functional theory methods. 1996 , 365, 75-80	26
1508	The evaluation of nitrogen containing bond dissociation energies using the ab initio and density functional methods. 1996 , 366, 103-108	79
1507	Phenyl rotation in diphenylether and diphenylmethane calculated with ab initio methods. 1996 , 366, 83-88	31

1506	The study of the isomerization of bicyclo[6.1.0]nona-3,5-diene into bicyclo-[6.1.0]nona-2,4-diene by ab initio and density functional theory (DFT) methods. 1996 , 366, 109-112	18
1505	The density functional theory investigation of the equilibrium structures of OOF, FOOF, OOF2, and FOOOF. 1996 , 366, 97-101	52
1504	A density functional study of CO adsorption on three- and five-coordinate Al in oxide systems. 1996 , 40, 183-188	26
1503	13C Hyperfine interactions in CD3C60 and the distribution of unpaired spin on the C60 cage. 1996 , 11, 325-333	4
1502	On assignment of fundamental vibrational modes of hypophosphite anion and its deuterated analogue. 1996 , 10, 325-329	6
1501	Theoretical and experimental studies of F3SiCO+ and F3SiOC+. 1996 , 153, 161-172	7
1500	Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study. 1996 , 206, 57-61	14
1499	Molecular structure and vibrational IR spectra of the system and its thio and seleno analogs: density functional theory versus conventional ab initio calculations. 1996 , 376, 325-342	31
1498	First principle analysis of the catalytic reaction pathways in the synthesis of vinyl acetate. 1996 , 51, 1691-1699	28
1497	What is the lowest-energy isomer of the C60 dimer?. 1996 , 257, 583-586	69
1496	Theoretical study of the structural evolution of small hydrogenated silicon clusters: Si6Hx. 1996 , 261, 346-352	47
1495	Non-empirical dynamical DFT calculation of the Berry pseudorotation of PF5. 1996 , 262, 74-79	13
1494	Structures and electronic states of endohedral dimetallofullerenes: M2@C80 (M = Sc, Y, La, Ce, Pr, Eu, Gd, Yb and Lu). 1996 , 262, 227-232	57
1493	Structures and molecular surface electrostatic potentials of high-density C, N, H systems. 1996 , 7, 273-280	7
1492	Thermochemical and theoretical study of some methyldiazines. 1996 , 7, 329-336	31
1491	Cooperative effects in water trimers. The performance of density functional approaches. 1996 , 371, 1-10	117
1490	Density functional study of the H3N?Cl2 systemthe importance of Hartree-Fock exchange in density functional methods. 1996 , 371, 11-16	14
1489	Applications of density functional theory approaching chemical accuracy to the study of typical carbon-carbon and carbon-hydrogen bonds. 1996 , 369, 29-37	11

1488	The determinant role of water in the ionic dissociation of HO2. 1996 , 371, 143-152	5
1487	Protonation of the Co?Rh bond in CoRh(ECO)(CO)2(Edppm)2. 1996 , 371, 37-43	3
1486	Theoretical study of the ScCO2 -fOScCO reaction. 1996 , 371, 79-84	15
1485	Acetamidine-Mg+(2S) complexes; the performance of different exchange and correlation functionals. 1996 , 371, 313-324	6
1484	Comparison of density functional calculations of C?NO2, N?NO2 and C?NF2 dissociation energies. 1996 , 388, 51-55	4
1483	A grid-free DFT implementation of non-local functionals and analytical energy derivatives. 1996 , 388, 277-284	11
1482	Structures of oxyfluoroaluminates in molten cryolite-alumina mixtures investigated by DFT-based calculations. 1996 , 368, 67-80	27
1481	Density functional studies of internal rotation: formamide as a prototype of the peptide bond. 1996 , 375, 181-188	2
1480	Density functional theory and ab initio study of bond dissociation energy for peroxonitrous acid and peroxyacetyl nitrate. 1996 , 370, 65-69	45
1479	Computations of 57Fe-NMR Chemical Shifts with the SOS-DFPT Method. 1996 , 79, 742-754	32
1478	An Analysis of the Bonding Properties of Benz[a]azulene by X-Ray, NMR, and Computational Studies. 1996 , 79, 837-854	9
1477	Analyse der verbl□ ffenden ekliptischen Konformation der Methylgruppe eines tricyclischen Orthoamid-Trihydrats. 1996 , 108, 200-202	7
1476	Beziehungen zwischen Struktur und Magnetismus bei zweikernigen d1-d1-Komplexen: Struktur und Magnetochemie von VIV-Zweikernkomplexen mit ferromagnetischen Wechselwirkungen. 1996 , 108, 699-703	8
1475	Komplexe mit Phosphor und Arsen als terminalen Liganden. 1996 , 108, 2637-2641	39
1474	A coupled density functional-molecular mechanics Monte Carlo simulation method: The water molecule in liquid water. 1996 , 17, 19-29	106
1473	The structure of 1-chlorosilatrane: An ab initio molecular orbital and a density functional theory study. 1996 , 17, 767-780	21
1472	Density functional Gaussian-type orbital approach in theoretical study of S2F2 isomerization. 1996 , 17, 835-840	49
1471	Base stacking in cytosine dimer. A comparison of correlated ab initio calculations with three empirical potential models and density functional theory calculations. 1996 , 17, 841-850	134

1470 Models for the description of the H3O+ and OHllons in water. 1996 , 17, 1099-1107	11
1469 Accurate estimation of correlation energies using locally dense basis sets. 1996 , 17, 1431-1443	4
Structure of the optimized effective KohnBham exchange potential and its gradient approximations. 1996 , 57, 17-33	15
On the conjoint gradient correction to the Hartree \mathbf{E} ock kinetic and exchange energy density functionals. 1996 , 57, 3-6	1
1466 Comparison shopping for a gradient-corrected density functional. 1996 , 57, 309-319	235
A study of the performance of numerical basis sets in DFT calculations on sulfur-containing molecules. 1996 , 57, 533-542	34
1464 Static and dynamic density functional investigation of hydrated beryllium dications. 1996 , 57, 655-662	19
DNA base amino groups and their role in molecular interactions: Ab initio and preliminary density functional theory calculations. 1996 , 57, 959-970	179
An ab initio study of the dioxygen binding site of hemocyanin: A comparison between CASSCF, CASPT2, and DFT approaches. 1996 , 58, 109-119	29
On the use of common effective core potentials in density functional calculations. I. Test calculations on transition-metal carbonyls. 1996 , 58, 147-152	32
1460 A density functional study of the electronic spectrum of permanganate. 1996 , 58, 681-687	34
Energetics of reactions involving radical species in solution: Calculation of relative electrode potentials for nitroimidazoles using density functional and continuum methods. 1996 , 59, 135-145	4
1458 Comparative study of DFT methods applied to small titanium/oxygen compounds. 1996 , 59, 427-443	50
Calculation of bond dissociation energies for oxygen containing molecules by ab initio and density functional theory methods. 1996 , 59, 495-501	58
Potential energy surfaces of pseudoaromatic molecules: An MMVB and CASSCF study of pentalene. 1996 , 60, 505-512	18
Stability and structure of rare-gas ionic clusters using density functional methods: A study of helium clusters. 1996 , 60, 593-608	20
The calculation of NMR shielding tensors based on density functional theory and the frozen-core approximation. 1996 , 60, 753-766	136
1453 Parallel electron correlation effect and Fermi hole structure. 1996 , 60, 853-857	

1452	Calculation of intramolecular force fields from second-derivative tensors. 1996 , 60, 1271-1277	164
1451	Reaction energetics of tetrahedrane and other hydrocarbons: Ab initio and density functional treatments. 1996 , 60, 1351-1360	3
1450	On the optimal mixing of the exchange energy and the electron-electron interaction part of the exchange-correlation energy. 1996 , 60, 1375-1384	22
1449	DFT calculations of alternative structures in the allyl-nickel catalyzed polymerization of butadiene. 1996 , 60, 1409-1417	2
1448	Electronic structure and properties of MCO and M5CO carbonyls (M = Fe, Ni, Cu) by density functional methods. 1996 , 60, 1429-1441	4
1447	Condensed-phase effects on the conformational equilibrium of ethylene glycol. 1996 , 60, 1651-1660	6
1446	Effects of relativity on the Ni?CO, Pd?CO, and Pt?CO bonding mechanism: a constrained space orbital variation analysis of density functional results. 1996 , 248, 109-115	31
1445	Ab initio molecular dynamics of retinals. 1996 , 248, 165-172	46
1444	Comparison of convetional and hybrid density functional approaches. Cationic hydrides of first-row transition metals as a case study. 1996 , 249, 290-296	40
1443	Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. Twelve test cases and application to three C2H4O2 isomers. 1996 , 249, 491-495	50
1442	On the performance of density functional methods for describing atomic populations, dipole moments and infrared intensities. 1996 , 250, 393-401	170
1441	Study of prototypical Diels-Alder reactions by a hybrid density functional/Hartree-Fock approach. 1996 , 251, 393-399	30
1440	Vibrational interactions at surfaces: H2O on Si(100). 1996 , 252, 230-235	63
1439	A computational study of the structures of Van der Waals and hydrogen-bonded complexes of ethene and ethyne. 1996 , 254, 135-140	21
1438	The covalently bound N3O2 molecule: Two possible isomers. 1996 , 253, 196-200	9
1437	Theoretical studies of tetrakaidecahedral structures of (H2O)24, (H2O)25 and (H2O)26 clusters. 1996 , 253, 299-304	25
1436	Static second hyperpolarizabilities of nitroxide radical and formaldehyde: evaluation of spatial contributions to by a hyperpolarizability density analysis. 1996 , 254, 158-164	51
1435	Electronic structure and thermodynamic properties of YIrC and YIrC2. 1996 , 254, 274-280	5

1434 On the nature of the cobalt-nitrogen bond in the CON+2 complex. A theoretical study. **1996**, 254, 314-320

1433 On the structure and vibrational frequencies of C24. 1996 , 255, 7-14	41
1432 C28: the smallest stable fullerene?. 1996 , 255, 1-6	35
1431 Hypermetallation is ubiquitous: MX6 molecules (M?C?Pb, X?Li?K). 1996 , 255, 363-366	37
1430 Density functional theory and ab initio study of CH3NC and HNC isomerization. 1996 , 256, 213-2	19 35
Treatment of electronic excitations within the adiabatic approximation of time dependent dens functional theory. 1996 , 256, 454-464	ity 47 ¹¹
Calculation of molecular electrostatic potentials and Fukui functions using density functional methods. 1996 , 256, 400-408	136
1427 Evaluation of transition state properties by density functional theory. 1996 , 256, 595-602	257
Density functional theory study of radical hydrogen abstraction with hydrogen and hydroxyl radicals. 1996 , 256, 603-608	88
1425 Vibrational frequency prediction using density functional theory. 1996 , 256, 391-399	1041
Structure and properties of X2O and XYO (X, Y? Cl, Br) molecules: DFT vs. Blassical b initio calculations. 1996 , 256, 609-615	22
1423 Relative stability of 1C4 and 4C1 chair forms of 毗-glucose: a density functional study. 1996 , 257,	, 49-60 78
On the electronic structure and bonding of the polynuclear aryl derivatives of the group IB meta Cu5(C6H5)5, Ag4(C6H5)4 and Au5(C6H5)5 by density functional theory. 1996 , 257, 41-48	als 25
Theoretical analysis of the triplet excited states of difluorosilylene. A density functional study. 1996 , 257, 61-67	4
1420 The structure of dichromium tetraformate. 1996 , 257, 238-248	38
Lithium- and chlorine-doped biphenyl dimers as models for interchain polarons and bipolarons I density functional study. 1996 , 257, 592-600	13
Density-functional and density-functional reaction field calculations of the molecular properties phenol. 1996 , 258, 436-444	of ₁₈
Theoretical studies of structures and stabilization energies of (H2O)26, (H2O)27 and (H2O)28 pentakaidecahedral clusters. 1996 , 258, 574-580	12

1416	Dimesitylketone O-oxide: verification of an unusually stable carbonyl oxide by NMR chemical shift calculations. 1996 , 260, 43-50	23
1415	The tautomeric equilibrium of benzotriazole: new evidence from the jet-cooled rotational spectrum and first principles calculations. 1996 , 260, 119-124	17
1414	Application of time-dependent density functional response theory to Raman scattering. 1996 , 259, 599-604	53
1413	Ab initio and density functional theory study of the diazene isomerization. 1996 , 261, 13-17	35
1412	Theoretical study of the effective exchange interactions between nitroxides via hydrogen atoms. 1996 , 261, 129-137	14
1411	Ab initio SCF and DFT models of met-car adducts: $Ti8C12(L)n$ (L = Cl, NH3, CO, C6H6; n = 4, 8). 1996 , 260, 577-581	22
1410	First-principles molecular dynamics simulation of water dissociation on TiO2 (110). 1996 , 261, 246-252	146
1409	Molecular electronic structure calculations employing a plane wave basis: A comparison with Gaussian basis calculations. 1996 , 261, 521-526	21
1408	Endohedral dimetallofullerenes Sc2@C84 and La2@C80. Are the metal atoms still inside the fullerence cages?. 1996 , 261, 502-506	99
1407	An ab initio study of VC: a comparison of different levels of theory including density functional methods. 1996 , 262, 87-90	17
1406	Electronic, vibrational and environmental effects on the hyperfine coupling constants of nitroside radicals. H2NO as a case study. 1996 , 262, 201-206	74
1405	Ab Initio ECP/DFT Calculation and Interpretation of Carbon and Oxygen NMR Chemical Shift Tensors in Transition-Metal Carbonyl Complexes. 1996 , 2, 24-30	47
1404	The Effect of Microsolvation on E2 and SN2 Reactions: Theoretical Study of the Model System FI C2H5F + nHF. 1996 , 2, 196-207	70
1403	Zintl Anions as Starting Compounds for the Synthesis of Polynuclear Transition Metal Complexes. 1996 , 2, 238-244	70
1402	NMR Chemical-Shift Anomaly and Bonding in Piano-Stool Carbonyl and Related Complexes Ab Initio ECP/DFT Study. 1996 , 2, 348-358	22
1401	Permethyltitanocene Derivatives with Naked Chalcogen Ligands: Synthesis of [(Cp*2Ti)2(E)] and [Cp*2Ti(Z-E2)] and the Role of the Terminal Chalcogenides [Cp*2Ti(E)] in Their Interconversion (E = Se, Te). 1996 , 2, 1221-1229	8
1400	A Combined Spectroscopic, Photophysical and Theoretical (DFT) Study of the Electronically Excited Inorganometallic Complexes [Ru(E)(E?)(CO)2(iPrDAB)] (E?Cl, Me, SnPh3, PbPh3; E??GePh3, SnR3, PbR3 (R?Me, Ph); iPrDAB=N,N'-discopropyl-1,4-diazar-1,3-butadiene): Evidence of an Exceptionally	48
1399	Long-Lived 3th Excited State for [Ru(SnPh3)2(CO)2(iPrDAB)]. 1996, 2, 1556-1565 Interpretation of 31P-NMR Coordination Shifts for Phosphane Ligands. Ab Initio ECP/DFT Study of Chemical Shift Tensors in M(CO)5L [M = Cr, Mo, W; L = PH3, P(CH3)3, PF3, PCl3]. 1996, 129, 535-544	35

1398	A density-functional study of van der Waals forces: He interaction with a semiconductor surface. 1996 , 97, 215-219	11
1397	Nonclassical furoxans 🖪 computational study. 1996 , 52, 743-752	15
1396	Theoretical study on crown compounds as a building block of the molecule with function II. Density functional approach to analyze Li+ selectivity of aza-12-crown-4 with a functionalized arm. 1996 , 52, 8199-820)8 ⁸
1395	Theoretical study of the structure and vibrational spectrum of 1,3-dithiole-2-thione. 1996 , 52, 279-286	5
1394	Density functional theory study of vibrational spectra part 5. Structure, dipole moment, and vibrational assignment of azulene. 1996 , 52, 1211-1220	8
1393	Computational materials design and processing: perspectives for atomistic approaches. 1996 , 37, 72-82	11
1392	Matrix and ab initio infrared spectra of germanium carbonyls. 1996 , 10, 139-146	14
1391	Theoretical evidence for reassignment of two fundamental vibrational modes of tetrafluorooxirane-16O and 🛮 8O. 1996 , 11, 159-162	
1390	Density functional theory study of vibrational spectra. 4. Comparison of experimental and calculated frequencies of all-trans-1,3,5,7-octatetraene IThe end of normal coordinate analysis?. 1996 , 12, 73-79	15
1389	Density functional theory study of vibrational spectra. 3. Assignment of fundamental vibrational modes of quadricyclane. 1996 , 12, 65-71	9
1388	Density functional theory study of vibrational spectra. 1. Performance of several density functional methods in predicting vibrational frequencies. 1996 , 12, 53-63	30
1387	Infrared spectra of thiouracils: experimental matrix isolation and ab initio Hartree-Fock, post-Hartree-Fock and density functional theory studies. 1996 , 13, 23-40	38
1386	Comparison of extended-H [□] ckel and ab initio calculations in predicting the hapticity of benzene in silica-supported NiI complexes. 1996 , 107, 137-143	4
1385	Theoretical study of the structures and racemization barriers of [n]helicenes (n = 3B, 8). 1996 , 204, 411-417	114
1384	Molecular and electrostatic properties of the N-methylated nucleic acid bases by density functional theory. 1996 , 204, 301-311	39
1383	Structure and anisotropy of ionic argon clusters using density functional models. 1996 , 208, 25-34	10
1382	Cationic, structural, and compositional effects on the surface structure of zeolitic aluminosilicate catalysts. 1996 , 208, 331-340	14
1381	Density functional based structure optimization for molecules containing heavy elements: analytical energy gradients for the Douglas-Kroll-Hess scalar relativistic approach to the LCGTO-DF method. 1996 , 210, 413-425	121

1380	Ab initio MP2 and DFT calculations of geometry and solution tautomerism of purine and some purine derivatives. 1996 , 211, 147-161	86
1379	Studies of the electron density in the highest occupied molecular orbitals of PH3, PF3 and P(CH3)3 by electron momentum spectroscopy and Hartree-Fock, MRSD-CI and DFT calculations. 1996 , 207, 173-192	28
1378	Ab initio calculation of ethylene insertion in zirconocene catalyst systems: A comparative study between bridged and unbridged complexes. 1996 , 37, 1663-1667	25
1377	Relationships between dissociation energies and electrostatic potentials of C?NO2 bonds: applications to impact sensitivities. 1996 , 376, 419-424	166
1376	Density functional studies of internal rotation: formamide as a prototype of the peptide bond. 1996 , 375, 181-188	8
1375	Experimental and theoretical studies of the single- and double-CO loss photoproducts of [CpCo(CO)]2(ECH2). 1996 , 252, 405-412	1
1374	Structures and energy barriers in small hydrocarbon molecules 🗈 density functional study. 1996 , 252, 1-8	17
1373	Investigations using the Becke95 correlation functional. 1996 , 252, 19-22	16
1372	Density functional calculation of core-electron binding energies of transition metal carbonyl and nitrosyl complexes. 1996 , 262, 733-736	12
1371	Density functional computations for inner-shell excitation spectroscopy. 1996 , 262, 729-732	37
1370	Potential energy surfaces from Kohn-Sham potentials. 1996 , 262, 533-538	4
1369	Ab initio and density functional study of the Jahn-Teller distortion in the silane radical cation. 1996 , 262, 782-788	13
1368	A CASSCF study of the S0 and S1 states of phenol. 1996 , 263, 126-132	33
1367	Solvent effects on the conformational behavior of model peptides. A comparison between different continuum models. 1996 , 263, 113-118	26
1366	Density functional theory description of excited-state intramolecular proton transfer. 1996 , 263, 414-422	26
1365	High-level ab initio calculations on the 1,2-dithioglyoxal/1,2-dithiete isomerism. 1996 , 263, 407-413	17
1364	Titanium-silicalite catalyzed epoxidation of ethylene with hydrogen peroxide. A theoretical study. 1996 , 32, 107-114	57
1363	Density functional theory study of vibrational spectra. 8. Assignment of fundamental vibrational modes of 9,10-anthraquinone and 9,10-anthraquinone-d8. 1996 , 52, 1803-1814	19

1362	Diyttrium: evidence for a 5Dlground state from pulsed-field ionizationzero electron kinetic energy photoelectron spectroscopy and density functional calculations. 1996 , 159, 65-74	20
1361	Mass spectrometry and density functional studies of neutral and anionic tin clusters. 1996 , 157-158, 329-343	23
1360	Orbital momentum profiles and binding energy spectra for the complete valence shell of molecular fluorine. 1996 , 212, 269-300	33
1359	Influence of rotation between agostic structures on ethene interaction with a zirconocene polymerization site. 1996 , 519, 277-280	30
1358	Matrix isolation and density functional studies of novel transition metal complexes. NO + Fe, Co, Ni, Cu, and Zn in argon matrices. 1996 , 384, 101-114	32
1357	Ab initio calculations of the NMR chemical shift. 1996 , 29, 229-278	209
1356	Dissociation and chain reaction in the pyrolysis of pyraine. 1996 , 26, 651-658	5
1355	Synthese, Kristallstruktur, Elektronenstruktur, spektroskopische und magnetische Eigenschaften von [VOCl2{P(SiMe3)3}2]: Ein Phosphankomplex mit fehlgeordneter VOCl2-Einheit. 1996 , 622, 1756-1764	6
1354	Adatom migrations and nucleations on reconstructed (001) surfaces I. Si. 1996 , 107, 18-24	4
1353	Density functional theory calculations of pericyclic reaction transition structures. 1996 , 1-24	70
1352	Electron Densities of Several Small Molecules As Calculated from Density Functional Theory. 1996 , 100, 6317-6324	33
1351	Structure, Stability, and Bonding of Transition-Metal B oryl Complexes. A Molecular Orbital Study. 1996 , 100, 6509-6517	61
1350	Theoretical Studies of Direct Exchange Couplings Between Transition Metal Ions I. Naked Binuclear Chromium(II) and Molybdenum (II) Systems. 1996 , 286, 193-200	4
1349	Quantum Chemical Study of CO and NO Bonding to Pd2, Cu2, and PdCu. 1996 , 100, 13506-13513	51
1348	Synthesis of N-Confused Porphyrin Analogues by beta-Azafulvenone Tetramerization. 1996 , 61, 8125-8131	13
1347	The Douglas-Kroll-Hess Approach to Relativistic Density Functional Theory: Methodological Aspects and Applications to Metal Complexes and Clusters. 1996 , 497-566	77
1346	Ionization of Bases in Water: Structure and Stability of the NH4+ ⁴⁴⁴ OH- Ionic Forms in Ammonia Water Clusters. 1996 , 100, 7398-7404	35
1345	Ab initiomolecular dynamics simulation of liquids and solutions. 1996 , 8, 9405-9409	23

1344	Density Functional Theory Study of Molecular Structures and Vibrational Spectra of 3,4- and 2,3-Pyridyne. 1996 , 100, 3430-3434	45
1343	Density Functional Theory. 1996 , 1-35	9
1342	Ligand Substitution: An Assessment of the Reliability of ab Initio Calculations. 1996 , 100, 18363-18370	21
1341	Structure and Vibrations of Small Carbon Clusters from Coupled-Cluster Calculations. 1996 , 100, 6047-6056	145
1340	Generalized gradient correction for exchange: Deduction from the oscillator model. <i>Physical Review A</i> , 1996 , 53, 3143-3150	8
1339	Theoretical study of the water pentamer. 1996 , 105, 6957-6971	114
1338	Ab initio calculations of the cohesive, elastic, and dynamical properties of CoSi2 by pseudopotential and all-electron techniques. 1996 , 54, 1729-1734	97
1337	Dissociative chemisorption of H2 on Cu(100): A four-dimensional study of the effect of parallel translational motion on the reaction dynamics. 1996 , 105, 5979-5998	37
1336	Kohn-Sham calculations with self-interaction-corrected local-spin-density exchange-correlation energy functional for atomic systems. <i>Physical Review A</i> , 1996 , 54, 3939-3947	71
1335	Generalized gradient approximation for the relativistic exchange-only energy functional. <i>Physical Review A</i> , 1996 , 53, 1367-1374	105
1334	Electronic structure of small copper oxide clusters: From Cu2O to Cu2O4. 1996 , 53, 8028-8031	97
1333	Simulation of nondynamical correlation in density functional calculations by the optimized fractional orbital occupation approach: Application to the potential energy surfaces of O3 and SO2. 1996 , 105, 4641-4648	68
1332	An interpolated unrestricted HartreeBock potential energy surface for the OH+H2-H2O+H reaction. 1996 , 104, 4600-4610	63
1331	Exploring chromium (VI) dioxodihalides chemistry: Is density functional theory the most suitable tool?. 1996 , 104, 9499-9510	27
1330	Comparison of density functional and coupled cluster methods in the study of metalligand systems: ScliO2 and CuNO2. 1996 , 105, 9966-9971	43
1329	Improved radial grids for quadrature in molecular density-functional calculations. 1996 , 104, 9848-9858	107
1328	Sum-over-states density functional perturbation theory: Prediction of reliable 13C, 15N, and 17O nuclear magnetic resonance chemical shifts. 1996 , 105, 8995-9006	60
1327	Structure and electronic properties of quinizarin chemisorbed on alumina. 1996 , 104, 8143-8150	17

1326	A KohnBham study of CH4, C6H6, and O3 using functionals incorporating exact exchange. 1996 , 104, 4166-4172	17
1325	Accuracy of approximate kinetic energy functionals in the model of KohnBham equations with constrained electron density: The FH???NCH complex as a test case. 1996 , 105, 9182-9190	115
1324	Ground State Properties of Hg2. 1. A Pseudopotential Configuration Interaction Study. 1996 , 100, 6147-6151	70
1323	Generalized-gradient functionals in adaptive curvilinear coordinates. 1996 , 54, 1568-1574	25
1322	An investigation of hydrogen transfer in water clusters. 1996 , 104, 5555-5557	20
1321	Excited state properties of Cr3+ in Cs2NaYCl6 and Cs2NaYBr6: A density functional study. 1996 , 104, 7624-7632	33
1320	NaxAu and CsxAu bimetal clusters: Finite size analogs of sodiumgold and cesiumgold compounds. 1996 , 105, 5574-5585	64
1319	Generalized gradient theory for silica phase transitions. 1996 , 76, 660-663	271
1318	Charge Localization and Dynamics in Rhodopsin. 1996 , 77, 4474-4477	44
1317	Adsorption of water and methanol on zeolite Bro/nsted acid sites: An ab initio, embedded cluster study including electron correlation. 1996 , 105, 3770-3776	67
1316	Laser-induced desorption of NO from NiO(100): Ab initio calculations of potential surfaces for intermediate excited states. 1996 , 104, 10030-10040	68
1315	An investigation of the quantum chemical description of the ethylenic double bond in reactions. I. The electrophilic addition of hydrochloric acid to ethylene. 1996 , 105, 6910-6920	6
1314	An analytical six-dimensional potential energy surface for dissociation of molecular hydrogen on Cu(100). 1996 , 104, 7344-7358	106
1313	Vibrational Spectra of N,N-Dimethylaniline and Its Radical Cation. An Interpretation Based on Quantum Chemical Calculations. 1996 , 100, 9678-9688	60
1312	Evaluating the accuracy of density functional methods for ClOO. 1996 , 104, 5345-5346	12
1311	Chlorine on Si(001)-(2 x 1): Bridge versus Terminal Bonding. 1996 , 77, 881-884	21
1310	Exchange-correlation potentials. 1996 , 105, 9200-9213	99
1309	Density functional theory study of some structural and energetic properties of small lithium clusters. 1996 , 105, 9933-9947	80

1308	Ab initio study of the adducts of carbon monoxide with alkaline cations. 1996 , 105, 4129-4139	102
1307	Proton transfer in the ground and lowest excited states of malonaldehyde: A comparative density functional and post-Hartree E ock study. 1996 , 105, 11007-11019	201
1306	Structures, thermochemistry, and electron affinities of the PFn and PFB series, n=1 B . 1996 , 104, 3676-3683	73
1305	Some reasons not to use spin projected density functional theory. 1996 , 105, 6574-6577	173
1304	Isomers of SO3: Infrared absorption of OSOO in solid argon. 1996 , 104, 5745-5753	38
1303	Investigation of the reliability of density functional methods: Reaction and activation energies for SiBi bond cleavage and H2 elimination from silanes. 1996 , 104, 148-158	107
1302	Acrylonitrile on Cu(100): A density functional theoretical study of adsorption and electrochemical grafting. 1996 , 105, 3278-3289	28
1301	Molecular exchange-correlation KohnBham potential and energy density from ab initio first- and second-order density matrices: Examples for XH (X=Li, B, F). 1996 , 104, 8535-8545	68
1300	Microwave spectrum, large-amplitude motions, and ab initio calculations for N2O5. 1996 , 105, 7249-7262	11
1299	Straightforward gradient approximation for the exchange energy of s-p bonded solids. 1996 , 54, 17392-17	401 11
1298	Experimental and Theoretical Study of the Rotation of Si Ad-dimers on the Si(100) Surface. 1996 , 77, 2518-2521	97
1297	Effect of molecular dissociation on the exchange-correlation Kohn-Sham potential. <i>Physical Review A</i> , 1996 , 54, 1957-1972	94
1296	IR and Raman Spectra, Conformational Flexibility, and Scaled Quantum Mechanical Force Fields of Sodium Dimethyl Phosphate and Dimethyl Phosphate Anion 1996 , 100, 1559-1568	66
1295	Relevance of relativistic exchange-correlation functionals and of finite nuclei in molecular density-functional calculations. <i>Physical Review A</i> , 1996 , 54, 4775-4782	5 84
1294	Competition between vibrational excitation and dissociation in collisions of H2 with Cu(100). 1996 , 53, 10397-10401	49
1293	Supported nickel and copper clusters on MgO(100): A first-principles calculation on the metal/oxide interface. 1996 , 104, 7329-7337	151
1292	Isomers of SO2: Infrared absorption of SOO in solid argon. 1996 , 105, 9454-9460	37
1291	Interaction of Water with Br listed Acidic Sites of Zeolite Catalysts. Ab Initio Study of 1:1 and 2:1 Surface Complexes. 1996 , 100, 6199-6211	152

1290	Anisotropic a-C:H from compression of polyacetylene. 1996 , 76, 2081-2084	31
1289	Fourier transform infrared and theoretical isotopic study of the $\Delta(\overline{u})$ and $\overline{B}(\overline{u})$ modes of linear C7. 1996 , 105, 5313-5320	35
1288	Simple spin correction of unrestricted density-functional calculation. <i>Physical Review A</i> , 1996 , 53, 3946-3 2 52	88
1287	Hydrogen adsorption on the (100) surfaces of rhodium and palladium: the influence of non-local exchange - correlation interactions. 1996 , 8, 7659-7675	52
1286	Quantum Chemical Study of the Properties of Molecular Hydrogen Complexes of Osmium(II): A Comparison of Density Functional and Conventional ab Initio Methods. 1996 , 100, 6023-6031	34
1285	Energetics and Dynamics for NO and CO Dissociation on Cu(100) and Cu(111). 1996, 100, 2279-2289	57
1284	Density Functional Theory Studies on Sulfur N itrogen Species. 1996 , 100, 17485-17489	16
1283	Density Functional Investigation of Methoxy-Substituted p-Benzoquinones: Conformational Analysis and Harmonic Force Fields of 2-Methoxy- and 2,3-Dimethoxy-1,4-benzoquinone. 1996 , 100, 14549-14	5 33
1282	Calculations of Isotropic Hyperfine Coupling Constants of Organic Radicals. An Evaluation of Semiempirical, Hartreeflock, and Density Functional Methods. 1996 , 100, 18371-18379	80
1281	Chapter 152 Electronic structure calculations for molecules containing lanthanide atoms. 1996 , 22, 607-729	33
1280	A Theoretical Study on the Mechanism of the Superacid-Catalyzed Unimolecular Isomerization of n-Alkanes and n-Alkenes. Comparison between ab Initio and Density Functional Results. 1996 , 100, 16514-165	2 ² 1 ³
1279	Theoretical Study of Effective Exchange Integrals for Ferromagnetic Phenylenevinylene Polymers with Nitroxddes. Possibilities of Organic Ferro-or Ferri-Magnetic Solids. 1996 , 279, 19-28	10
1278	Solvation Free Energy Calculations Using a Continuum Dielectric Model for the Solvent and Gradient-Corrected Density Functional Theory for the Solute. 1996 , 100, 1515-1523	40
1277	The high-pressure phase transitions of silicon and gallium nitride: a comparative study of Hartree - Fock and density functional calculations. 1996 , 8, 3993-4000	34
1276	Ammonium Nitrate Cluster Ions. 1996 , 100, 5281-5285	11
1275	Electron Affinity of Hydrogen Peroxide and the [H2,O2] Potential Energy Surface. A Comparative DFT and ab Initio Study. 1996 , 100, 100-110	56
1274	Validation of Hybrid Density Functional/Hartreeflock Approaches for the Study of Homogeneous Catalysis. 1996 , 100, 2094-2099	32
1273	Negative Ion Thermochemistry: The Sulfur Fluorides SFn/SFn- (n = 111). 1996 , 100, 6061-6068	96

1272	Formamide 1996, 100, 3965-3973	23
1271	Reference-State Density Functional Theory. 1996 , 100, 6104-6106	9
1270	Structure and Dynamics of the Cr(CO)3 Complexes of Triquinacene and Dimethylenecyclobutene by HartreeEock and Density Functional Methods. 1996 , 100, 6111-6115	8
1269	Toward Stable Silylenes. 1996 , 100, 6262-6265	24
1268	Photochemistry of Deuterated Acetylketenes: Matrix Isolation Infrared Spectroscopic and ab Initio Studies. 1996 , 100, 3917-3922	13
1267	Structural Investigations of trans-Rh(PY3)2(CO)X ($X = F$, Cl, NCO; $Y = H$, Me, Ph) Using Density Functional Theory and X-ray Analysis. 1996 , 100, 11250-11254	16
1266	Electron Diffraction and Vibrational Spectra of Difluorodioxirane, CF2O2. 1996 , 100, 3983-3988	16
1265	A Cycloaddition Model for Fullerene Formation. 1996 , 100, 6492-6498	58
1264	Laser-Evaporated Aluminum Atom Reactions with Halogen Molecules. Infrared Spectra of AlXn (X = F, Cl, Br, I; n = 1B) in Solid Argon. 1996 , 100, 7317-7325	21
1263	Ab Initio Studies on the Structure of Silyl Isocyanate in the Gas Phase, in Solution, and in the Crystalline State. 1996 , 100, 9619-9623	4
1263 1262		99
	Crystalline State. 1996 , 100, 9619-9623 Trimethylenemethane. Comparison of Multiconfiguration Self-Consistent Field and Density	
1262	Crystalline State. 1996, 100, 9619-9623 Trimethylenemethane. Comparison of Multiconfiguration Self-Consistent Field and Density Functional Methods for a Non-Kekul 'Hydrocarbon. 1996, 100, 9664-9670 Reactions of Nitric Oxide with Sulfur Species. Infrared Spectra and Density Functional Theory	99
1262	Crystalline State. 1996, 100, 9619-9623 Trimethylenemethane. Comparison of Multiconfiguration Self-Consistent Field and Density Functional Methods for a Non-Kekul 'Hydrocarbon. 1996, 100, 9664-9670 Reactions of Nitric Oxide with Sulfur Species. Infrared Spectra and Density Functional Theory Calculations for SNO, SNO+, SSNO, and SNNO in Solid Argon. 1996, 100, 8273-8279	99
1262 1261 1260	Crystalline State. 1996, 100, 9619-9623 Trimethylenemethane. Comparison of Multiconfiguration Self-Consistent Field and Density Functional Methods for a Non-Kekul 'Hydrocarbon. 1996, 100, 9664-9670 Reactions of Nitric Oxide with Sulfur Species. Infrared Spectra and Density Functional Theory Calculations for SNO, SNO+, SSNO, and SNNO in Solid Argon. 1996, 100, 8273-8279 Theoretical Study of the Structure and Vibrational Spectrum of N,N-Dimethylformamide. 1996, 100, 16822-1 Characterization of New Cumulenes C2NX2 (X = O or S): Tandem Mass Spectrometry and ab Initio	99 30 683 3
1262 1261 1260 1259	Trimethylenemethane. Comparison of Multiconfiguration Self-Consistent Field and Density Functional Methods for a Non-Kekul□'Hydrocarbon. 1996, 100, 9664-9670 Reactions of Nitric Oxide with Sulfur Species. Infrared Spectra and Density Functional Theory Calculations for SNO, SNO+, SSNO, and SNNO in Solid Argon. 1996, 100, 8273-8279 Theoretical Study of the Structure and Vibrational Spectrum of N,N-Dimethylformamide. 1996, 100, 16822-1 Characterization of New Cumulenes C2NX2 (X = O or S): Tandem Mass Spectrometry and ab Initio Studies. 1996, 100, 10536-10541 Metal-to-Ligand Charge Transfer (MLCT) Photochemistry of fac-Mn(Cl)(CO)3(H-DAB): A Density	99 30 68387
1262 1261 1260 1259	Trimethylenemethane. Comparison of Multiconfiguration Self-Consistent Field and Density Functional Methods for a Non-Kekul□'Hydrocarbon. 1996, 100, 9664-9670 Reactions of Nitric Oxide with Sulfur Species. Infrared Spectra and Density Functional Theory Calculations for SNO, SNO+, SSNO, and SNNO in Solid Argon. 1996, 100, 8273-8279 Theoretical Study of the Structure and Vibrational Spectrum of N,N-Dimethylformamide. 1996, 100, 16822-1 Characterization of New Cumulenes C2NX2 (X = O or S): Tandem Mass Spectrometry and ab Initio Studies. 1996, 100, 10536-10541 Metal-to-Ligand Charge Transfer (MLCT) Photochemistry of fac-Mn(Cl)(CO)3(H-DAB): A Density Functional Study. 1996, 100, 15346-15357 Combining Multiconfigurational Wave Functions with Density Functional Estimates of Dynamic	99 30 68387 12 28

1254	Reactions of Laser-Ablated Iron Atoms with N2O, NO, and O2in Condensing Nitrogen. Infrared Spectra and Density Functional Calculations of Ternary Iron Nitride Oxide Molecules. 1996 , 100, 11235-11241	33
1253	Analysis of X-ray Photoelectron Spectra of Eight Polymers by deMon Density-Functional Calculations Using the Model Oligomers. 1996 , 100, 19455-19460	49
1252	Density Functional Studies of Vibrational Properties of HCN, H2O, CH2O, CH4, and C2H4. 1996 , 100, 16530-16537	21
1251	Two, Three, and Four Water Chain Models for the Nucleophilic Addition Step in the Wacker Process. 1996 , 100, 14672-14680	53
1250	Calculated Gas-Phase Acidities Using Density Functional Theory: Is It Reliable?. 1996 , 100, 17465-17471	89
1249	Platinum-Modified Nucleobase Pairs in the Solid State: A Theoretical Study. 1996 , 100, 17797-17800	50
1248	Ab Initio Study of Pernitric Acid: Comparison with Experimental Spectra. 1996 , 100, 15731-15734	16
1247	Density Functional Investigation of Structures and Harmonic Force Fields of Methyl-Substituted p-Benzoquinones. 1996 , 100, 20148-20155	7
1246	Functional Groups in Quantum Chemistry. 1996 , 163-222	51
1245	Embedded-cluster calculations for transition-metal impurities in. 1996 , 8, 1687-1704	7
1244	Computing Transition State Structures with Density Functional Theory Methods. 1996 , 709-741	41
1243	Molecular Structures and Harmonic Vibrational Frequencies of M2O3 (M = Ga, In, Tl). 1996 , 100, 18078-18082	11
1242	Alternative density functional theory for atoms and molecules. 1996 , 29, L173-L179	15
1241	Density functional theory, the exchange hole, and the molecular bond. 1996 , 207-238	10
1240	Charge-Transfer Complexes: Stringent Tests for Widely Used Density Functionals. 1996 , 100, 12265-12276	176
1239	Concerning the applicability of density functional methods to atomic and molecular negative ions. 1996 , 105, 862-864	186
1238	Calculation of the atomic kinetic energy from a density functional virial relationship. 1997 , 30, 2039-2045	5
1237	A study of sulphur-containing molecules using Hartree-Fock, MP2 and DFT (hybrid) methodologies. 1997 , 92, 339-352	37

1236	Proposal of a Micro-Fabrication Process for Al Nanostructures. 1997 , 36, 4049-4052	8
1235	Comparative application of different approaches for band structure calculations on polyparaphenylene in the Pariser-Parr-Pople model: II. MI ler-Plesset and coupled cluster methods. 1997 , 56, 506-526	2
1234	Density-functional exchange-correlation potential and orbital eigenvalues for the Ne-Atom. 1997 , 55, 459-463	1
1233	Formation of localized hole states in complex oxides: I. Hole states in. 1997 , 9, 6359-6370	6
1232	Numerical application of the coupled-cluster theory with localized orbitals to polymers: III. Bond alternation intrans-polyacetylene. 1997 , 9, 2043-2063	9
1231	Ab initio study of the CoSi2 (110) surface. 1997 , 55, 10805-10813	12
1230	Relativistic calculations on the adsorption of CO on the (111) surfaces of Ni, Pd, and Pt within the zeroth-order regular approximation. 1997 , 56, 13556-13562	139
1229	The effects of electron correlation on the degree of bond alternation and electronic structure of oligomers of polyacetylene. 1997 , 107, 6712-6721	136
1228	Six-dimensional quantum dynamics of dissociative chemisorption of H2 on Cu(100). 1997 , 107, 3309-3323	68
1227	The gas-phase infrared spectra of anthracene-h10 and anthracene-d10. 1997 , 106, 9004-9012	35
1226	On-Ball Doping of Fullerenes: The Electronic Structure of C59N Dimers from Experiment and Theory. 1997 , 78, 4249-4252	72
1225	Xe129 adsorbed in AlPO4-11 molecular sieve: Molecular dynamics simulation of adsorbate dynamics and NMR chemical shift. 1997 , 107, 6470-6478	19
1224	Theoretical analysis of the vibronic structure of the zero-kinetic-energy photoelectron spectra from single vibronic levels of the S1-state manifold of naphthalene. 1997 , 107, 4827-4843	19
1223	Novel Structures for the Excess Electron State of the Water Hexamer and the Interaction Forces Governing the Structures. 1997 , 79, 2038-2041	93
1222	Theoretical investigation of structural and thermodynamic properties of lanthanum carbides LaCn (n=2B). 1997 , 106, 158-164	48
1221	Density functional study of polypropylene and its submolecules. 1997 , 106, 8545-8551	18
1220	A density functional theory estimation of the heat of formation for FOOCl. 1997 , 106, 2555-2556	38
1219	CH5+: The story goes on. An explicitly correlated coupled-cluster study. 1997 , 106, 1863-1869	95

1218	Fourier transform infrared observation of the vibrational spectrum of the linear SiCCH radical in Ar at 10 K. 1997 , 106, 6222-6230	10
1217	Solid-State Polymerization of Acetylene under Pressure: Ab Initio Simulation. 1997 , 78, 2008-2011	62
1216	Six-Dimensional Quantum Dynamics of Dissociative Chemisorption of (v=0, j=0) H2 on Cu(100). 1997 , 78, 3583-3586	109
1215	High-Temperature Magnetic Ordering in a New Organic Magnet. 1997 , 79, 2336-2339	129
1214	Improving harmonic vibrational frequencies calculations in density functional theory. 1997 , 106, 10175-10183	74
1213	A matrix isolation FTIR and quasirelativistic density functional theory investigation of the reaction products of laser-ablated uranium atoms with NO, NO2 and N2O. 1997 , 106, 5894-5903	36
1212	Theoretical study of the water tetramer. 1997 , 106, 7193-7207	78
1211	Cohesive properties of alkali halides. 1997 , 56, 10121-10127	37
1210	Density-functional theory with optimized effective potential and self-interaction correction for ground states and autoionizing resonances. <i>Physical Review A</i> , 1997 , 55, 3406-3416	147
1209	The electron affinities of the perfluorocarbons C2Fn, n=1B. 1997 , 107, 8536-8544	35
1208	Laser spectroscopy and density functional calculations on niobium monocarbide. 1997 , 107, 307-318	50
1207	Local correlation energies of two-electron atoms and model systems. <i>Physical Review A</i> , 1997 , 56, 290-2 26 6	59
1206	Numerical application of the coupled cluster theory with localized orbitals to polymers. IV. Band structure corrections in model systems and polyacetylene. 1997 , 106, 10248-10264	49
1205	Excited-state energies and distortions of d0 transition metal tetraoxo complexes: A density functional study. 1997 , 107, 4606-4617	47
1204	DielsAlder reactions: An assessment of quantum chemical procedures. 1997, 106, 8727-8732	43
1203	Equilibrium yield for helium incorporation into buckminsterfullerene: Quantum-chemical evaluation. 1997 , 106, 1796-1799	56
1202	A density functional especially designed for hydrogen-only systems. 1997 , 107, 10643-10651	48
1201	The dynamics of proton transfer in H5O2+. 1997 , 107, 8461-8468	75

1200	Solid Molecular Hydrogen: The Broken Symmetry Phase. 1997 , 78, 2783-2786		77
1199	Critical assessment of the self-interaction-corrected[bcal-density-functional method and its algorithmic implementation. <i>Physical Review A</i> , 1997 , 55, 1765-1771	2.6	146
1198	Natural variables for density functionals. <i>Physical Review A</i> , 1997 , 55, 4589-4592	2.6	8
1197	High Accuracy Molecular Heats of Formation and Reaction Barriers: Essential Role of Electron Correlation. 1997 , 79, 4353-4356		49
1196	A first-principles simulation of the semiconductor/water interface. 1997 , 106, 2811-2818		21
1195	Density Functional Theory: A Useful Tool for the Study of Free Radicals. 1997 , 293-309		13
1194	The calculation of 17O chemical shielding in transition metal oxo complexes. I. Comparison of DFT and ab initio approaches, and mechanisms of relativity-induced shielding. 1997 , 106, 9201-9212		68
1193	Phonon Softening and Elastic Instabilities in the Cubic-to-Orthorhombic Structural Transition of CsH. 1997 , 78, 4958-4961		10
1192	Combined ab initio and density functional study on polaron to bipolaron transitions in oligophenyls and oligothiophenes. 1997 , 107, 3021-3031		49
1191	Two Dimensional Ice Adsorbed on Mica Surface. 1997 , 78, 2855-2858		254
	Two Dimensional Ice Adsorbed on Mica Surface. 1997 , 78, 2855-2858 Ab initio molecular dynamics simulation of liquid hydrogen fluoride. 1997 , 106, 4658-4664		² 54
	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. 1997 , 106, 4658-4664		
1190	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. 1997, 106, 4658-4664 A study of Hel photoelectron spectroscopy on the electronic structure of the nitrate free radical		87
1190 1189	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. 1997, 106, 4658-4664 A study of Hel photoelectron spectroscopy on the electronic structure of the nitrate free radical NO3. 1997, 106, 3003-3006 Energetics and structures of neutral and charged Sins(n?10) and sodium-doped Sin Na clusters.		87
1190 1189 1188	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. 1997, 106, 4658-4664 A study of Hel photoelectron spectroscopy on the electronic structure of the nitrate free radical NO3. 1997, 106, 3003-3006 Energetics and structures of neutral and charged Sins(n?10) and sodium-doped Sin Na clusters. 1997, 55, 7935-7944 Density functional calculations of molecular g-tensors in the zero-order regular approximation for		87 41 65
1190 1189 1188 1187	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. 1997, 106, 4658-4664 A study of Hel photoelectron spectroscopy on the electronic structure of the nitrate free radical NO3. 1997, 106, 3003-3006 Energetics and structures of neutral and charged Sins(n?10) and sodium-doped Sin Na clusters. 1997, 55, 7935-7944 Density functional calculations of molecular g-tensors in the zero-order regular approximation for relativistic effects. 1997, 107, 2488-2498 High-pressure phases of SiO2 using local-density and generalized-gradient approximations. 1997,		87 41 65 268
1190 1189 1188 1187 1186	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. 1997, 106, 4658-4664 A study of Hel photoelectron spectroscopy on the electronic structure of the nitrate free radical NO3. 1997, 106, 3003-3006 Energetics and structures of neutral and charged Sins(n?10) and sodium-doped Sin Na clusters. 1997, 55, 7935-7944 Density functional calculations of molecular g-tensors in the zero-order regular approximation for relativistic effects. 1997, 107, 2488-2498 High-pressure phases of SiO2 using local-density and generalized-gradient approximations. 1997, 55, 11003-11005 Predicting electron affinities with density functional theory: Some positive results for negative		87 41 65 268

1182	Density functional theory investigation of hyperfine coupling constants in peroxyl radicals. 1997 , 106, 7738-7748		39
1181	An ab initio study of CrC: A comparison of different levels of theory including density functional methods. 1997 , 106, 1491-1494		23
1180	Electronic-structure-based molecular-dynamics method for large biological systems: Application to the 10 basepair poly(dG)?poly(dC) DNA double helix. 1997 , 55, 6880-6887		66
1179	Ab initio calculations on small lithium clusters. <i>Physical Review A</i> , 1997 , 56, 617-625	2.6	41
1178	Exact hydrogenic density functionals. <i>Physical Review A</i> , 1997 , 56, 2726-2730	2.6	25
1177	Coupled cluster calculations for HC9NH+, a cation of interest to astrochemistry. 1997 , 107, 9702-9703		5
1176	Ab initio molecular dynamics study of polyfluoride anions. 1997 , 107, 8012-8019		27
1175	Simplified generalized-gradient approximation and anharmonicity: Benchmark calculations on molecules. 1997 , 55, 7454-7459		117
1174	Geometric and electronic properties of small vanadium clusters: A density functional study. 1997 , 107, 10620-10625		63
1173	Density functional study of mononitrosyls of first-row transition-metal atoms. 1997 , 106, 8778-8787		43
1172	Direct subsurface absorption of hydrogen on Pd(111): Quantum mechanical calculations on a new two-dimensional potential energy surface. 1997 , 106, 9286-9296		39
1171	Laser spectroscopy of the □ ② -X 2 = transition of ytterbium monoacetylide. 1997 , 107, 2720-2727		14
1170	Hartree-Fock energy-density functionals generated by local-scaling transformations: Applications to first-row atoms. 1997 , 107, 6722-6731		13
1169	Density functional results for isotropic and anisotropic multipole polarizabilities and C6, C7, and C8 Van der Waals dispersion coefficients for molecules. 1997 , 106, 5091-5101		100
1168	The low-lying electronic states of CrF and CrCl: Analysis of the A $6H$ -K $6H$ system of CrCl. 1997 , 106, 6231-6239		29
1167	Ab initio molecular dynamics study of solid- to liquidlike transitions in Li9+, Li10, and Li11+ clusters. 1997 , 107, 6321-6334		31
1166	Transition State Structure for the Hydrolysis of NAD Catalyzed by Diphtheria Toxin. 1997 , 119, 12079-12	2088	80
1165	Electron Affinity of SF6. 1997 , 28, 189-203		8

1164	Magnetism of free and supported vanadium clusters. 1997 , 9, 10739-10748	18
1163	Doping high Tc superconductors with oxygen and metallic atoms: A molecular dynamics study. 1997 , 12, 2901-2906	
1162	High Pressure Studies of Mantle Minerals by Ab initio Variable Cell Shape Molecular Dynamics. 1997 , 39-61	1
1161	Energetics of the [N]Phenylenes with Application to Helical Conformers. 1997 , 101, 5596-5599	37
1160	Paramagnetic States of Four Ironflour Sulfur Clusters. 1. EPR Single-Crystal Study of 3+ and 1+ Clusters of an Asymmetrical Model Compound and General Model for the Interpretation of the g-Tensors of These Two Redox States. 1997 , 119, 9757-9770	28
1159	Ab initio molecular dynamics simulation of H5 O2+ and H7 O3+ gas phase clusters based on density functional theory. 1997 , 91, 963-975	8
1158	Simulation of C1s Spectra of C- and O-Containing Polymers in XPS by ab initio MO Calculations Using Model Oligomers. 1997 , 29, 171-181	27
1157	Chapter 13 Density-functional theory of epitaxial growth of metals. 1997 , 8, 490-544	16
1156	A High-Level ab Initio and Density Functional Investigation of Cyclopropenyl Anion and Its Mono-, Di-, and Trisubstituted Derivatives. 1997 , 119, 12322-12337	28
1155	Extension of a predictive substrate model for human cytochrome P4502D6. 1997 , 27, 357-68	24
1154	Quantum Chemical Investigation of Ethylene Insertion into the Crl H3 Bond in CrCl(H2O)CH3+ as a Model of Homogeneous Ethylene Polymerization. 1997 , 16, 2514-2522	23
1153	Casci and Casscf Studies of Dinuclear Transition Metal Systems with Quadruple Metal-Metal Bonds (M=Cr(li), Mo(li)). 1997 , 306, 321-330	
1152	Self-consistent density-functional approach to the correlated ground states and an unrestricted many-body perturbation theory. 1997 , 76, 145-192	16
1151	Solid molecular phases of Hydrogen via constant-pressure first-principles Molecular Dynamics. 1997 , 499, 329	1
1150	Ab-Initio Simulation of Solid State Polymerization of Acetylene Under Pressure. 1997 , 499, 407	
1149	First Principles Simulations of Glucose in Aqueous Solution. 1997 , 489, 67	
1148	Cleavage of C⊞ Bond of Methane on Intermediate Q of Methane Monooxygenase. 1997 , 26, 1213-1214	12
1147	Investigation of the structure sensitivity of nitrogen adsorption on single crystal ruthenium clusters using density functional theory. 1997 , 109, 251-259	2

1146	Identification of the Borirene Molecule, (CH)2BH: Matrix Isolation FTIR and DFT Calculations for Five Vibrational Modes of Six Isotopic Molecules. 1997 , 119, 12402-12403	19
1145	Transition State Structure of the Solvolytic Hydrolysis of NAD+ 🛘 1997 , 119, 12069-12078	42
1144	Exchange energy functionals based on the density matrix expansion of the Hartree-Fock exchange term. 1997 , 92, 601-608	12
1143	A density functional water dimer potential surface. 1997 , 92, 667-676	16
1142	CationInteraction in Al(L)+ Complexes (L = C6H6, C5H5N, C5H6, C4H4NH, C4H4O). 1997 , 101, 3800-3807	47
1141	Infrared Spectrum and Structure of Me2TiCl2 and Quantum Mechanical Calculations of Geometries and Force Fields for MeTiCl3 and Me2TiCl2. 1997 , 101, 1951-1968	20
1140	Ab Initio Study of the Hydrogen Bonding between Pyrrole and Hydrogen Fluoride: A Comparison of NH-F and FH-Interactions. 1997 , 101, 1982-1988	26
1139	Energy Storage in the Primary Photoproduct of Vision. 1997 , 101, 2954-2958	53
1138	Evidencing Intermolecular Effects with Core-Level Photoelectron Spectroscopy via the Accurate Density Functional Calculation of CoreElectron Binding Energies on Model Systems: 即PS as a Test. 1997 , 101, 10254-10261	17
1137	Coupled cluster calculations for HC7N, HC7NH+ and C7N, molecules of interest to astrochemistry. 1997 , 92, 381-392	40
1136	Theory of Substituent Effects on Pericyclic Reaction Rates: Alkoxy Substituents in the Claisen Rearrangement. 1997 , 119, 2877-2884	62
1135	Computational and EXAFS Study of the Nature of the Ti(IV) Active Sites in Mesoporous Titanosilicate Catalysts. 1997 , 101, 4232-4237	106
1134	Effect of Lewis Acid Catalysis on the Diels-Alder Reaction between Methyl (Z)-(S)-4,5-(2,2-Propylidenedioxy)pent-2-enoate and Cyclopentadiene. A Theoretical Study. 1997 , 62, 3049-3054	43
1133	Analysis of C1s Spectra of N-, O-, and X-Containing Polymers in X-Ray Photoelectron Spectroscopy by ab initio Molecular Orbital Calculations Using Model Molecules. 1997 , 29, 255-260	21
1132	Evaluation of the performance of non-local and hybrid density functional theory methods for pi-radical hyperfine structures. 1997 , 91, 827-834	9
1131	The Cℍ activation reaction of methane for all transition metal atoms from the three transition rows. 1997 , 107, 4318-4328	90
1130	Structure and dynamics of the silacyclobutane radical cation, studied by ab initio and density functional theory and electron spin resonance spectroscopy. 1997 , 107, 297-306	17
1129	NMR Properties of Formamide: A First Principles and Experimental Study. 1997 , 101, 5069-5081	45

1128	CO2 Coordination to Nickel Atoms: Matrix Isolation and Density Functional Studies. 1997, 101, 2626-2633	57
1127	Edge-Bridged Tetrahedral Geometry of Five-Coordinate d0 Complexes, Relatives of the Bent [MCp2L3] Family: A Theoretical and Structure-Correlation Study. 1997 , 119, 11974-11985	17
1126	Stereoelectronic Control on the Kinetic Stability of 卧cetoxy-Substituted (卧-Allyl)palladium Complexes in a Mild Acidic Medium. 1997 , 16, 3779-3785	24
1125	Correlated Capped Subsystem Method for the Calculation of Substituent Effects on Bond Energies. 1997 , 101, 1193-1197	24
1124	Oligomerization of the PH(3)CuC&tbd1CCuPH(3) Acetylide toward the Formation of (PH(3)CuC)(n)() (n = 4, 6, 8) Metal Carbides: A Theoretical Study Based on Density Functional Theory. 1997 , 36, 2018-2022	4
1123	Density Functional Study of the [2+2]- and [2+3]-Cycloaddition Mechanisms for the Osmium-Catalyzed Dihydroxylation of Olefins. 1997 , 16, 13-19	101
1122	Unimolecular Dissociation in Allene and Propyne: The Effect of Isomerization on the Low-Pressure Rate. 1997 , 101, 4057-4071	53
1121	Prediction of SingletIIriplet Splittings for Aryne Biradicals from 1H Hyperfine Interactions in Aryl Radicals. 1997 , 101, 9191-9194	36
1120	Structure of the First Solvation Shell of the Hydroxide Anion. A Model Study Using OH-(H2O)n(n= 4, 5, 6, 7, 11, 17) Clusters. 1997 , 101, 7842-7853	77
1119	Quantum Chemical Investigation of Structures, Rotational Barriers, and Vibrational Spectra of the Rotamers of Ethyl Nitrite (CH3CH2ONO). 1997 , 101, 5580-5586	13
1118	Coordinative Behavior of the CNCN Ligand. Experimental and Density Functional Study of Spectroscopic Properties and Bonding in the Cr(CO)5CNCN Complex. 1997 , 16, 2254-2262	10
1117	Solvent Effects on the Conformer Distribution of 2-Methoxypropanal and Chloroacetaldehyde. A Model Case for the Conformational Analysis in Solution of Chiral Aldehydes Including Polar Groups. 1997 , 62, 6485-6492	21
1116	Reactions of Laser-Ablated Mg, Ca, Sr, and Ba Atoms with Hydrogen Cyanide in Excess Argon. Matrix Infrared Spectra and Density Functional Calculations on Novel Isocyanide Products. 1997 , 101, 9666-9672	24
1115	Molecular Structure of C(GeBr3)4 Determined by Gas-Phase Electron Diffraction and Density Functional Theory Calculations: Implications for the Length and Stability of Gett Bonds in Crystalline Semiconductor Solids. 1997 , 36, 5198-5201	9
1114	Density Functional Study of the Neutral Hypoxanthine Tautomeric Forms. 1997 , 101, 8309-8318	47
1113	Theoretical Study of the 15- and 17-Electron Structures of Cyclopentadienylchromium(III) and Cyclopentadienylmolybdenum(III) Complexes. Dichloride and Dimethyl Compounds. 1997 , 101, 9801-9812	24
1112	Theoretical Studies of CO and NO Adsorption on Cu+\(\mathbb{Z}\)SM-5 Zeolite. 1997 , 101, 7691-7701	40
1111	Reactions of Diarylnitrenium Ions with Electron Rich Alkenes: An Experimental and Theoretical Study. 1997 , 62, 2742-2751	25

1110	Characterization of Low-Barrier Hydrogen Bonds. 7. Relationship between Strength and Geometry of Short-Strong Hydrogen Bonds. The Formic Acidflormate Anion Model System. An ab Initio and DFT Investigation. 1997 , 119, 11277-11281	68
1109	Binding of Nitric Oxide to First-Transition-Row Metal Cations: An ab Initio Study. 1997 , 101, 8530-8539	64
1108	IR Matrix Isolation and ab Initio Identification of Products of the Reactions of CH3Cl and CH3Br with Mg. 1997 , 101, 8625-8630	26
1107	Density Functional Theory Study of the Methylperoxy Radical Isomerization. 1997 , 101, 2345-2349	20
1106	Benzenium Ion Chemistry on Solid Metal Halide Superacids: In Situ13C NMR Experiments and Theoretical Calculations. 1997 , 119, 406-414	31
1105	A Density Functional Study of the Vibrations of Three Oligomers of Thiophene. 1997 , 101, 7283-7291	33
1104	Self-Assembled Peptide Nanotubes from First Principles. 1997 , 79, 761-764	49
1103	Reactions of H2XXH2 and H2XO Double Bonds (X = Si, Ge, Sn, Pb): Are 1,3-Dioxa-2,4-dimetaletanes Unusual Molecules?. 1997 , 36, 4241-4246	38
1102	Exact Kohn-Sham Exchange Potential in Semiconductors. 1997 , 79, 2089-2092	313
1101	CoCF3+ Is Really (FCo+#F2C). 1997 , 16, 4020-4022	12
	CoCF3+ Is Really (FCo+#F2C). 1997, 16, 4020-4022 Proton Affinity and Acidity of Hypohalous Acids: A Density Functional Study. 1997, 101, 5022-5025	12
1100	Proton Affinity and Acidity of Hypohalous Acids: A Density Functional Study. 1997 , 101, 5022-5025 Solid State 15N and 13C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes.	14
1100	Proton Affinity and Acidity of Hypohalous Acids: A Density Functional Study. 1997 , 101, 5022-5025 Solid State 15N and 13C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes. 1997 , 119, 7114-7120	14 31
1100	Proton Affinity and Acidity of Hypohalous Acids: A Density Functional Study. 1997, 101, 5022-5025 Solid State 15N and 13C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes. 1997, 119, 7114-7120 Tetrafluorophosphate Anion. 1997, 119, 3918-3928 Monodeprotonated Free Base Porphyrin. 1997, 101, 1496-1497	14 31 29
1100 1099 1098 1097	Proton Affinity and Acidity of Hypohalous Acids: A Density Functional Study. 1997, 101, 5022-5025 Solid State 15N and 13C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes. 1997, 119, 7114-7120 Tetrafluorophosphate Anion. 1997, 119, 3918-3928 Monodeprotonated Free Base Porphyrin. 1997, 101, 1496-1497 Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Glycine Radical in	14 31 29
1100 1099 1098 1097	Proton Affinity and Acidity of Hypohalous Acids: A Density Functional Study. 1997, 101, 5022-5025 Solid State 15N and 13C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes. 1997, 119, 7114-7120 Tetrafluorophosphate Anion. 1997, 119, 3918-3928 Monodeprotonated Free Base Porphyrin. 1997, 101, 1496-1497 Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution. 1997, 119, 12962-12967 Binding of Ethylene to Anionic, Neutral, and Cationic Nickel(II), Palladium(II), and Platinum(II)	14 31 29 15

1092	Enough Activation by the 14-Electron $M(X)(PH3)/2(M = RN, Ir; X = CH3, H, Cl)$ Complex. A Density Functional Study. 1997 , 119, 10178-10185	43
1091	Structures and Conformations of CF3SC(O)F and CF3SC(O)Cl: Gas-Phase Electron Diffraction, Vibrational Analysis, and Theoretical Calculations. 1997 , 101, 2173-2177	13
1090	Hydrogen-bonding in glycine and malonaldehyde: Performance of the Lap1 correlation functional. 1997 , 107, 6770-6781	89
1089	Distinctive Normal Harmonic Vibrations of [2.2]Paracyclophane. 1997 , 101, 8233-8241	29
1088	Origins of Stereoselective Carbene 1,2-Shifts and Cycloadditions of 1,2-Dichloroethylidene: A Theoretical Model Based on CBS-Q and B3LYP Calculations. 1997 , 119, 10805-10809	50
1087	Comparison of the BeckelleeNangParr and BeckePerdewWang Exchange-Correlation Functionals for Geometries of CyclopentadienyllTransition Metal Complexes. 1997 , 101, 2502-2508	19
1086	Theoretical Characterization of the Vibrational Properties at the Aluminum/trans-Polyacetylene Interface. 1997 , 101, 4193-4202	11
1085	Density Functional Theory Study of Transition-Metal Compounds Containing Metal Metal Bonds. 1. Molecular Structures of Dinuclear Compounds by Complete Geometry Optimization. 1997 , 119, 7514-7520	94
1084	Structures, Automerizations, and Isomerizations of C3H2Isomers. 1997 , 119, 5847-5856	126
1083	Theoretical and (e,2e) Experimental Investigation into the Complete Valence Electronic Structure of [1.1.1]Propellane. 1997 , 119, 2896-2904	26
1082	Inverse Electron Demand DielsAlder Reactions: 'Cycloaddition of Enol Ethers and Enamines with 4-Substituted 6-Nitrobenzofuroxans and a Nitroethylene Model. Anab Initioand Semiempirical Theoretical Study. 1997 , 62, 8687-8692	28
1081	Benchmarks of the PC-UNIX Computer with Electronic Structure Calculation. 1997 , 37, 1111-1114	3
1080	Atomic Sulfur and Chlorine Interaction with Pdn Clusters (n = 1日): A Density Functional Study. 1997 , 101, 1969-1974	22
1079	Molecular Conformation and Nanomechanics of Self-Assembled Alkylsiloxane Monolayers. 1997 , 13, 58-64	18
1078	The Force Field of Porphycene: A Theoretical and Experimental Approach. 1997, 101, 8409-8416	39
1077	Ab Initio and Resonance Raman Studies of Hexafluoro-1,3-butadiene. 1997 , 101, 1455-1459	19
1076	H-Bridged Structures for Tetrahedranes A4H4 (A = C, Si, Ge, Sn, and Pb). 1997 , 119, 12968-12973	17
1075	The Remarkably Stabilized Trilithiocyclopropenium Ion, C3Li3+, and Its Relatives. 1997 , 119, 9504-9512	28

1074	Quantum Chemical Study of the Different Forms of Nitric Acid Monohydrate. 1997, 101, 8871-8876	19
1073	The torsional conformations of butane: Definitive energetics from ab initio methods. 1997 , 106, 5143-5150	145
1072	Bonding of M-Acetylide Ligands to Electron-Rich Ruthenium Centers: Can Electron-Withdrawing Ligands Induce Significant Metal-to-Ligand Back-Bonding?. 1997 , 16, 4004-4011	70
1071	Probing the Balance between Localization and Delocalization of the Metal-Based Electrons in Face-Shared Bioctahedral Complexes. 1997 , 36, 3242-3247	52
1070	EDonor Substituent Effects on Calculated Structures, Spin Properties, and Vibrations of Radical Anions ofp-Chloranil,p-Fluoranil, andp-Benzoquinone. 1997 , 101, 8351-8359	54
1069	A Theoretical Study of Stereochemistry of 1,3-Migration in Allylsilane and Related Allylmetallic Compounds. 1997 , 119, 1948-1953	24
1068	Molecular Cluster Bowl To Enclose a Single Electron. 1997 , 119, 9329-9330	76
1067	Isomers of P2S2. 1997 , 101, 201-207	6
1066	Molecular and Vibrational Structure of 1,6,6a\(\textit{B}\)-Trithiapentalene. Infrared Linear Dichroism Spectroscopy and ab Initio Normal-Mode Analyses\(\textit{D}\) 1997, 101, 4475-4480	16
1065	Theoretical Analysis of CO2 Adducts on the Native El©enter in Ion-Bombarded Porous Silica. 1997 , 101, 9695-9702	2
1064	Exotic Structures of Si2B2H4. 1997 , 101, 919-925	14
1063	A Density Functional Study of the Mechanism of the DiimineNickel-Catalyzed Ethylene Polymerization Reaction. 1997 , 119, 367-374	162
1062	M(2)L(6) Complexes with Triple Mo-Mo and W-W Bonds: Molecular Topology and Inverted Pyramidality Effect. 1997 , 36, 1055-1060	9
1061	Theoretical Investigation of the Reaction between Aluminum and Propene. Comparison between Calculated and Experimental ESR Results. 1997 , 101, 4814-4820	5
1060	Quantum Mechanical Methods and the Interpretation and Prediction of Pericyclic Reaction Mechanisms. 1997 , 101, 8378-8388	196
1059	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 11. Migratory Insertion of Coordinated Nitric Oxide into Cobaltarbon Bonds. 1997 , 119, 3077-3086	29
1058	MP2 and Density Functional Studies of Hydrogen Bonding in Model Trioses: d-(+)-Glyceraldehyde and Dihydroxyacetone. 1997 , 101, 1542-1548	45
1057	IR Matrix Spectroscopy of Pentachlorocyclopentadienyl Cation C5Cl5+. Effect of Chlorine as a Substituent. 1997 , 101, 1523-1525	11

1056	Infrared Matrix Isolation and Theoretical Studies on Glutarimide. 1997 , 101, 7834-7841	62
1055	Systematic Study of the Potential Energy Surface for the Base-Induced Elimination Reaction of Fluoride Ion with Ethyl Fluoride Using Density Functional Theory. 1997 , 101, 208-218	31
1054	HOCl Adsorption on Ice Surfaces. 1997, 101, 6308-6312	27
1053	Polar Effect in Hydrogen Abstraction Reactions from Halo-Substituted Methanes by Methyl Radical: A Comparison between Hartreeflock, Perturbation, and Density Functional Theories. 1997, 101, 1912-1919	14
1052	Structural and Solvent Effects on the Mechanism of the Thermal Decarboxylation of 2-Oxetanones. A Limiting Case between Concerted and Stepwise Pathways in Pericyclic Reactions. 1997 , 119, 816-825	27
1051	Hydrogen-Bond Networks for Hydrolyses of Anhydrides. 1997 , 62, 7049-7053	16
1050	Boron Dibromide and Boron Diiodide Ground State Neutral and Cation. Use of Effective Core Potentials Combined with ab Initio and Density Functional Theory. 1997 , 101, 1374-1377	11
1049	Comparison between CASPT2 and DFT in the Study of Ni(C2H4)2 Complexes. 1997, 101, 6310-6314	35
1048	A Solid-State 1NMR and Theoretical Study of the Chemical Bonding in Disilenes. 1997 , 119, 4972-4976	58
1047	Structure and Stability of 2-Aza-21-carbaporphyrin Tautomers Prearranged for Coordination. 1997 , 36, 6287-6291	61
1046	Incorrect Dissociation Behavior of Radical Ions in Density Functional Calculations. 1997 , 101, 7923-7925	282
1045	Origin of the Stereoselectivity of the Intramolecular 1,2-Hydrogen Shift in Singlet Chlorocarbenes. A Theoretical Study. 1997 , 101, 2509-2513	21
1044	Structures and Energetics of Vn(C6H6)m+ Clusters: Evidence for a Quintuple-Decker Sandwich. 1997, 101, 8207-8213	129
1043	性 Electronic Transition of the Di- and Trinuclear Complexes Ru(E)(EI(CO)2(iPr-DAB): Resonance Raman, Electronic Absorption, Emission, and Density Functional Study (E = Me, SnPh3, M(CO)5; Eほ M(CO)5; M = Mn, Re; iPr-DAB = N,NiDiisopropyl-1,4-diaza-1,3-butadiene). 1997 , 16, 2055-2062	21
1042	Density Functional Study of Hydrogen-Bonded Systems: The WaterCarbon Monoxide Complex. 1997 , 101, 5004-5009	79
1041	A Density Functional Study of	42
1040	Substituent Effects on 103Rh NMR Chemical Shifts and Reactivities. A Density Functional Study. 1997 , 16, 261-267	30
1039	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 12. Intramolecular Carbon Hydrogen Bond Activation in (Butenyl) manganese Tricarbonyl. 1997 , 16, 2318-2324	17

1038	An IR Matrix Isolation and DFT Theoretical Study of the First Steps of the Ti(0) Ethylene Reaction: Vinyl Titanium Hydride and Titanacyclopropene. 1997 , 101, 9650-9659	49
1037	Geometry of Coordinatively Unsaturated Two-Legged Piano Stool Complexes with 16 Valence Electrons: A Theoretical Study 1997 , 16, 3207-3215	78
1036	Interactions of anesthetics with the water-hexane interface. A molecular dynamics study. 1997 , 101, 782-91	79
1035	The Chemical Nature of Atomic Oxygen Adsorbed on Rh(111) and Pt(111): A Density Functional Study. 1997 , 101, 10051-10057	36
1034	Electronic and Magnetic Properties of Neutral and Charged Quinone and Plastoquinone Radicals. 1997 , 101, 9496-9504	48
1033	Examination of MetalBilicon Bonding through Structural and Theoretical Studies of an Isostructural Set of Five-Coordinate Silyl Complexes, Os(SiR3)Cl(CO)(PPh3)2 (R = F, Cl, OH, Me). 1997, 16, 5076-5083	34
1032	A Density Functional Study of Metal-Ligand Bonding in $[(PR(3))(2)M](+)$ and $[PR(3)MCl]$ (M = Ag, Au; R = H, Me) Complexes. 1997 , 36, 1754-1757	49
1031	Theoretical Study of the Oxidation of Alcohol to Aldehyde by d0 Transition-Metal©xo Complexes: Combined Approach Based on Density Functional Theory and the Intrinsic Reaction Coordinate Method. 1997 , 16, 716-724	41
1030	14N and 2H NMR Study of the Mesophases of Cetyltrimethylammonium Bromide in Formamide. 1997 , 101, 32-38	25
1029	Static and ab Initio Molecular Dynamics Study of the Titanium(IV)-Constrained Geometry Catalyst (CpSiH2NH)Ti-R+. 2. Chain Termination and Long Chain Branching. 1997 , 16, 3454-3468	111
1028	Reactions of Laser-Ablated Al, Ga, In, and Tl Atoms with Hydrogen Cyanide in Excess Argon. Matrix Infrared Spectra and Density Functional Theory Calculations on New Cyanide and Isocyanide Products. 1997 , 101, 9660-9665	39
1027	The Naphthylcarbene Potential Energy Hypersurface. 1997 , 119, 1370-1377	42
1026	Infrared Spectra of Perdeuterated Naphthalene, Phenanthrene, Chrysene, and Pyrene. 1997 , 101, 2414-2422	57
1025	Calculation of Static Third-Order Polarizabilities of Large Organic Molecules. 1997 , 101, 2207-2214	30
1024	Study of the Stability of Cl2O3 Using ab Initio Methods. 1997 , 101, 7145-7153	15
1023	Electronic Structure of Cycloheptatrienyl Sandwich Compounds of Actinides: An(可-C7H7)2 (An = Th, Pa, U, Np, Pu, Am). 1997 , 119, 9021-9032	84
1022	Theoretical Study of the Interaction of the Ti Atom with CO2: Cleavage of the CD Bond. 1997 , 101, 4465-4471	70
1021	Structure and Bonding of the Isoelectronic Hexacarbonyls [Hf(CO)6]2-, [Ta(CO)6]-, W(CO)6, [Re(CO)6]+, [Os(CO)6]2+, and [Ir(CO)6]3+: A Theoretical Study1. 1997 , 16, 4807-4815	116

1020	Ab Initio and Nonlocal Density Functional Study of 1,3,5-Trinitro-s-triazine (RDX) Conformers. 1997 , 101, 8720-8726	124
1019	Characterization of Low-Barrier Hydrogen Bonds. 5. Microsolvation of Enol-Enolate. An ab Initio and DFT Investigation. 1997 , 62, 8171-8176	35
1018	Quantum Chemical Reaction Path and Transition State for a Model Cope (and Reverse Cope) Elimination. 1997 , 101, 3554-3560	28
1017	Density Functional Study of Geometry and Vibrational Spectra for the Isoelectronic and Cr(CO)6Molecules. 1997 , 101, 6273-6279	24
1016	X-ray-Induced Transformation of o-Vinylbenzaldehyde and 2-Methylbenzocyclobutenone to ano-Quinoid Ketene and Its Radical Cation. 1997 , 119, 2825-2831	9
1015	Interaction of Methane with a [Li]0 Center on MgO(100): HF, Post-HF, and DFT Cluster Model Studies. 1997 , 101, 10028-10034	19
1014	Structure and Relative Spin-State Energetics of [Fe(H2O)6]3+: A Comparison of UHF, M\[] [ler\textbf{P}] lesset, Nonlocal DFT, and Semiempircal INDO/S Calculations. 1997, 101, 3959-3965	38
1013	Competing Reaction Mechanisms for the Carbonylation of Neutral Palladium(II) Complexes Containing Bidentate Ligands: A Theoretical Study. 1997 , 16, 3199-3206	29
1012	Density Functional Study of the Mechanism of the Palladium(II)-Catalyzed Ethylene Polymerization Reaction. 1997 , 16, 1933-1945	96
1011	Density Functional Study of 59Co Chemical Shielding Tensors Using Gauge-Including Atomic Orbitals. 1997 , 101, 3637-3640	15
1010	First-Principles Analysis of Elementary Steps in the Catalytic Decomposition of NO by Cu-Exchanged Zeolites. 1997 , 101, 4353-4357	58
1009	Relationship between H D Spin S pin Coupling and Internuclear Distance in Molecular Hydrogen Complexes. 1997 , 119, 1717-1719	34
1008	Theoretical Study of the Elimination Kinetics of Carboxylic Acid Derivatives in the Gas Phase. Decomposition of 2-Chloropropionic Acid. 1997 , 101, 1859-1865	44
1007	Structure and Binding of Neutral and Charged SinH2O (n = 1, 2, 7) Clusters. 1997 , 101, 5035-5037	
1006	Experimental and Theoretical Studies on 1,4,5,7-Dithiadiazepinyl Radicals: Preparation and X-ray Structure of 5-(Trimethylsilyl)tetrachlorobenzo-1,4,5,7-dithiadiazepine. 1997 , 36, 4772-4777	14
1005	Theoretical Model for Insertion of the 16-Electron Species (E5-C5H5)M(L) into Saturated Hydrocarbons. A (E5-C5H5)M(CO) + CH4 (M = Ru-, Os-, Rh, Ir, Pd+, Pt+) Case Study. 1997 , 16, 1621-1627	30
1004	Assessment of Procedures for Calculating Radical Hyperfine Structures. 1997 , 101, 1352-1359	66
1003	Interaction of Alkene Radical Cations with Solvent Molecules As Described with Density Functional Theory. 1997 , 101, 8942-8948	27

1002	Density Functional and Hartree B ock Calculations on the Cyclopropane Ring Intermediates Involved in the Zeolite-Catalyzed Skeletal Isomerization of Hydrocarbons and in the Carbon Isotope Scrambling in 2-Propyl Cation. 1997 , 101, 5346-5351	36
1001	Crtto Photodissociation in Cr(CO)6: Reassessment of the Role of Ligand-Field Excited States in the Photochemical Dissociation of Metalligand Bonds. 1997 , 119, 7324-7329	82
1000	A Theoretical Study of the Reaction H2 + Fe(CO)4 ? H2Fe(CO)4. 1997 , 101, 2358-2363	38
999	Importance of Quantum Effects for Cℍ Bond Activation Reactions. 1997, 119, 9891-9896	57
998	Prediction of Alternative Structures of the Molybdenum Site in the Xanthine Oxidase-Related Aldehyde Oxido Reductase. 1997 , 119, 3159-3160	40
997	Endohedral Metallofullerenes. Are the Isolated Pentagon Rule and Fullerene Structures Always Satisfied?. 1997 , 119, 12693-12694	141
996	Generation and Decay of Aryl Sulfinyl and Sulfenyl Radicals: A Transient Absorption and Computational Study 1. 1997 , 101, 6855-6863	35
995	Ab Initio Study of the Structures and Vibrational Spectra of Some Diamine Radical Cations. 1997 , 101, 3626-3633	35
994	Adsorption of water on Si(100)-(2 \square 1): A study with density functional theory. 1997 , 106, 2426-2435	182
993	Gas-Phase Reactions of Fe(CH2O)+ and Fe(CH2S)+ with Small Alkanes: An Experimental and Theoretical Study. 1997 , 119, 12879-12888	14
992	Acylation of Lactams by Class A Lactamase: An ab Initio Theoretical Study on the Effects of the Oxy-Anion Hole. 1997 , 119, 6423-6431	30
991	A Contribution to the Understanding of Carbonyl Migration in Mn2(CO)10 via the Pairwise Exchange Mechanism. 1997 , 101, 8734-8740	23
990	Molecular Mechanics/Continuum Reaction Field/Quantum Mechanics Study of the Intramolecular Diels Alder Reaction of 2-Furfuryl Derivatives. 1997 , 62, 1439-1448	12
989	A DFT Study of the SimmonsBmith Cyclopropanation Reaction. 1997 , 119, 12300-12305	53
988	Systematic Theoretical Study of Structures and Bondings of the Charge-Transfer Complexes of Ammonia with HX, XY, and X2 (X and Y are Halogens). 1997 , 101, 2879-2885	39
987	Pt+-Catalyzed Oxidation of Methane: Theory and Experiment. 1997 , 101, 1567-1579	143
986	A Density Functional and Thermochemical Study of MIX Bond Lengths and Energies in [MX6]2-Complexes: LDA versus Becke88/Perdew86 Gradient-Corrected Functionals. 1997 , 101, 4793-4798	19
985	Molecular Vibrations of Solvated Uracil. Ab Initio Reaction Field Calculations and Experiment. 1997 , 101, 10923-10938	33

984	A Density Functional Study of Nickel(II) Diimide Catalyzed Polymerization of Ethylene. 1997 , 119, 1094-1100	176
983	NMR Chemical Shifts of [email´protected]28. How Shielded Can 91Zr Get?. 1997 , 101, 2514-2517	11
982	Theoretical Approaches to Direct Exchange Couplings between Divalent Chromium Ions in Naked Dimers, Tetramers, and Clusters. 1997 , 101, 705-712	124
981	Bi- and Trimetallic EAcetylide Complexes Connected through a Phenyl Ring in the Fe(Cp*)(dppe) Series. 1997 , 16, 2024-2031	115
980	Anomeric Effects in Bis(fluorooxy)difluoromethane. 1997 , 119, 803-806	10
979	Synergy of Theory and Experiment in the Remote Functionalization of Aliphatic Nitriles by B are□ Fe(I) and Co(I) Cations in the Gas Phase□ 1997 , 16, 3135-3147	23
978	Assessment of Modified Gaussian-2 (G2) and Density Functional Theories for Molecules Containing Third-Row Atoms Ga K r (1997, 101, 8701-8705)	46
977	Density Functional Study of the Primary Photoprocesses of Manganese Pentacarbonyl Chloride (MnCl(CO)(5)). 1997 , 36, 1541-1551	25
976	Horbidden Four-Center Reactions: Molecular Orbital Considerations for N2 + N2 and N2 + N2+. 1997 , 101, 8255-8263	15
975	Reactions of Laser-Ablated Beryllium Atoms with Hydrogen Cyanide in Excess Argon. FTIR Spectra and Quantum Chemical Calculations on BeCN, BeNC, HBeCN, and HBeNC. 1997 , 119, 6392-6398	27
974	Ligand Effects in the Models and Mimics of Oxyhemocyanin and Oxytyrosinase. A Density Functional Study of Reversible Dioxygen Binding and Reversible O-O Bond Cleavage. 1997 , 36, 4831-4837	58
973	Density Functional Study on the Electronic Structures of Model Peroxidase Compounds I and II. 1997 , 119, 11442-11451	88
972	Hartreeflock and Density Functional Methods and IR and NMR Spectroscopies in the Examination of Tautomerism and Features of Neutral 9-Acridinamine in Gaseous and Condensed Media. 1997 , 101, 283-292	38
971	Static Dipole Polarizabilities through Density Functional Methods. 1997 , 101, 4231-4235	28
970	Structure and Bonding of the Noble GasMetal Carbonyl Complexes M(CO)5Mg (M = Cr, Mo, W and Ng = Ar, Kr, Xe). 1997 , 16, 4896-4902	47
969	Why the Classical and Nonclassical Norbornyl Cations Do Not Resemble the 2-endo- and 2-exo-Norbornyl Solvolysis Transition States(1)(,). 1997 , 62, 4216-4228	51
968	Structure and Energetics of Ionized Water Clusters: (H2O)n+, n = 2 B . 1997 , 101, 164-169	68
967	Calculation of NMR Chemical Shifts and SpinBpin Coupling Constants in the Monosaccharide Methyl-軠-xylopyranoside Using a Density Functional Theory Approach 1997, 101, 9756-9762	40

966	Structure and Fluxional Behavior of (\text{M-butadiene})Fe(CO)2L (L = CO, PH3, PMe3) Complexes. A Density Functional Study. 1997 , 16, 475-481	12
965	Dissociation Energies, Vibrational Frequencies, and 13C NMR Chemical Shifts of the 18-Electron Species [M(CO)6]n(M = Hflr, Mo, Tc, Ru, Cr, Mn, Fe). A Density Functional Study. 1997 , 36, 5031-5036	89
964	A Theoretical Study of the Favorskii Rearrangement. Calculation of Gas-Phase Reaction Paths and Solvation Effects on the Molecular Mechanism for the Transposition of the Echlorocyclobutanone. 1997, 119, 1941-1947	22
963	Possible Nitrogen Fixation by Disilabutadiene. 1997 , 16, 5058-5063	9
962	A Quantum Chemical View of Density Functional Theory. 1997 , 101, 5383-5403	511
961	Density Functional Theory/GIAO Studies of the13C,15N, and1H NMR Chemical Shifts in Aminopyrimidines and Aminobenzenes: Relationships to Electron Densities and Amine Group Orientations. 1997 , 119, 8699-8711	134
960	Electron-Energy-Loss Spectroscopy and Theoretical Study of Triplet and Singlet Excited States of Fulvene. 1997 , 101, 2089-2095	18
959	Mechanism of Cℍ Activation by Diiron Methane Monooxygenases: ´Quantum Chemical Studies. 1997, 119, 3103-3113	276
958	Calculation of 125Te Chemical Shifts Using Gauge-Including Atomic Orbitals and Density Functional Theory. 1997 , 101, 4121-4127	45
957	Trans- and Cis-Water Reactivities in d(6) Octahedral Ruthenium(II) Pentaaqua Complexes: Experimental and Density Functional Theory Studies(1)(,)(2). 1997 , 36, 6009-6020	38
956	The ClO4 radical: Experiment versus theory. 1997 , 106, 4028-4037	26
955	Assessment of Gaussian-2 and density functional theories for the computation of enthalpies of formation. 1997 , 106, 1063-1079	1822
954	Theoretical Study of CIL Bond Formation in the Methanol-to-Gasoline Process. 1997, 119, 5020-5027	128
953	Methanol adsorption and activation by zeolitic protons. 1997 , 105, 1707-1714	2
952	Ab Initio Study of RDX Decomposition Mechanisms. 1997 , 101, 8675-8679	100
951	Density functional theory with approximate kinetic energy functionals applied to hydrogen bonds. 1997 , 106, 8516-8526	126
950	Density Functional Calculations of Structures, Vibrational Frequencies, and Normal Modes of transand cis-Azobenzene. 1997 , 101, 5555-5566	147
949	Porphyrin Isomers: Geometry, Tautomerism, Geometrical Isomerism, and Stability. 1997 , 62, 9240-9250	74

948	Catalytic Mechanism of the Enzyme Papain: Predictions with a Hybrid Quantum Mechanical/Molecular Mechanical Potential. 1997 , 119, 12285-12291	119
947	Structure and gas phase stability of complexes L M, where $M = Li+$, $Na+$, $Mg2+$ and L is formaldehyde, formic acid, formate anion, formamide and their sila derivatives. 1997 , 91, 929-936	9
946	Comparison of Hartreeflock, Density Functional, M\leftilerflesset Perturbation, Coupled Cluster, and Configuration Interaction Methods for the Migratory Insertion of Nitric Oxide into a Cobaltflarbon Bond. 1997 , 101, 1360-1365	43
945	Theoretical Study of the Mechanism of Surface Methoxy and Dimethyl Ether Formation from Methanol Catalyzed by Zeolitic Protons. 1997 , 101, 2292-2305	149
944	Broken-Symmetry and Approximate Spin-Projected Potential Energy Curves for Bimetallic Systems: A Density Functional Study of M2Cl9, M = CrIII, MoIII, WIII, and ReIV. 1997 , 101, 6265-6272	56
943	Experimental and Theoretical Studies of SiFn(CO)2+ Cations with n = 2 and 3: A Search for Pentacoordinate Cationic Silicon. 1997 , 101, 7258-7264	7
942	Recent Developments in Multiple Scattering Theory and Density Functional Theory for Molecules and Solids. 1997 , 1-58	
941	Van Der Waals Interactions from Density Functional Theories:. 1997 , 337-382	3
940	Identification of the True Product of the Urate Oxidase Reaction. 1997 , 119, 5435-5442	122
939	The alkali metal trifluorides M+F3 [how well can theory predict experiment?. 1997 , 90, 515-524	6
938	Ab Initio Conformational Analysis of 1,4-Dioxane. 1997 , 101, 3382-3387	63
937	Relationships between bond dissociation energies, electron density minima and electrostatic potential minima. 1997 , 90, 425-430	9
936	Calculated Properties of Ag Clusters on Silver Halide Cubic Surface Sites. 1997 , 101, 8180-8190	35
935	A Combined Car P arrinello QM/MM Implementation for ab Initio Molecular Dynamics Simulations of Extended Systems: Application to Transition Metal Catalysis. 1997 , 101, 7877-7880	87
934	A Quantum Chemical Study of Hydrogen Abstraction from Manganese-Coordinated Water by a Tyrosyl Radical: A Model for Water Oxidation in Photosystem II. 1997 , 119, 8285-8292	116
933	Describing van der Waals Interaction in diatomic molecules with generalized gradient approximations: The role of the exchange functional. 1997 , 107, 7921-7925	262
932	Density Functional Theory-Based Molecular Dynamics Simulation of Acid-Catalyzed Chemical Reactions in Liquid Trioxane. 1997 , 119, 7218-7229	82
931	Vibrational Analysis of 1,3,3-Trinitroazetidine Using Matrix Isolation Infrared Spectroscopy and Quantum Chemical Calculations. 1997 , 101, 7742-7748	13

930	冊ydrogen-Containing Zirconium Alkyls with the Doubly-Bridged Bis(dimethylsilanediyl)dicyclopentadienyl Ligand. X-ray Molecular Structures of [Zr{(SiMe2)2(卧-C5H3)2}ClEt] and [Zr{(SiMe2)2(卧-C5H3)2}Et]2(ЮH2CH2). 1997 , 16, 1553-1561	29
929	Do Localized Structures of [14]- and [18]Annulenes Exist?. 1997 , 119, 11994-11995	33
928	Density Functional Theory Predictions of Second-Order Hyperpolarizabilities of Metallocenes. 1997 , 101, 9391-9398	77
927	Metal P hosphorus Bonding in Fe(CO)4PR3 Complexes. A Density Functional Study. 1997 , 16, 5556-5562	47
926	Vibrational Circular Dichroism Study of (♪Sparteine. 1997 , 101, 9783-9790	24
925	Density-Functional Studies on the Structure and Vibrational Spectra of Transient Intermediates of p-Benzoquinone. 1997 , 101, 4449-4459	69
924	Comparative Study of Benzene (X = O2, N2, CO) Complexes Using Density Functional Theory: The Importance of an Accurate Exchange Correlation Energy Density at High Reduced Density Gradients. 1997 , 101, 7818-7825	221
923	Assessment of Basis Set and Functional Dependencies in Density Functional Theory: Studies of Atomization and Reaction Energies. 1997 , 101, 1927-1934	58
922	Structures and Vibrational Spectra of p-Benzoquinone in Different Oxidation and Protonation States: A Density Functional Study. 1997 , 101, 1235-1246	42
921	Toward the Prediction of Magnetic Coupling in Molecular Systems: Hydroxo- and Alkoxo-Bridged Cu(II) Binuclear Complexes. 1997 , 119, 1297-1303	773
9 2 0	Density Functional Calculations of Magnetic Exchange Interactions in Polynuclear Transition Metal Complexes. 1997 , 36, 5022-5030	203
919	A Density Functional Theory Study of Secondary Orbital Overlap in Endo Cycloaddition Reactions. An Example of a Diels-Alder Reaction between Butadiene and Cyclopropene. 1997 , 62, 3046-3048	37
918	An experimental and theoretical investigation of the electronic structure of Pd and Pt bis(carbene) complexes. 1997 , 1963	121
917	Ab Initio Calculations of the Ground Electronic States of Polyiodide Anions. 1997 , 101, 2192-2197	60
916	Analysis of Substituent Effects on the Claisen Rearrangement with Ab Initio and Density Functional Theory. 1997 , 62, 6121-6128	46
915	Applications of the generalized-gradient approximation to atoms, clusters, and solids. 1997 , 56, 7197-7205	101
914	Characterization of Low-Barrier Hydrogen Bonds. 1. Microsolvation Effects. An ab Initio and DFT Investigation. 1997 , 119, 7561-7566	71
913	Effect of Substituents on the Structure of the Vinyl Radical: Calculations and Experiments. 1997 , 62, 4072-4077	78

912	Antiferromagnetic Exchange Interactions from Hybrid Density Functional Theory. 1997 , 79, 1539-1542	252
911	Isotope and temperature effects on the 13C and 77Se nuclear shielding in carbon diselenide. 1997 , 107, 1350-1361	28
910	Conformational Information from Vibrational Spectra of Styrene, trans-Stilbene, and cis-Stilbene. 1997 , 101, 3823-3831	261
909	CuDinitrosyl Species in Zeolites: A Density Functional Molecular Cluster Study. 1997 , 101, 6903-6913	48
908	In-Plane Aromaticity in 1,3-Dipolar Cycloadditions. 1997 , 62, 7033-7036	123
907	Ab initio dynamics of surface chemistry. 1997 , 48, 243-70	58
906	Theoretical Studies of Ethylene Polymerization Reactions Catalyzed by Zirconium and Titanium Chelating Alkoxide Complexes. 1997 , 119, 7190-7196	109
905	A Multiplet Analysis of Fe K-Edge 1s -f3d Pre-Edge Features of Iron Complexes. 1997 , 119, 6297-6314	1073
904	Structure and Bonding in Carbon Clusters C14 to C24: Chains, Rings, Bowls, Plates, and Cages. 1997 , 79, 443-446	163
903	A refined substrate model for human cytochrome P450 2D6. 1997 , 10, 41-8	66
902	Computed 13C NMR Chemical Shifts via Empirically Scaled GIAO Shieldings and Molecular Mechanics Geometries. Conformation and Configuration from 13C Shifts. 1997 , 119, 9483-9494	272
901	Rearrangements of C(7)H(6) Isomers: Computational Studies of the Interconversions of Bicyclo[3.2.0]hepta-1,3,6-triene, Bicyclo[3.2.0]hepta-3,6-diene-2-ylidene, Bicyclo[3.2.0]hepta-2,3,6-triene, and Cyclohepta-1,2,4,6-tetraene. 1997 , 62, 4398-4405	37
900	Nanotubules of bare boron clusters: Ab initio and density functional study. 1997 , 39, 527-532	143
899	Density Functional Study of the Electronic Structures of [Co(NH3)5X](3+n)+ Complexes. Insight into the Role of the 3d and 4s Orbitals in Metalligand Interactions. 1997 , 101, 4196-4201	9
898	Molecular Geometries and Vibrational Spectra of Phenol, Benzaldehyde, and Salicylaldehyde:´ Experimental versus Quantum Chemical Data. 1997 , 101, 2254-2263	148
897	Ab Initio Characterization of [H3N·BH3]2, [H3N·AlH3]2, and [H3N·GaH3]2. 1997 , 36, 5358-5362	78
896	Chromium dichloride: the unusually flat bending potential of the 5½-derived 5B2 ground state. 1997 , 91, 131-138	10
895	Origin of Solvent Acceleration in Organolithium Metal Halogen Exchange Reactions. 1997 , 16, 6021-6023	24

894	Coordination Chemistry and Mechanisms of Metal-Catalyzed CC-Coupling Reactions. 10. Ligand Dissociation in Rhodium-Catalyzed Hydroformylation: A Theoretical Study 1997 , 16, 701-708	69
893	Pentalene: Formation, Electronic, and Vibrational Structure. 1997 , 119, 1869-1875	100
892	Linkage Isomerism and the Relativistic Effect in Interaction of Lanthanoid and Carbon Monoxide. 1997 , 101, 9314-9317	8
891	Calculation of the G-Tensor of Electron Paramagnetic Resonance Spectroscopy Using Gauge-Including Atomic Orbitals and Density Functional Theory. 1997 , 101, 3388-3399	227
890	A Density Functional Study of the Rotational Barrier of Tricarbonyl(eta(4)-norbornadiene)iron. Effect of the Torsional Angle on the Carbonyl Stretching Spectra. 1997 , 36, 2922-2924	16
889	Theoretical studies of large water clusters: (H2O)28, (H2O)29, (H2O)30, and (H2O)31 hexakaidecahedral structures. 1997 , 106, 5537-5540	27
888	Systematic Density Functional Study of the Adsorption of Transition Metal Atoms on the MgO(001) Surface. 1997 , 101, 2786-2792	252
887	Structural Modeling and Magneto-Structural Correlations for Hydroxo-Bridged Copper(II) Binuclear Complexes. 1997 , 36, 3683-3688	364
886	A new gradient-corrected exchange-correlation density functional. 1997 , 91, 847-860	17
885	Adsorption of Water and Methanol on Silica Hydroxyls: Ab Initio Energy and Frequency Calculations. 1997 , 101, 1178-1187	55
884	Reactions of Laser-Ablated Nickel Atoms with Dioxygen. Infrared Spectra and Density Functional Calculations of Nickel Oxides NiO, ONiO, Ni2O2, and Ni2O3, Superoxide NiOO, Peroxide Ni(O2), and Higher Complexes in Solid Argon. 1997 , 101, 3109-3118	82
883	On the Quantum Nature of the Shared Proton in Hydrogen Bonds. 1997 , 275, 817-20	617
882	Dissociation of methane into hydrocarbons at extreme (planetary) pressure and temperature. 1997 , 275, 1288-90	128
881	Electric quadrupole second-harmonic generation spectra in epitaxial vanadyl and titanyl phthalocyanine films grown by molecular-beam epitaxy. 1997 , 107, 1687-1691	21
880	CarbonDxygen Bond Strength in Diphenyl Ether and Phenyl Vinyl Ether: An Experimental and Computational Study. 1997 , 101, 5404-5411	50
879	The Role of Bulky Substituents in Brookhart-Type Ni(II) Diimine Catalyzed Olefin Polymerization: A Combined Density Functional Theory and Molecular Mechanics Study. 1997 , 119, 6177-6186	304
878	Structures of the 12-Vertex Oxa- and Thia-nido-dodecaborates and B(13)H(13)(2)(-): A Theoretical DFT/GIAO/NMR Investigation. 1997 , 36, 4897-4899	23
877	Calculation of ionization energies, electron affinities, electronegativities, and hardnesses using density functional methods. 1997 , 106, 3270-3279	128

876	Ultrasoft pseudopotentials applied to magnetic Fe, Co, and Ni: From atoms to solids. 1997 , 56, 15629-15646	302
875	On the mechanism of HOONO to HONO2 conversion. 1997 , 1, 494-501	16
874	Organometallic Analogs of the Cyclobutadiene Dication: An Ab Initio MO and Density Functional Study of the Symmetrical Planar and Puckered [WL2(ECR)]2 Complexes (L = H, Me, F, OH; R = H, F, Me). 1997 , 16, 1425-1429	8
873	Calculation of total energies in multicomponent oxides. 1997 , 8, 142-152	12
872	Fluorination of diamond IC4F9I and CF3I photochemistry on diamond (100). 1997 , 370, 209-231	20
871	New quasi-planar surfaces of bare boron. 1997 , 370, 355-363	173
870	Density functional study of acetylene and ethylene adsorption on Ni(111). 1997 , 371, 53-62	41
869	A molecular dynamics study of the chemisorption of C2H2 and CH3 on the SI(001)-(2 \square \square 1) surface. 1997 , 375, 45-54	42
868	Vibrational frequencies for NO chemisorbed on different sites: DFT calculations on Pd clusters. 1997 , 380, 83-90	52
867	Theoretical investigation of the adsorption of alkali metals on a Cu(111) surface. 1997 , 385, 24-36	29
866	Trends in atom/molecule-surface van der Waals interactions. 1997, 383, 88-94	16
865	H2 adsorption/desorption at Si(111)-(7 🗆 🗗): a density functional study. 1997 , 383, L779-L784	16
864	Energetics of void enlargement in thermally grown ultrathin Si-oxide on Si(001). 1997 , 387, L1057-L1061	4
863	Is CO chemisorbed on Pt anomalous compared with Ni and Pd? An example of surface chemistry dominated by relativistic effects. 1997 , 392, 173-184	58
862	Quantum chemical studies of the effects on silicate mineral dissolution rates by adsorption of alkali metals. 1997 , 61, 2577-2587	40
861	Calculated One-Electron Reduction Potentials and Solvation Structures for Selected p-Benzoquinones in Water. 1997 , 101, 623-631	62
860	Exchange and correlation energy in density functional theory: Comparison of accurate density functional theory quantities with traditional Hartree Bock based ones and generalized gradient approximations for the molecules Li2, N2, F2. 1997 , 107, 5007-5015	177
859	Density Functional Study of N2 Activation by Molybdenum(III) Complexes. Unusually Strong Relativistic Effects in 4d Metal Compounds. 1997 , 16, 995-1000	62

858	Density Functional Calculations of g Values and Molybdenum Hyperfine Coupling Constants for a Series of Molybdenum(V) Oxyhalide Anions. 1997 , 36, 5348-5357	47
857	Remarks on the Proper Use of the Broken Symmetry Approach to Magnetic Coupling. 1997 , 101, 7860-7866	396
856	Spin Density Maps for the Ferrimagnetic Chain Compound MnCu(pba)(H2O)3•2H2O (pba = 1,2-Propylenebis(oxamato)): Polarized Neutron Diffraction and Theoretical Studies. 1997 , 119, 3500-3506	62
855	Single-Bond Torsional Potentials in Conjugated Systems: A Comparison of abInitio and Density Functional Results. 1997 , 101, 7426-7433	247
854	Mn+(H2)n and Zn+(H2)n Clusters: Influence of 3d and 4s Orbitals on Metalligand Bonding. 1997 , 101, 2809-2816	58
853	Theoretical studies of CO adsorption on H-ZSM-5 and hydrothermally treated H-ZSM-5. 1997 , 121, 45-62	29
852	Reactions of Laser-Ablated Scandium Atoms with Dioxygen. Infrared Spectra of ScO, OScO, (O2)ScO, (ScO)2, and Sc(O2)2 in Solid Argon. 1997 , 101, 9085-9091	66
851	The gas phase reactivity and theoretical structures of germanium ions generated by direct laser vaporisation. 1997 , 164, 45-69	36
850	N2O2, N2O2land N2O22listructures, energetics and N?N bonding. 1997 , 221, 1-10	60
849	Highly optimized tight-binding model of silicon. 1997 , 55, 1528-1544	172
848	Reactions of Laser-Ablated Cobalt Atoms with O2. Infrared Spectra of Cobalt Oxides in Solid Argon. 1997 , 101, 8793-8802	67
847	From clusters to bulk: A relativistic density functional investigation on a series of gold clusters Aun, n=6, 147. 1997 , 106, 5189-5201	316
846	Electrical properties of molybdenum disulfide MoS2. Experimental study and density functional calculation results. 1997 , 90, 165-172	51
845	Preparation and characterization of pyridinium-n-carboxylate trioxochromate (VI) (n=3, 4) and pyridinium-4-carboxylic pyridine-4 carboxylate trioxochromate (VI) hemihydrate. 1997 , 258, 53-63	9
844	Imaging of the HOMO electron density in Cr(CO)6, Mo(CO)6 and W(CO)6 by electron momentum spectroscopy: a comparison with Hartree-Fock and DFT calculations. 1997 , 215, 191-205	36
843	Structures and potential energy surface of faujasitic zeolite/water. 1997 , 215, 77-87	20
842	Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (II). Confirmation with a total of seventy-six cases. 1997 , 216, 91-98	14
841	Accurate density-functional calculation of core-electron binding energies with a scaled polarized triple-zeta basis set. (III). Extension to open-shell molecules. 1997 , 216, 99-104	8

840	Insight into the stabilization of A-DNA by specific ion association: spontaneous B-DNA to A-DNA transitions observed in molecular dynamics simulations of d[ACCCGCGGGT]2 in the presence of hexaamminecobalt(III). 1997 , 5, 1297-311	97
839	The determination of the equilibrium structures of oxygen, ozone, and hydrogen peroxide using the ab initio and density functional theory methods. 1997 , 389, 251-256	32
838	The conformational space of selected aldo-pyrano-hexoses. 1997 , 395-396, 29-40	26
837	Theoretical investigation of thionyl and sulfuryl dihalide structures using density functional theory methods. 1997 , 389, 75-81	28
836	A density functional study of bonding of water to copper and nickel atoms. 1997 , 389, 83-89	17
835	Modified local exchange and kinetic energy functionals for atomic systems. 1997 , 390, 1-9	4
834	Compared performances of the molecular orbital and density functional theories for fragments of biomolecules. 1997 , 390, 11-21	17
833	Local and nonlocal density functional calculations of the molecular structure of isomeric thiadiazoles. 1997 , 390, 67-78	23
832	Conformational and thermodynamic studies of alkaline subhalides M2X (M = Li, Na, K, Rb; X = F, Cl, Br, I). 1997 , 390, 121-126	12
831	Molecular conformations and harmonic force field of 1,3,5-benzenetriol molecule from ab initio and density functional theory investigations. 1997 , 390, 139-148	28
830	Equilibrium structure of the carbon dioxide-water complex in the gas phase: an ab initio and density functional study. 1997 , 390, 157-167	19
829	Theoretical study of the diffusion of alkali metals on a Cu(111) surface. 1997 , 390, 183-192	6
828	An MP2 and density functional study of the oxides of nitrogen. 1997 , 391, 231-240	14
827	Computation of the heats of formation of cyclopropane and cyclobutane derivatives using density functional theory methods. 1997 , 391, 75-83	26
826	Theoretical studies of thermal syn elimination reaction of organic amine oxide, sulfoxide and phosphoxide by ab initio and density functional methods. 1997 , 389, 257-263	11
825	The quest for a planar and pyramidal carbon atom Part 4: An unsuccessful search for pyramidal carbon atoms in hypothetical unsaturated conjugated paddlane. 1997 , 391, 201-205	5
824	Density functional modelling for the conformers of 2-methoxyethanol. 1997 , 401, 181-187	3
823	Review of quantum Monte Carlo methods and their applications. 1997 , 394, 75-85	19

822	Electronic structure and properties of transition metal complexes MCH2 and M5 CH2 (M = Fe, Ni, Cu;) by density functional methods. 1997 , 394, 249-258	5
821	An ab initio and density functional study of nitrosomethane and its rearrangement products formaldonitrone and formaldoxime. 1997 , 401, 141-150	15
820	Computational study of the addition of molecular oxygen to benzene. 1997 , 397, 13-20	8
819	A comparative study of the calculation of 59Co NMR shielding constants of hexacoordinated diamagnetic Co(III) complexes using DFT-IGLO and DFT-GIAO methods. 1997 , 393, 93-96	12
818	Double water and double ammonia proton complexations studied with ab initio and density functional theory methods. 1997 , 393, 1-7	12
817	Computing electron affinities of radicals with density functional theory methods. 1997 , 394, 19-23	19
816	Hybrid and gradient-corrected density functional theory computations of the cubane infrared and raman spectra. 1997 , 394, 15-18	26
815	An ab initio study of the structure and energetics of the bisulfite ion in the gas phase and in aqueous solution. 1997 , 394, 1-9	13
814	Bond and atomization energies of C60 and C70 fullerenes. 1997 , 398-399, 301-305	5
813	A computational study of the bent hydrogen bond in the formaldehyde-hydrogen chloride complex. 1997 , 401, 127-132	1
812	Study on europium chalcogenides by means of density functional theory. 1997 , 417, 9-17	1
811	Properties of some weakly bound complexes obtained with various density functionals. 1997 , 397, 191-197	3
810	Density functional studies of conformational properties of conjugated systems containing heteroatoms. 1997 , 393, 39-58	35
809	The potential energy surface for the oxywater radical cation transformation to hydrogen peroxide radical cation studied by density functional theory and ab initio methods. Are hybrid density functional methods as accurate as coupled-cluster ab initio methods?. 1997 , 401, 45-54	9
808	Spin densities, conformations and rotational energy barriers around the C(O)?N bond in acylaminoxyl (RC(?O)?N(?O)R?; R,R??H,CH3) radicals: ab initio and density functional study. 1997 , 401, 55-68	2
807	Rationalization of the anomalous 1H NMR chemical shifts in 1,3-diheterocyclohexanes. 1997 , 418, 231-241	36
806	Intramolecular sulfur-oxygen interactions: An ab initio molecular orbital and density functional theory investigation. 1997 , 418, 139-154	19
805	Pseudopotentials including part of the atomic correlation energy. 1997 , 401, 93-105	9

804	Ab initio and density functional study of azidoacetone. 1997 , 397, 223-230	4
803	A density functional theory study on stability of carbonylmetallate monoanions Mn(CO)6 HFe(CO)4 and Co(CO)4 1997, 417, 247-254	4
802	Computational studies of formaldehyde dissociation and protonated carbon monoxide isomerization with density functional theory methods. 1997 , 418, 11-16	6
801	Optimum geometry of CO dimer and FT-IR spectra of CO in solid argon. 1997 , 418, 1-10	13
800	Geometrical and electronic properties of dibenzoporphycenes. 1997 , 398-399, 325-332	10
799	Ab initio model potentials and their application to the thermal stability of metal clusters. 1997 , 398-399, 333-340	8
798	The density functional theory evaluation of the heats of formation of some aromatic compounds through the isodesmic approach. 1997 , 417, 99-106	25
797	Density functional theory and ab initio study of oxywater isomerization into hydrogen peroxide. 1997 , 417, 81-88	9
796	Density functional calculations on the heats of formation of cyclic hydrocarbons. 1997 , 417, 107-115	14
795	Density functional theory studies of the structures of some compounds having 12 valence electrons with a central sulfur atom. 1997 , 418, 165-169	14
794	Density functional study of hydrogen-bonded systems: Energetic and vibrational features of some gas-phase adducts of hydrogen fluoride. 1997 , 419, 227-238	32
793	DFT analysis of interfacial processes occurring in the first steps of electrodeposition of nickel from chloride melt. 1997 , 419, 1-10	12
792	Hydrogen fluoride: a critical comparison of theoretical and experimental results. 1997, 400, 69-92	35
791	Ab initio effective core potential calculations on lanthanide complexes: basis sets and electron correlation effects in the study of [Gd-(H2O)9]3+. 1997 , 392, 75-85	15
790	Di-Ethloro-bis[dicarbonylpalladium(I)] molecular structure characterization by Hartree-Fock and local spin density methods. 1997 , 392, 223-230	3
789	Structure, stability, and vibrational properties of small silver cluster. 1997 , 40, 479-482	62
788	Ab-initio molecular dynamics based on non-local density functional procedure with Gaussian basis; study of structural and temperature behaviour of metallic clusters. 1997 , 40, 486-489	7
787	Electronic structure of Lanthanum-carbon clusters. 1997 , 41, 69-72	15

786	Calculation of heats of sublimation and solid phase heats of formation. 1997 , 91, 923-928	195
7 ⁸ 5	Accurate numerical determination of Kohn-Sham potentials from electronic densities: I. Two-electron systems. 1997 , 106, 9659-9667	39
784	Toward Improved Force Fields. 1. Multipole-Derived Atomic Charges. 1997 , 101, 5437-5445	39
783	Size dependence of bond length and binding energy in palladium and gold clusters. 1997 , 101, 1640-1643	47
782	Density functional study of model species for nucleic acids and lipids. 1997 , 101, 1828-1835	2
781	Density-functional thermochemistry. V. Systematic optimization of exchange-correlation functionals. 1997 , 107, 8554-8560	1447
780	A hybrid Gaussian and plane wave density functional scheme. 1997 , 92, 477-488	828
779	Molecular Structure of Free Molecules of the Fullerene C70 from Gas-Phase Electron Diffraction. 1997 , 119, 5314-5320	78
778	Electron affinities of p-benzoquinone, p-benzoquinone imine and p-benzoquinone diimine, and spin densities of their p-benzosemiquinones computed by several quantum chemical models. 1997 , 11, 345-56	15
777	The Water Dimer: Post-Hartree-Fock and Density Functional Calculations on the Potential Energy Surface. 1997 , 7, 317-348	2
776	Density functional theory studies of zeolite structure, acidity, and reactivity. 1997 , 4, 157-171	64
775	Comparative calculations on the hyperfine parameters of bond-centered impurities in silicon using high-level ab initio techniques. 1997 , 105, 351-355	
774	The muonium adduct to biacetyl 🗈 initio calculations and vibrational averaging. 1997 , 106, 169-174	4
773	Theoretical analysis of thermally stable adsorption forms of oxygen on silver. 1997 , 38, 519-527	9
772	On the molecular models of lewis acid sites on the surface of Al2O3 and in zeolites: a density functional study of CO adsorption. 1997 , 38, 698-702	1
771	The structure of astatine azide, AtN3A theoretical study. 1997 , 8, 421-423	2
770	Structure and dynamics of protonated methane: CH +5 at finite temperatures. 1997 , 41, 253-260	27
769	Adsorption of isolated Cu, Ni and Pd atoms on various sites of MgO(001): Density functional studies. 1997 , 19, 1743-1748	45

768	Adsorption of water on silica hydroxyls: DFT calculations (*). 1997 , 19, 1749-1758	3
767	Reaction coordinate analyses of transition metal catalyzed CH and CS activation steps. 1997 , 160, 169-184	19
766	Parallel biomolecular simulation: Theory, algorithms and implementation. 1997 , 5, 573-603	1
765	The T1 resonance Raman spectra of biochemically relevant chromophores a theoretical investigation. 1997 , 105, 209-216	6
764	Computational chemistry predictions of reaction processes in organometallic vapor phase epitaxy. 1997 , 35, 117-149	42
763	Vibrational spectroscopic and force field studies of N,N-dimethylthioformamide, N,N-dimethylformamide, their deuterated analogues and bis(N,N-dimethylthioformamide)mercury(II) perchlorate. 1997 , 14, 207-227	49
762	Modelling of structure, sorption, synthesis and reactivity in catalytic systems1Communication presented at the First Francqui Colloquium, Brussels, 19½0 February 1996.1. 1997 , 115, 431-448	11
761	Synthesis and characterization of cyanocobalamin conjugates with Pt(II) complexes towards potential therapeutic applications. 2023 , 230, 116230	O
760	A comprehensive benchmark investigation of quantum chemical methods for carbocations.	0
759	Non-soluble chalcones and their potential application as corrosion coatings on carbon steel exposed to 1 M HCl solutions. 2023 , 16, 104459	Ο
758	Structural and electronic properties of Ln2Si6q: (Sm, Eu, Yb; q´=´0, 🗓) clusters. 2023 , 566, 111782	0
757	Understanding the role of host-guest interactions in enhancing oil recovery through tyclodextrin and adamantane modified copolymer. 2023 , 369, 120841	O
756	Liquid formulations of local anesthetics through Deep Eutectics based on monoterpenoids. 2023 , 369, 120852	O
755	New members of radical bridged Ln2 metallocene single-molecule magnets based on the unsubstituted 1,2,4,5-tetrazine ligand. 2022 , 10, 259-266	O
754	Magneto-structural correlations of dinickel(II) complexes with phenoxido/azido coligands: A theoretical investigation. 2023 , 811, 140241	1
753	Theoretical study on the structure and properties of Au-Au interlocking gold(I) thiolate [2]catenanes.	O
752	Ab initio simulation of amorphous GeSe3 and GeSe4. 2023 , 601, 121998	О
751	Efficient regulation of active layer morphology and interfacial charge-transfer process by porphyrin-based additive in organic solar cells. 2023 , 659, 130818	O

75 ⁰	Coupled effect of Cr and Al on interactions between a prismatic interstitial dislocation loop and an edge dislocation line in Fe-Cr-Al alloy. 2023 , 245, 118651	1
749	Density functional theory study of the sensing of ozone gas molecules by using fullerene-like Group-III nitride nanostructures. 2023 , 650, 414553	Ο
748	Density functional theory study of formation and diffusion of hydrogen, deuterium, and tritium in Pd-V intermetallic compounds. 2023 , 218, 111976	Ο
747	Theoretical investigation of the electronic absorption spectra of the glucosides. 2023 , 293, 106945	Ο
746	The catalytic performance enhanced via Electron cloud interaction of polymerized cobalt phthalocyanine/3D-graphene as bifunctional oxygen catalysts for Zn-air battery. 2023 , 556, 232471	О
745	Experimental and theoretical calculation of pKa values of substituted-2,4,6-trinitrodiphenylamines. 2023 , 371, 120926	O
744	Synthesis, biological activities and theoretical studies of a new macroacyclic Schiff base ligand and its related Co(II), Ni(II), and Cu(II) complexes: The X-ray crystal structure of the Co(II) complex. 2023 , 1276, 134770	2
743	Role of supramolecular steric compression during photoinduced intramolecular hydrogen abstraction reactions of ketones and thioketones. 2023 , 437, 114442	О
742	Dihydrolevoglycosenone as a novel bio-based nanofluid for thermal energy storage: Physiochemical and quantum chemical insights. 2023 , 59, 106365	О
741	Impact of Co doping on electronic response, momentum densities and localisation of d electrons of TiO2: Compton profiles and first-principles calculations. 2023 , 34, 105144	O
740	Toward the design of inorganicBrganic hybrid Ir(III) complexes containing borazine and benzene ligands with excellent second-order NLO responses: An appropriate substitution and Econjugated extension. 2023 , 371, 121081	Ο
739	Electron scattering and ionization of astrophysical molecules. 2023 , 204, 110686	O
738	Growth, structural, vibrational, characterization and DFT investigations of 2-methylimidazolium hydrogen oxalate dihydrate (2MIO) single crystal-towards third order NLO applications. 2023 , 1275, 134665	О
737	Crystal engineering of Pb(II)-salen coordination polymer enforced for the selective fluorescence NACs sensing activity in a dispersed aqueous medium: A combined experimental and theoretical DFT monologue. 2023 , 1276, 134717	1
736	Spectroscopic, computational, anti-bacterial studies of bivalent metal complexes of N-picolyl-amine dithiocarbamate. 2023 , 1276, 134730	1
735	A comparative analysis of different van der Waals treatments for molecular adsorption on the basal plane of 2H-MoS2. 2023 , 729, 122226	Ο
734	A DFT studies on absorbing and sensing possibilities of glucose on graphene surface doped with Ag, Au, Cu, Ni & amp; Pt atoms. 2023 , 13, 100287	0
733	An expedient synthesis spectral characteristic computational studies and target prediction through insilco studies of 24\textbf{E}thylcholest-5, 22E-dien-3-yl-2- mercapto-benzoate and 11, 17 di-hydroxy preg-4-ene-3, 20-dione-21-yl-2-mercapto-benzoate. 2023 , 1275, 134591	О

732	Reliable prediction of association (free) energies of supramolecular complexes with heavy main group elements I the HS13L benchmark set. 2022 , 24, 28831-28843	O
731	Self-diffusion and molecular association in the binary systems dimethyl sulfoxide Ethloroform and acetone Ethloroform. 2022 , 4, 100673	Ο
730	Benzaldehyde derivatives on tin electroplating as corrosion resistance for fabricating copper circuit. 2022 , 11, 3125-3137	О
729	Enzyme-substrate interactions in orotate-mimetic OPRT inhibitor complexes: A QM/MM analysis.	Ο
728	Revealing incorporation of NH2 group into the edge of carbon dots for H2O2 sensing via CN 444 hydrogen bond interaction.	O
727		Ο
726	Quantum-Chemical Calculations of the Stability of Zeolite P hosphate Complexes as Pigments of Paint Coatings. 2022 , 58, 12-19	О
725	Density Functional Theory Investigation on the Molecular Structure and Vibrational Spectra of Triclosan. 2022 , 23-32	0
724	The Effect of Molecular Structure on the Strength of CNO2 Bonds of Nitropentanes. 2022, 16, 862-868	О
723	Gas-Phase Computational Spectroscopy: The Challenge of the Molecular Bricks of Life. 2023 , 74,	O
722	Threshold Photoelectron Spectrum of the Phenoxy Radical. 2022 , 126, 9022-9030	О
721	Combining a Low Valent Molybdenum(0) Center with a Strongly Donating Mesoionic Carbene Chelate Ligand Synthesis and Structural Characterization. 2022 , 10, 216	Ο
720	Comment on Multiple locations of boron atoms in the exohedral and endohedral C60 fullerene 2022 , 106,	0
719	Analytical gradients and derivative couplings for the TDDFT-1D method.	O
718	Synthesis and Theoretical Calculations of Benzoic Acid-Based New Mono Azo Dye. 2022 , 17, 559-567	O
717	Nature of Beryllium, Magnesium, and Zinc Bonds in Carbene?MX2 (M = Be, Mg, Zn; X = H, Br) Dimers Revealed by the IQA, ETS-NOCV and LED Methods. 2022 , 23, 14668	1
716	Protocols for Understanding the Redox Behavior of Copper-Containing Systems. 2022 , 7, 45057-45066	О
715	Spin-State Splittings in 3d Transition-Metal Complexes Revisited: Benchmarking Approximate Methods for Adiabatic Spin-State Energy Differences in Fe(II) Complexes. 2022 , 18, 7442-7456	1

714	Biomimetic Approach toward Visible Light-Driven Hydrogen Generation Based on a Porphyrin-Based Coordination Polymer Gel.	O
713	Selective coordination behaviors of Uranium(VI) with novel asymmetrical tetra-alkylcarbamides. 2022 , 120924	O
712	Epoxidized Cassia fistula Seed Oil as Bio-Based Plasticizer for Poly(vinyl chloride) Soft Films. 2022 , 4, 8926-8941	1
711	Mechanism of Photocatalytic CO2 Reduction by Iron Spin-Crossover Complex with Copper Photosensitizer. 2022 , 41, 3568-3580	O
710	How Does Spin Play with the Cycloaddition to Paramagnetic Endohedral Metallofullerenes? The Curious Case of TiSc2N@C80. 2022 , 61, 19183-19192	O
709	The Role of the Redox Non-Innocent Hydroxyl Ligand in the Activation of O2 Performed by [Ni(H)(OH)]+.	O
708	DielsAlder Reactivity of Allenylboronic Acid Pinacol Ester and Related Dienophiles: Mechanistic Studies and Distortion/Interaction-Activation Strain Model Analysis. 2022 , 87, 16776-16784	O
707	Potential SARS-CoV-2 RdRp inhibitors of cytidine derivatives: Molecular docking, molecular dynamic simulations, ADMET, and POM analyses for the identification of pharmacophore sites. 2022 , 17, e0273256	1
706	Infrared Spectra and Phototransformations of meta-Fluorophenol Isolated in Argon and Nitrogen Matrices. 2022 , 27, 8248	0
705	Theoretical study of nickel-doped zinc oxide interaction with methylene blue and methyl orange using DFT methods.	O
704	Surface-Enhanced Infrared Absorption Spectroscopy for Analyzing Nucleophilic Molecules Using Ethylene Glycol Decorated TiO2 Nanosheet. 2022 , 14, 54313-54319	O
703	Two Theorems and Important Insight on How the Preferred Mechanism of Free Radical Scavenging Cannot Be Settled. Comment on Pandithavidana, D.R.; Jayawardana, S.B. Comparative Study of Antioxidant Potential of Selected Dietary Vitamins; Computational Insights. Molecules 2019, 24,	O
702	Toward Reliable and Insightful Entropy Calculations on Flexible Molecules. 2022 , 18, 7166-7178	O
701	Development of QSRR model for hydroxamic acids using PCA-GA-BP algorithm incorporated with molecular interaction-based features. 10,	O
700	Novel di and tripeptide side groups bearing acrylate polymers: synthesis, characterization, and their theoretical, and electrical properties. 2022 , 29,	O
699	Joint Studies of Spin Frustration Induced by Doping Small ZnSe Nanoparticles with Fe Atoms. 2200011	O
698	Structure I romaticity Deactivity relationship of one- and two-dimensional polyaromatic hydrocarbons and polyborazines.	O
697	Occurrence and stability of anionInteractions between phosphate and nucleobases in functional RNA molecules. 2022 , 50, 11455-11469	O

696	Testing of Exchange-Correlation Functionals of DFT for a Reliable Description of the Electron Density Distribution in Organic Molecules. 2022 , 23, 14719	1
695	Polymorphism and Mechanochromism in 2-Phenylbenzothiazole Cyclometalated PtII Complexes with Chelating N?O Ligands. 2022 , 61, 20043-20056	O
694	Rhenium Tricarbonyl Complexes of Azodicarboxylate Ligands. 2022, 27, 8159	O
693	Resolving a Half-Century-Long Controversy between (Magneto)optical and EPR Spectra of Single-Electron-Reduced [PcFe][[PcFeL][]and [PcFeX]2[Complexes: Story of a Double Flip. 2022 , 61, 20177-20199	O
692	Performance of Screened-Exchange Functionals for Band Gaps and Lattice Constants of Crystals.	O
691	Some Tautomers of Amrinone and their Interaction with Calcium Cation - DFT Treatment. 209-226	O
690	Synthesis, Structure, and Spectral-Luminescent Properties of Peripherally Fluorinated Mg(II) and Zn(II) Octaphenyltetraazaporphyrins. 2022 , 27, 8619	О
689	The chemical reaction of thioindole and [20] fullerene and the use of DFT to estimate some quantum chemical descriptors. 1-12	O
688	A theoretical evaluation for new fused remote N-heterocyclic silylenes (RNHSis) using density functional theory.	0
687	Adsorption of thioindole as a biologically active anti-cancer to C 20 fullerene in different reaction media using density functional theory.	O
686	Chemical Bonding Perspective on Low-Lying SiC4H2 Isomers: Conceptual Quantum Chemical Views. 2022 , 126, 9366-9374	O
685	The thermodynamic and kinetic aspects of midazolam ring closure from benzophenone to benzodiazepine form, its acid ${\bf B}$ ase equilibria and aromaticity: a quantum-chemical study.	O
684	Solvent-Induced Spin-State Change in Copper Corroles. 2022 , 61, 20288-20298	0
683	Triplets with a Twist: Ultrafast Intersystem Crossing in a Series of Electron Acceptor Materials Driven by Conformational Disorder.	O
682	Catalytic Dehydrogenation of Liquid Organic Hydrogen Carrier Model Compounds by CpM+ (M = Fe, Co, Ni) in the Gas Phase. 2022 , 41, 3823-3833	0
681	Crystallographic and/or magnetic properties of neutral and cationic uranium(IV) sandwiched phthalocyanine complexes. 2022 , 134870	O
680	A computational study of Aln[and Aln[and] Pt[and the effects of doping and a uniform tuning gauge for single-atom nanocatalysts. 2022 , 76,	О
679	A theoretical study of solvent effect on the excited state intramolecular proton transfer of 3-hydroxyflavone.	O

678	Preparation and Characterization of a Formally NiIVIDxo Complex with a Triplet Ground State and Application in Oxidation Reactions. 2022 , 144, 22698-22712	O
677	Soft-x-ray spectroscopy of coronene+ and (coronene+H)+ cations: The influence of hydrogenation on electronic structure and ph. 2022 , 106,	O
676	Synchrotron-based techniques for characterizing STCH water-splitting materials. 10,	O
675	N2-Reduction vs H2-Evolution in a Molybdenum- or Tungsten-Based Small-Molecule Model System of Nitrogenase.	O
674	Charge Transfer as Bridging Correlator for DSSC Efficiency and NLO Property. 2022, 7,	O
673	Manganese(II) Bromide Compound with Diprotonated 1-Hydroxy-2-(pyridin-2-yl)-4,5,6,7-tetrahydrobenzimidazole: Dual Emission and the Effect of Proton Transfers. 2022 , 10, 245	2
672	Tetrafluorosubstituted Metal Phthalocyanines: Study of the Effect of the Position of Fluorine Substituents on the Chemiresistive Sensor Response to Ammonia. 2022 , 10, 515	1
671	Superoxide intermediate in the oxygen reduction on a zinc hydroxide model corrosion product. 2022 , 157, 224702	1
670	A theoretical and experimental approaches to the use of benzoyl carbamothioyl alanine as a new ionophore for development of various mercury selective electrodes. 2022 , 121043	0
669	One-dimensional nanospace confinement effects on the chemical properties of organic molecules in carbon nanotubes: Quantum chemical calculation analyses. 2022 , 1, 175-187	O
668	Ag(III)Ag(III) Argentophilic Interaction in a Cofacial Corrole Dyad.	0
667	Electronic, vibrational, and rotational analysis of 1,2-benzanthracene by high-resolution spectroscopy referenced to an optical frequency comb. 2022 , 157, 234303	O
666	Suppressing Deep Oxidation by Detached Nano-sized Boron Oxide in Oxidative Dehydrogenation of Propane Revealed by the Density Functional Theory Study. 2022 , 126, 21263-21271	0
665	Bridges and Vertices in Heteroboranes. 2023 , 28, 190	O
664	Heterometallic Porphyrin Conjugated Polymer Thin Films Gas-Phase Approach for the Engineering of New Fused Porphyrin Systems. 2202237	O
663	Hydroxylated buckminsterfullerene complexes with endohedral europium atom. 2022, 76,	O
662	Structure, Magnetic, Opto-electronic and thermoelectric properties of A3In2As4 and A5In2As6 (A = Sr and Eu) Zintl phase compounds. 2022 , 168614	0
661	Relationship between the Structure of Fluorine-Containing Phenoxy-Imine Complexes, Their Spectral Properties and Activity in Ethylene Polymerization.	O

660	Stability of Dibromo-Dipyrromethene Complexes Coordinated with B, Zn, and Cd in Solutions of Various Acidities. 2022 , 27, 8815	O
659	Accelerated constant-voltage quantum mechanical/molecular mechanical method for molecular systems at electrochemical interfaces. 2022 , 157, 234107	O
658	Transition-metal-catalyzed synthesis of organophosphate-appended cyclobutanofullerenes from C60 and secondary propargylic phosphates. 2022 , 154299	0
657	Mechanistic Details of the Pd-catalyzed and MPAA Ligand-Enabled 땂(sp3)-H Acetoxylation of Free Carboxylic Acid.	O
656	Nitrogen- and Boron-Doped Polycyclic Aromatic Hydrocarbons as Hole Transporting Materials for Perovskite Solar Cells.	0
655	Thermochemical evaluation of adaptive and fixed density functional theory quadrature schemes. 2022 , 157, 234106	0
654	Copper Complexes with Diazoolefin Ligands and their Photochemical Conversion into Alkenylidene Complexes.	1
653	Fully tin coated coinage metal ions 🖪 pincer type bis-stannylene ligand for exclusive tetrahedral complexation.	1
652	Spectroscopic, DFT study, and molecular docking investigation of N-(3-methylcyclohexyl)-2-phenylcyclopropane-1-carbohydrazide as a potential antimicrobial drug. 2022 , 100806	0
651	Preparation and Characterization of 2,7-Diaminophenazine Supported on Nanocellulose as Novel Recyclable Nanocatalyst for Synthesis of Isoxazolo[4,3-e]indazole Derivatives and Theoretical Study on the Mechanism using a DFT Method. 1-17	Ο
650	On the Origin of the Blue Color in The Iodine/Iodide/Starch Supramolecular Complex. 2022 , 27, 8974	0
649	Divergent Mechanistic Pathways for Copper(I) Hydrophosphination Catalysis: Understanding That Allows for Diastereoselective Hydrophosphination of a Tri-substituted Styrene. 550-562	0
648	Building on the Strengths of a Double-Hybrid Density Functional for Excitation Energies and Inverted Singlet-Triplet Energy Gaps.	0
647	Salt Sensitive Purely Zwitterionic Physical Hydrogel for Prevention of Postoperative Tissue Adhesion. 2022 ,	0
646	Synthesis of Quinoline-Pyrene Derivatives and Theoretical Investigation of Their Fluorescence and Electronic Properties. 2022 , 7,	0
645	Steric and Electronic Analyses of Ligand Effects on the Stability of EMethane Coordination Complexes: A DFT Study. 2022 , 41, 3834-3844	0
644	Synthesis and Characterization of Yttrium Methanediide Silanide Complexes.	0
643	Adsorption behavior of hydrogen selenide gas on the surfaces of pristine and Ni-doped X12Y12 (X=Al, B and Y=N, P) nano-cages: a first-principles study.	0

642	Theoretical Photoelectron Spectroscopy of Low-Valent Carbon Species: A \sim 6 eV Range of Ionization Potentials among Carbenes, Ylides, and Carbodiphosphoranes.	O
641	Germanium speciation in experimental and natural sphalerite: implications for critical metal enrichment in hydrothermal Zn-Pb ores. 2022 ,	o
640	Halogen Bonds between Diiodotetrafluorobenzenes and Halide Anions: Theoretical Analysis.	1
639	Impact of Dispersion Force Schemes on Liquid Systems: Comparing Efficiency and Drawbacks for Well-Targeted Test Cases. 2022 , 27, 9034	O
638	Mechanism of Friedellarafts Acylation Using Metal Triflate in Deep Eutectic Solvents: An Experimental and Computational Study.	0
637	Samarium Diiodide Acting on AcetoneModeling Single Electron Transfer Energetics in Solution. 2022 , 27, 8673	O
636	Selective Incorporation of 5-Hydroxytryptophan Blocks Long Range Electron Transfer in Oxalate Decarboxylase.	О
635	Magneto-Structural Correlations in a Mixed Porphyrin(Cu2+)/Trityl Spin System: Magnitude, Sign and Distribution of the Exchange Coupling Constant.	0
634	Diantimony Complexes [(CpR)2Mo2(CO)4(E2-Sb2)] (CpR = C5H5, C5H4tBu) as Unexpected Ligands Stabilizing Silver(I)n (n = 1-4) Monomers, Dimers and Chains.	0
633	Development of Nonlocal Kinetic-Energy Density Functional for the Hybrid QM/MM Interaction.	o
632	Identification of Histidine-Ni (II) metal complex by Raman spectroscopy.	0
631	Solution, Crystal and in-Silico Structures of the Organometallic Vitamin B12-Derivative Acetylcobalamin and of its Novel Rhodium-Analogue Acetylrhodibalamin.	o
630	Simulation Reveals the Chameleonic Behavior of Macrocycles.	0
629	Insights into molecular cluster materials with adamantane-like core structures by considering dimer interactions.	O
628	Elucidation of the Roles of Water on the Reactivity of Surface Intermediates in Carboxylic Acid Ketonization on TiO2.	0
627	Spin-Dependent Interactions of Fe2On Clusters with H2 and O2 Molecules. 2022 , 67, 2003-2008	O
626	Use of the Far Infrared Spectroscopy for NaCl and KCl Minerals CharacterizationA Case Study of Halides from KBdawa in Poland. 2022 , 12, 1561	О
625	Hotspots and Tendencies of Energy Optimization Based on Bibliometric Review. 2023 , 16, 158	o

624	Behavior of HF and (HF) 2 inside a fullerene cage: An in silico study using different density functionals.	O
623	Are benzoylium and nitrilium ions produced from substituted 2-arene-2-oxazolines during mass spectrometry? A study based on DFT calculations, QTAIM, and ESI-MS/MS.	Ο
622	Structural Investigation of DHICA Eumelanin Using Density Functional Theory and Classical Molecular Dynamics Simulations. 2022 , 27, 8417	O
621	A Mechanistic Study on the Formation of Acetone (CH3COCH3), Propanal (CH3CH2CHO), Propylene Oxide (c-CH3CHOCH2) along with Their Propenol Enols (CH3CHCHOH/CH3C(OH)CH2) in Interstellar Analog Ices. 2022 , 941, 103	O
620	Interexcited State Photophysics I: Benchmarking Density Functionals for Computing Nonadiabatic Couplings and Internal Conversion Rate Constants.	О
619	Photocatalytic nitrogen fixation under an ambient atmosphere using a porous coordination polymer with bridging dinitrogen anions.	1
618	A multi-fidelity machine learning approach to high throughput materials screening. 2022, 8,	0
617	Study of Human Lipoxygenase by the Method of Molecular and Quantum Mechanics. 2022 , 16, 1089-1093	O
616	Experimental and Computational Studies of Ruthenium Complexes Bearing Z-Acceptor Aluminum-Based Phosphine Pincer Ligands. 2022 , 61, 20690-20698	0
615	Copper Complexes with Diazoolefin Ligands and their Photochemical Conversion into Alkenylidene Complexes.	O
614	Photomediated core modification of diaryl dihydrophenzines through three-component alkylarylation of alkenes toward organocatalyzed ATRP. 2022 ,	0
613	Investigating the Heaviest Halogen: Lessons Learned from Modeling the Electronic Structure of Astatine Small Molecules.	Ο
612	Bond Activation by a Bimetallic Gal Complex: Avenue to Intermetallic Compounds.	Ο
611	Efficient implementation of time-dependent auxiliary density functional theory.	Ο
610	A multiconfigurational approach to the electronic structure of electro-generated species of the Re 2 (EP.h 2 PCH 2 PPh 2)(S 2 CNEt 2) 4 complex.	0
609	Computational evaluation of relevant species in inorganic sulfur biochemistry.	Ο
608	CD Bond Activation in Mononuclear Lanthanide Oxocarbonyl Complexes OLn(\boxtimes -CO) (Ln = La, Ce, Pr, and Nd).	0
607	Influence of Number of Ligands and Point Group on the Electronic Structure of Co2+ Aqua-Complexes. 2022 , 61, 20743-20756	Ο

606	Solvent-free synthesis and antibacterial evaluation of novel mercaptobenzenesulfonamides.	0
605	High photocatalytic hydrogen evolution via strong built-in electric field induced by high molecular dipoles of heteroatom-annulated perylene imide supramolecule. 2022 ,	O
604	praphyne: a promising electron acceptor for organic photovoltaics. 2022 , 111526	0
603	Electronic Structure and Magnetic Properties of a High-Spin Mn III Complex: [Mn(mesacac) 3] (mesacac=1,3-Bis(2,4,6-trimethylphenyl)-propane-1,3-dionato).	O
602	Photochemical Study and Vibrational Spectra of Propiolamide Isolated in Low-Temperature Ar, Xe, and N2 Matrices. 2022 , 114487	O
601	Substituent and Solvent Effects on Excited-State Intramolecular Proton Transfer Reactions of Orotic and Isoorotic Azo Dyes.	O
600	Synthesis, antibacterial evaluation, and in silico investigations of novel 3-amino-1,2-dihydroisoquinoline derivatives.	О
599	Heterodinuclear M1M2 Complexes (M1 = Ni, Pd, Pt; M2 = Rh, Ir) Supported by a Tetradentate Phosphine Ligand and Their Application for Hydrosilylation.	O
598	A Spur to Molecular Geometry Optimization: Gradient-Enhanced Universal Kriging with On-the-Fly Adaptive Ab Initio Prior Mean Functions in Curvilinear Coordinates.	O
597	Efficient Antibacterial/Antifungal Activities: Synthesis, Molecular Docking, Molecular Dynamics, Pharmacokinetic, and Binding Free Energy of Galactopyranoside Derivatives. 2023 , 28, 219	4
596	Diantimony Complexes [(CpR)2Mo2(CO)4(脛-Sb2)] (CpR = C5H5, C5H4tBu) as Unexpected Ligands Stabilizing Silver(I)n (n = 1-4) Monomers, Dimers and Chains.	0
595	Oligomerization of ethylene promoted by methylaluminoxane activated arylchalcogenyl-sulfonate nickel(II) complexes.	O
594	Synthesis of TSF Donors Substituted with the meso-dimethylethylenedithio Group: Structures and Conducting Properties of (meso-DM-BETS)2X (XI PF6I and AsF6II	O
593	The dominant nature of Herzberg Teller terms in the photophysical description of naphthalene compared to anthracene and tetracene. 2022 , 12,	O
592	Computational Study of Iron-Catalyzed Intramolecular [2 + 2] Cycloaddition and Cycloisomerization of Enyne Acetates: Mechanism and Selectivity.	O
591	Photosensitized activation of diazonium derivatives for CB bond formation. 2023, 100490	O
590	A Thermodynamic Cycle-Based Electrochemical Windows Database of 308 Electrolyte Solvents for Rechargeable Batteries. 2212342	1
589	Thiosemicarbazonecopper/Halido Systems: Structure and DFT Analysis of the Magnetic Coupling. 2023 , 11, 31	O

588	On TAML Catalyst Resting State Lifetimes: Kinetic, Mechanistic, and Theoretical Insight into Phosphate-Induced Demetalation of an Iron(III) Bis(sulfonamido)bis(amido)-TAML Catalyst. 2023 , 62, 639-647	O
587	Luminescent Metal-Organic Framework with 2,1,3-Benzothiadiazole Units for Highly Sensitive Gossypol Sensing. 2023 , 11, 52	O
586	Solvent Phase Optimizations Improve Correlations with Experimental Stability Constants for Aqueous Lanthanide Complexes. 1-11	0
585	Switch from Local to Global Aromatic Character in MI Bius Carbon Nanobelts upon Dioxidation. Evaluation of Magnetic Behavior in Neutral and Charged species.	Ο
584	Synthesis, crystal structure, DFT, Hirshfeld surface analysis, energy framework, docking and molecular dynamic simulations of (E)-4-(4-methylbenzyl)-6-styrylpyridazin-3(2H)-one as anticancer agent. 1-20	0
583	Design and computational study of the novel nano-buds of C20@C60 with high NLO properties. 2023 , 134961	O
582	Pyridine derivatives complexes of Co (II) and Ni (II) 3-Bromobenzoates: Crystal Structure, in silico Anti-SARS-CoV-2 potential, Serum Albumin Binding Properties and Cytotoxicity.	O
581	Molecular Modelling of Ionic Liquids: Situations When Charge Scaling Seems Insufficient. 2023 , 28, 800	О
580	Understanding the Role of Intramolecular Ion-Pair Interactions in Conformational Stability Using an Ab Initio Thermodynamic Cycle.	О
579	Evaluation of Zerumbone as an EGFR Tyrosine Kinase Inhibitor by Molecular Docking Method. 2023 , 47, 18-18	O
578	Degradation by hydrolysis of three triphenylmethane dyes: DFT and TD-DFT study. 2023, 142,	0
577	First principles study on stability of base and precious metals pentlandite-like compounds. 2023 , 142,	O
576	CO gas adsorption and detection ability of boron nitride nanosheet doping with group 8B transition metal: A theoretical investigation. 2023 , 109694	1
575	Adsorption of 6-MHO on two indoor relevant surface materials: SiO2 and TiO2.	Ο
574	Diazoxide and its Tautomers - A DFT Treatment. 249-265	0
573	Spectroscopic, structural, and intermolecular interactions of 4-(2-hydroxy-3-methoxybenzylideneamino)-N-(5-methylisoxazol-3-yl)benzenesulfonamide enol-imine and keto-amine isomers. 2023 , 134978	O
572	Terminal and bridging ligand effects on M(I)?M(I) multiple bonding: A DFT investigation of the coordination in (X)[M 2 Cl] L 2 complexes (M = Cr , Fe.	О
571	Quantitative Descriptions of Dewar-Chatt-Duncanson Bonding Model: A Case Study of Zeise and Its Family Ions.	O

57°	Electronic and Steric Effects on L-Lactide Ring-Opening Polymerization with NSSN-type Zr(IV) Complexes.	O
569	Auto-accelerated dehydrogenation of alkane assisted by in-situ formed olefins over boron nitride under aerobic conditions. 2023 , 14,	0
568	4-(3-oxo-1,3-dihydroisobenzofuran-1-yl)aminobenzoic acid and its complexes: Synthesis, Crystal Structures, Theoretical Calculations and In Vitro and In silico Antibacterial Properties. 2023 , 134932	0
567	Nature-Derived Epoxy Resin Monomers with Reduced Sensitizing Capacity-Isosorbide-Based Bis-Epoxides.	O
566	Bonding in PdCl(NO) and Related Nitrosylmetal Species of the Enemark Eeltham (MNO)10 Type.	0
565	Accurate and Efficient Prediction of Vibrational Circular Dichroism Spectra of Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method.	O
564	The DNA Radical Code. Resolution of Identity in Dissociations of Trinucleotide Codon Cation Radicals in the Gas Phase.	1
563	Synthesis and Structures of Facial and Meridional Stereoisomers of [2-N,S-Chelated Ruthenium Borate Complexes.	O
562	Investigation of enhanced Am selectivity for Eu in solvent extraction using a BTPhen ligand substituted with halogen. 2023 , 13, 2476-2482	0
561	A Conformational Equilibrium in the Nitrogenase MoFe Protein with an 🖰 701 Amino Acid Substitution Illuminates the Mechanism of H2 Formation.	O
560	Investigating the Solvent Effects on Binding Affinity of PAHs E xBox4+ Complexes: An Alchemical Approach. 2023 , 127, 249-260	0
559	Ab initio study of boron-rich amorphous boron carbides.	O
558	Theoretical Study of the Reaction Mechanism of Phenol E poxy Ring-Opening Reaction Using a Latent Hardening Accelerator and a Reactivity Evaluation by Substituents. 2023 , 28, 694	0
557	Combining ab initio and ab initio molecular dynamics simulations to predict the complex refractive index of organic polymers.	O
556	Understanding Density-Driven Errors for Reaction Barrier Heights.	1
555	Gallic Acid Accelerates the Oxidation Ability of the Peracetic Acid/Fe(III) System for Bisphenol A Removal: Fate of Various Radicals.	O
554	Optical Physical Mechanisms of Helicene Carbon Nanohoop with M□ Bius Topology.	0
553	Latonduine-1-Amino-Hydantoin Hybrid, Triazole-Fused Latonduine Schiff Bases and Their Metal Complexes: Synthesis, X-ray and Electron Diffraction, Molecular Docking Studies and Antiproliferative Activity. 2023 , 11, 30	O

552	Raman microscopy tracks maturity of melanin intermediates in Botrytis cinerea, a plant pathogen. 2023 , 13, 1381-1391	О
551	Decontamination of Enoxacin containing Aqueous Phase through Hydrophobic Deep Eutectic Solvents: Solvent Regeneration and Quantum Chemical Insights. 2023 , 121254	Ο
550	Theoretical and Cyclic Voltammetric Analysis of Asparagine and Glutamine Electrocatalytic Activities for Dopamine Sensing Applications. 2023 , 13, 100	4
549	Discovery and Computational Studies of Potent Covalent Kinase Inhibitors with Bubstituent Electrophiles Targeting Cysteine.	Ο
548	Incorporation of a BoronNitrogen Covalent Bond Improves the Charge-Transport and Charge-Transfer Characteristics of Organoboron Small-Molecule Acceptors for Organic Solar Cells. 2023 , 28, 811	О
547	Synthesis, X-Ray Crystal Structure, and Identification of Potential Drug Candidate against COVID-19 Main Protease through Structure-Guided Modeling and Simulation Approach. 1-18	Ο
546	Tracking the Delocalized Proton in Concerted Proton Transfer in Bulk Water.	0
545	Multi Stimuli-Responsive Aggregation-Induced Emission Active Polymer Platform Based on Tetraphenylethylene-Appended Maleic Anhydride Terpolymers. 2023 , 15, 3543-3557	O
544	Corrosion Inhibition Potential of Thiosemicarbazide Derivatives on ALuminium: Insight from Molecular Modelling and QSARs Approaches. 915	0
543	Computational Studies of CuAAC Reaction Mechanism with Diimine and Phosphorus Ligands for Synthesis of 1,4-Disubstituted 1,2,3-Triazoles.	Ο
542	An Unusual Core Engineering on A Copper Hydride Nanoball.	0
541	Projection-Based Density Matrix Renormalization Group in Density Functional Theory Embedding. 716-722	Ο
540	In-situ observation of CGHAZ microstructure evolution of hot-rolled ship plate steel containing 0.012 yttrium under high-heat-input welding.	О
539	Dinitrogen reduction using ruthenium coordinated by nitrogen-doped graphene and cobalt complex coordinated by anionic PNP pincer ligand as catalysts and Frustrated Lewis Pair as a co-catalyst: Density Functional Theory studies.	1
538	Computational insight into a mechanistic overview of water exchange kinetics and thermodynamic stabilities of bis and tris-aquated complexes of lanthanides. 2023 , 13, 1516-1529	О
537	Nanozyme-like single-atom catalyst combined with artesunate achieves photothermal-enhanced nanocatalytic therapy in the near-infrared biowindow. 2023 ,	O
536	Machine Learning for Fast, Quantum Mechanics-Based Approximation of Drug Lipophilicity. 2023 , 8, 2046-20	<u></u> 56 ₀
535	Relativistic Effects from Heavy Main Group p-Elements on the NMR Chemical Shifts of Light Atoms: From Pioneering Studies to Recent Advances. 2023 , 9, 24	2

534	Enhanced hydrogen storage performance of Li and Co functionalized h-GaN nanosheets: DFT study. 2023 , 108415	0
533	Full Implementation, Optimization, and Evaluation of a Range-Separated Local Hybrid Functional with Wide Accuracy for Ground and Excited States.	Ο
532	Enhanced reversibility of fluorine substituted bis-BN cyclohexane for hydrogen storage: A first-principles approach. 2023 ,	0
531	Improving Lurasidone Hydrochloride Solubility and Stability by Higher-Order Complex Formation with Hydroxypropyl-tyclodextrin. 2023 , 15, 232	O
530	Some Thiocyanate Containing Heterocyclic Compounds: Synthesis, Bioactivity and Molecular Docking Study. 2023 , 8,	0
529	Synthesis and Characterization of New o -Carboranes-Based Aggregation-Induced Emission Molecules with Ultra-Large Stokes Shift. 2023 , 8,	O
528	Mechanistic Insights into the Reactive Uptake of Chlorine Nitrate at the Air Water Interface. 2023 , 145, 944-952	0
527	Synthesis and Characterization of a Bridging Cerium(IV) Nitride Complex. 2023, 145, 781-786	Ο
526	Two-photon absorption in imidazo[1,2-a]pyridine derivatives: study of nonlinear optical response and dipolar properties. 2023 , 121250	Ο
525	Inter and intra molecular dynamics in Poly(trimethylene 2,5-furanoate) as revealed by infrared and Broadband Dielectric Spectroscopies. 2023 , 125699	Ο
524	On the accuracy of orbital based multi-level approaches for closed-shell transition metal chemistry.	О
523	A Practical and Robust Zwitterionic Cooperative Lewis Acid / Acetate / Benzimidazolium Catalyst for Direct 1,4-Additions.	Ο
522	Tuning functionalized hexagonal boron nitride quantum dots for full visible-light fluorescence emission.	Ο
521	Comprehensive Study of the Ammonium SulfamateDrea Binary System. 2023 , 28, 470	1
520	Multireference Wavefunction-Based Investigation of the Ground and Excited States of LrF and LrO. 2023 , 127, 107-121	Ο
519	Computational Study of the Inhibition of RgpB Gingipain, a Promising Target for the Treatment of Alzheimer Disease.	O
518	Anisotropically Fused Clusters Form a 2D Superatomic Sheet Exhibiting Polarized Light Emission.	0
517	One-electron self-interaction error and its relationship to geometry and higher orbital occupation.	O

516	Cooperative Asymmetric Dual Catalysis Involving a Chiral N-Heterocyclic Carbene Organocatalyst and Palladium in an Annulation Reaction: Mechanism and Origin of Stereoselectivity. 1133-1148	O
515	Intramolecular Interactions (O-HD, C-HD, N-HDin Isomers of Neutral, Cation, and Anion Dopamine Molecules - A DFT Study on the Influence of Solvents (Water and Ethanol).	O
514	Synthesis and photophysical properties of BN-benzo[b]triphenylene. 2023, 813, 140313	O
513	Investigation of the anionic polyacrylamide as a potential adsorbent of crystal violet dye from aqueous solution: Equilibrium, kinetic, thermodynamic, DFT, MC and MD approaches. 2023 , 372, 121220	O
512	The effect of side chain variations on quinazoline-pyrimidine G-quadruplex DNA ligands. 2023 , 248, 115103	О
511	Quantum mechanics/molecular mechanics studies on the photoprotection mechanisms of three chalcones. 2023 , 372, 121165	O
510	QM/MM study of N501 involved intermolecular interaction between SARS-CoV-2 receptor binding domain and antibody of human origin. 2023 , 102, 107810	O
509	Recent progress in homogeneous molecular photoredox catalysis towards hydrogen evolution reaction and future perspective. 2023 , 651, 119010	O
508	A combined molecular dynamics simulation, DFT calculations, and experimental study of the adsorption of Rhodamine B dye on kaolinite and hydroxyapatite in aqueous solutions. 2023 , 36, 102647	O
507	Computational investigation of tuning the electronic ability and featured for heterofullerene based dye sensitized solar cells. 2023 , 100, 100870	O
506	A pentagonal bipyramidal Co(II) single-ion magnet based on an asymmetric tetradentate ligand with easy plane anisotropy. 2023 , 232, 116275	О
505	Multifunctional Cd-CP for fluorescence sensing of Cr(VI), MnO4pacetylacetone and ascorbic acid in aqueous solutions. 2023 , 291, 122369	O
504	A DMRG-CASPT2 investigation on the electronic states of NiSi/IO/+ (n´=´1B) clusters. 2023 , 1221, 114031	O
503	Understanding the electro-cocatalytic peroxymonosulfate-based systems with BDD versus DSA anodes: Radical versus nonradical dominated degradation mechanisms. 2023 , 309, 123120	O
502	SnS2/AuNPs surface-enhanced Raman scattering sensor for rapid and selective quantification of methimazole in serum and meat samples. 2023 , 380, 133325	O
501	The influence of double lanthanide metal atoms on the stability of germanium-based clusters. 2023 , 567, 111819	O
500	On the protonated forms of alkyl-bonded polycyclic aromatic heterocycles: Structure prediction and characterization using density functional theory. 2023 , 175, 111181	О
499	Adsorption difference of sodium alginate on marmatite (1 1 0) and galena (1 0 0): A DFT study. 2023 , 615, 156370	O

498	Triazolato Pd(II) and Pt(II) complexes of 2,6-bis(1-ethylbenzimidazol-2?-yl)pyridine formed via catalyst-free $[3'+2]$ click reactions. 2023 , 548, 121379	0
497	Insights into the HCl formation and volatilization mechanism from organochlorine in coal: A DFT study. 2023 , 338, 127271	О
496	Nanoscale synthesis, structural elucidation, DFT, and biological activity of amide appended transition metal(II) macrocyclic complexes in drug delivery system. 2022 , 75, 2843-2857	0
495	Electrochemical, computational, chemical and surface investigation on novel synthesized imine surfactants as an eco-friendly inhibitor for carbon steel corrosion in 1 M HCl.	О
494	ab initio determination of molecular geometry AND vibrational frequencies of benzotrifluoride.	0
493	The Effect of the Ancillary Ligand on Optical and Redox Properties of Cyclometalated Iridium(III) 2,5-Diphenyloxazole Complexes. 2022 , 48, 846-858	О
492	Interaction energy of Cl 2 and Br 2 with H 2 O : Exchange, dispersion and density the crucial ingredients.	O
491	Analysis of degradation products of Novichok agents in human urine by hydrophilic interaction liquid chromatographytandem mass spectrometry.	О
490	Theoretical insights into the synthesis mechanism of two amino-substituted derivatives of FOX -7.	O
489	Synthesis of Novel 1,3,4-Oxadiazole-Derived Aminophosphonates/Aminophosphonic Acids and Evaluation of Their In Vitro Antiviral Activity against the Avian Coronavirus Infectious Bronchitis Virus. 2023 , 15, 114	Ο
488	Synthesis, DFT and X-ray Studies of Trans CuCl2L2 with L Is (E)-(4-Chlorophenyl)-N-(3-phenyl-4H-1,2,4-triazol-4-yl)methanimine. 2023 , 11, 18	O
487	Synthesis and Chemistry of Dihydridoborate Group 7 Metal Complexes with Varied N,E-Chelated Ligands (E = O, NH, or S). 2023 , 62, 160-169	О
486	Ab-initio and molecular dynamics simulation of a discotic liquid crystal in ionic solution. 1-10	Ο
485	Nonfused Dimethoxybenzene Electron Acceptors in Organic Solar Cells: From Molecular Design to Structure Performance Relationship. 2023 , 127, 110-124	О
484	HONO Formation from the Oxidation Reactions of ClO, NO, and Water in the Gas-Phase and at the Air-Water Interface. 2023 , 14, 30	0
483	QM/MM Modeling of Vibrational Polariton Induced Energy Transfer and Chemical Dynamics. 2023 , 145, 377-384	1
482	Molecular Modeling Based on Time-Dependent Density Functional Theory (TD-DFT) Applied to the UV-Vis Spectra of Natural Compounds. 2023 , 5, 41-53	0
481	In-Silico Device Performance Prediction of Cosensitizer Dye Pairs for Dye-Sensitized Solar Cells. 2203536	О

480	Discovery of potent Plasmodium falciparum protein kinase 6 (PfPK6) inhibitors with a type II inhibitor pharmacophore. 2022 , 115043	1
479	Alternating Ring-Opening Metathesis Polymerization Promoted by Ruthenium Catalysts Bearing Unsymmetrical NHC Ligands. 2023 , 13, 34	O
478	Plasmonic Gradient and Plexcitonic Effects in Single-Molecule Tip-Enhanced (Resonance) Raman Spectroscopy. 2023 , 127, 476-489	0
477	Molecular modelling framework of metal-organic clusters for conserving surfaces: Langmuir sorption through the TD-DFT/ONIOM approach. 1-12	2
476	Antioxidant activity of caffeic acid: thermodynamic and kinetic aspects on the oxidative degradation pathway. 1-14	0
475	BO2 substituted novel alkyl biphenyl liquid crystalline series: dependence of geometrical and electronic properties on the alkyl chain length. 2023 , 142,	O
474	Reversible Single Electron Redox Steps Convert Polycycles with a C3P3 core to a Planar Triphosphinine.	O
473	Mechanism and Reaction Channels of Iron-Catalyzed Primary Amination of Alkenes by Hydroxylamine Reagents. 2023 , 13, 1863-1874	O
472	A computational study of the gas-phase interstellar formose-like reactions. 2023, 2431, 012091	О
471	Lithium, Tin(II), and Zinc Amino-Boryloxy Complexes: Synthesis and Characterization.	O
470	Highly Efficient Light-Driven CO 2 to CO Reduction by an Appropriately Decorated Iron Porphyrin Molecular Catalyst.	O
469	Trinuclear and Cyclometallated Organometallic Dinuclear Pt-Pyrazolato Complexes: A Combined Experimental and Theoretical Study. 2023 , 5, 187-200	O
468	Deciphering Swift Reversal of Multifaceted Photodynamics of a Novel Pyrene Appended Unsymmetrical Salicylaldehyde Azine Derivative in Aqueous and Protein Environments.	О
467	The Perfluoro Cage Effect: A Search for Electron-Encapsulating Molecules. 2023 , 8, 4972-4975	O
466	Hydrogen-Atom Electronic Basis Sets for Multicomponent Quantum Chemistry. 2023, 8, 5033-5041	O
465	Molecular cyclo-P3 complexes of the rare-earth elements via a one-pot reaction and selective reduction.	O
464	A non expected alternative Ni(0) Species in the Ni-Catalytic Aldehyde and Alcohol Arylation Reactions Facilitated by a 1,5-Diaza-3,7-diphosphacyclooctane Ligand.	0
463	Introducing a novel C50N10 azafullerene with chained nitrogen atoms on a buckyball pole; structure, stability, vibration and electronic properties.	O

462	Potential of Single Transition Metal Atom Embedded C 2 N as Efficient Catalysts for N 2 O Reduction: Theoretical Investigation. 2200680	O
461	The Highly Exothermic Hydrogen Abstraction Reaction H2Te + OH -fH2O + TeH: Comparison with Analogous Reactions for H2Se and H2S.	Ο
460	Spectroscopic and DFT Study of Alizarin Red S Complexes of Ga(III) in Semi-Aqueous Solution. 2023 , 3, 61-81	0
459	One-Pot Synthesis, E-/Z-Equilibrium in Solution of 3-Hetarylaminomethylidenefuran-2(3H)-ones and the Way to Selective Synthesis of the E-Enamines. 2023 , 28, 963	O
458	Tuning the Selectivity of Metal Oxide Gas Sensors with Vapor Phase Deposited Ultrathin Polymer Thin Films. 2023 , 15, 524	0
457	Luminescent Anionic Cyclometalated Organoplatinum (II) Complexes with Terminal and Bridging Cyanide Ligand: Structural and Photophysical Properties. 2023 , 62, 1513-1529	O
456	Five-Membered N-Heterocyclic Beryllium(I) Compounds: Fluctuating Electronic Structure with Ambiphilic Reactivity.	Ο
455	The core ionization energies calculated by delta SCF and Slater's transition state theory.	O
454	Influence of the Element and Substituent Effects on the Reactivity of Catching Reactions of Difluorocarbene by Benzene-Bridged and Group-13/Group-15-Based Frustrated Lewis Pairs. 2023 , 62, 1018-1031	0
453	Enhance Hydrogen Isotopes Separation by Alkali Earth Metal Dopant in Metal©rganic Framework. 2023 , 14, 1198-1207	1
452	Iridium-Catalyzed Chemo-, Diastereo-, and Enantioselective AllylAllyl Coupling: Accessing All Four Stereoisomers of (E)-1-Boryl-Substituted 1,5-Dienes by Chirality Pairing.	0
451	Power Efficiency Enhancement of Organic Light-Emitting Diodes Due to the Favorable Horizontal Orientation of a Naphthyridine-Based Thermally Activated Delayed Fluorescence Luminophore.	Ο
450	Role of Noncovalent Interactions in Inducing High Enantioselectivity in an Alcohol Reductive Deoxygenation Reaction Involving a Planar Carbocationic Intermediate. 2023 , 145, 2884-2900	0
449	Structural and photoelectron spectroscopic study on the heterotrinuclear nickellitanium dioxide carbonyl complexes Ni2TiO2(CO)n[$n = 24$). 2023 , 13, 3164-3172	O
448	Redox Potentials with COSMO-RS: Systematic Benchmarking with Different Databases.	0
447	Protonation of Imino Moiety in Aminoguanidine by Heterolytic OH Bond Cleavage on Phthalic Acid: Theoretical, Experimental and DNA Binding Studies. 2023 , 35, 406-416	O
446	Birth of the Hydrated Electron via Charge-Transfer-to-Solvent Excitation of Aqueous Iodide. 2023 , 14, 870-878	0
445	Quantifiable polarity match effect on CH bond cleavage reactivity and its limits in reaction design. 2023 , 52, 1399-1412	1

444	Intra- and Inter-molecular Interactions between 1-Alkanol and Benzonitrile: Computational and Thermodynamic Study.	0
443	5-Vinyl-1H-tetrazole. 2023 , 2023, M1565	O
442	Cobalt complexes with multi-dentate N-donor ligands: Redox, X-ray photoelectron spectroscopic and theoretical study. 2023 , 5, 100818	О
441	Effect of protonation on the UV/VUV photostability of cyano-substituted anthracene and phenanthrene.	O
440	Machine learning based implicit solvent model for aqueous-solution alanine dipeptide molecular dynamics simulations. 2023 , 13, 4565-4577	1
439	Conformations of Steroid Hormones: Infrared and Vibrational Circular Dichroism Spectroscopy. 2023 , 28, 771	1
438	IDType Tilted Quasi-One-Dimensional Assembly of Actinide-Embedded Coinage Metal Near-Plane Superatoms and Their Optical Properties. 2206899	О
437	Effect of void-carbon on blue-shifted luminescence in TADF molecules by theoretical simulations.	O
436	A rotational investigation of the three isomeric forms of cyanoethynylbenzene (HCC-C6H4-CN): Benchmarking experiments and calculations using the ''Lego brick'' approach.	1
435	Cyclohexane-1,3-dione Derivatives as Future Therapeutic Agents for NSCLC: QSAR Modeling, In Silico ADME-Tox Properties, and Structure-Based Drug Designing Approach. 2023 , 8, 4294-4319	O
434	Conjugated porphyrin polymer films with nickel single sites for the electrocatalytic oxygen evolution reaction.	О
433	Calculation of bandgaps in bulk and 2D materials using Harbola-Sahni and van Leeuwen-Baerends potentials. 2023 , 73-87	O
432	Semisynthetic Sesquiterpene Lactones Generated by the Sensibility of Glaucolide B to Lewis and Br listed lowry Acids and Bases: Cytotoxicity and Anti-Inflammatory Activities. 2023 , 28, 1243	О
431	Slow magnetic relaxation in a homoaxially phosphine oxide coordinated pentagonal bipyramidal Dy(iii) complex.	O
430	Binder-Driven Cathode E lectrolyte Interphase via Displacement Reaction for High Voltage Na3V2(PO4)2F3 Cathode in Sodium-Ion Batteries.	0
429	Prediction and Characterization of Two-Dimensional Zn2VN3. 2023, 14, 1148-1155	1
428	?????????. 2023,	O
427	Unprecedented Ir(iii) cationic complexes based on tridentate tetrazolate ligands: synthesis, photophysics and encapsulation in SiO2 nanoparticles.	O

426	Thomas-Fermi and Other Density-Functional Theories. 2023, 297-308	O
425	Development of quantitative structurelictivity relationship models based on electrophilicity index: a conceptual DFT-based descriptor. 2023 , 219-229	Ο
424	Glass transition, topology, and elastic models of Se-based glasses.	0
423	Noncollinear density functional theory. 2023 , 5,	O
422	Excitation energies of polycylic aromatic hydrocarbons by double-hybrid functionals: Assessing the PBE0-DH and PBE-QIDH models and their range-separated versions. 2023 , 158, 044105	1
421	Double-Hybrid Density Functional Theory for Core Excitations: Theory and Benchmark Calculations.	O
420	Synthesis and Properties of 2-Halo-1,3-diether-propanes: Diversifying the Range of Functionality in Glycerol-Derived Compounds.	0
419	Enhancing the Nlo Response of the Benzodiazepine Derivative with Different Solvents: Theoretical and Experimental Approach.	Ο
418	Prediction of the enantiomeric excess value for asymmetric transfer hydrogenation based on machine learning.	О
417	Advances in the homogeneous catalyzed alcohols homologation: The mild side of the Guerbet reaction. A mini-review. 2023 ,	O
416	Copper(ii) and silver(i) complexes with dimethyl 6-(pyrazine-2-yl)pyridine-3,4-dicarboxylate (py-2pz): the influence of the metal ion on the antimicrobial potential of the complex. 2023 , 13, 4376-4393	0
415	Computational Molecular Design to Assist Modification of Single LWalled Carbon Nanotubes with B, N, Al, Si, P, and S Dopant Atoms for Cl2 Gas Sensor Application. 2023 , 122264	O
414	Accuracy of Intermolecular interaction Energies, Particularly Those of Hetero Atom Containing Molecules Obtained by van der Waals DFT Calculations. 2023 , 8,	Ο
413	Experimental FTIR-MI and Theoretical Studies of Isocyanic Acid Aggregates. 2023 , 28, 1430	O
412	Theoretical studies on the reaction mechanisms of the oxidation of tetramethylethylene using MO3Cl (M=Mn, Tc and Re). 2023 , 120, 108419	0
411	Electronic Effect on Phenoxide Migration at a Nickel(II) Center Supported by a Tridentate Bis(phosphinophenyl)phosphido Ligand.	O
410	Tris(polypyridine)nickel(II) complexes: Synthesis, DFT and electrochemistry. 2023 , 549, 121422	0
409	Nature of the dative Nitrogen-Coinage metal bond in molecular Motors. Evaluation of NHC-M pyrazine bond (M´=´Cu, Ag, Au) from relativistic DFT. 2023 , 549, 121401	O

408	New thioether-hydrazide based ONS donor Schiff base and its Pd(II) complex: Synthesis, crystal structure, thermal analysis, hirshfeld surface analysis, quantum chemical studies and molecular docking. 2023 , 1281, 135041	0
407	Unveiling the tartrazine binding mode with dsDNA by UVDisible spectroscopy, electrochemical, and QM/MM methods. 2023 , 292, 122400	О
406	The synthesis and the mechanism of a five-membered ring formation between an isothiocyanate and an amide leading to the yield of Enzalutamide anticancer API; a joint experimental and theoretical study. 2023 , 1280, 135057	O
405	Mechanistic insights into the electroreduction of CO2 by a phosphine-nitrogen-coordinated manganese carbonyl complex for CO2-to-CO conversion over H2 formation. 2023 , 549, 121419	O
404	Using Stationary Points on Potential Energy Surfaces to Model Intermolecular Interactions and Retention in Gas Chromatography. 2004 , 59, 329-334	0
403	Structural Evolution of Monoanionic Hafnium-Doped Tin Clusters. 2022 , 58, 1249-1256	O
402	Infinitene as two fused helicoidal trails of fused rings: evaluation of the magnetic behavior of [12]infinitene and anionic species displaying global aromaticity and antiaromaticity. 2023 , 25, 8190-8197	O
401	Accelerated screening and assembly of promising MOFs with open Cu sites for isobutene/isobutane separation using a data-driven approach. 2023 , 25, 8608-8623	Ο
400	Spin polarization assisted facile CH activation by an $S = 1$ iron(iv)Bisimido complex: a comprehensive spectroscopic and theoretical investigation. 2023 , 14, 2808-2820	O
399	Superoxide targeted Burn-onl'fluorescence sensing enabled by a diselenide based quinoline probe and its in vitro anticancer activity in cancer cells. 2023 , 47, 6653-6660	O
398	Molecular dynamics study of plasmon-mediated chemical transformations.	O
397	A quinoline-benzotriazole derivative: Synthesis, crystal structure and characterization by using spectroscopic, DFT and molecular docking methods. 2023 , 5, 100916	O
396	Carbonyl (C?O)/N-based thermally activated delayed fluorescent materials with high efficiency and fast reverse intersystem crossing rate: a theoretical design and study.	0
395	Modulation of chiral spectral deflection by van der Waals force-induced molecular electropolarization in catenane oligomers. 2023 , 13, 11055-11061	O
394	Tribological performance of electrically conductive and self-lubricating polypropylenelbnic-liquid composites. 2023 , 13, 8000-8014	O
393	Magneto-structural studies on a number of doubly end-on cyanate and azide bridged dinuclear nickel(ii) complexes with {N3O} donor Schiff base ligands. 2023 , 13, 11311-11323	O
392	Theoretical and solid-state structures of three new macroacyclic Schiff base complexes and the investigation of their anticancer, antioxidant and antibacterial properties. 2023 , 13, 9418-9427	O
391	Halogen bonds with carbenes acting as Lewis base units: complexes of imidazol-2-ylidene: theoretical analysis and experimental evidence. 2023 , 25, 9636-9647	O

390	Monocarboxylate-Protected Two-Electron Superatomic Silver Nanoclusters with High Photothermal Conversion Performance.	O
389	Effect of hydration of a room temperature ionic liquid on the cationDation interaction of UO22+ and NpO2+ ions. 2023 , 47, 7391-7398	O
388	Molecular and electronic structure analysis of $[Fe(CO)4(SiX)]$ (X = O, S, Se and Te): a DFT study. 2023 , 135,	0
387	Pyrene-Based Fluorescent Probe for Dff-on-OffDequential Detection of Cu2+ and CNDwith HeLa Cells Imaging. 2023 , 11, 115	O
386	Catalytic Mechanism of Pyridoxal 5?-Phosphate-Dependent Aminodeoxychorismate Lyase: A Computational QM/MM Study. 2023 , 63, 1313-1322	0
385	Elucidating the Roles of Distinct Chemical Factors in the Hydrolytic Activities of Hetero- and Homonuclear Synthetic Analogues of Binuclear Metalloenzymes. 2023 , 13, 3131-3147	O
384	Driving a Third Generation Molecular Motor with Electrons Across a Surface. 2023 , 17, 3931-3938	0
383	Ultrafast structural changes direct the first molecular events of vision. 2023 , 615, 939-944	O
382	Consequences of Overfitting the van der Waals Radii of Ions. 2023 , 19, 2064-2074	О
381	Exchange Interactions and Magnetic Properties of a Molecular Mn18-Ring Complex.	Ο
380	Quadripartite bond length rule applied to two prototypical aromatic and antiaromatic molecules. 2023 , 29,	O
379	Cooperativity-Driven Reactivity of a Dinuclear Copper Dimethylglyoxime Complex.	Ο
378	Structure and function of the metagenomic plastic-degrading polyester hydrolase PHL7 bound to its product. 2023 , 14,	0
377	Experimental and Modeling Studies of Local and Nanoscale para-Cresol Behavior: A Comparison of Classical Force Fields.	O
376	Spectroscopic study on size-dependent optoelectronics of N-type ultra-high conductive polymer PBFDO. 2023 , 122744	0
375	Ion-Neutral Collision Cross Section as a Function of the Static Dipole Polarizability and the Ionization Energy of the Ion.	O
374	Electrophilicity-based charge transfer for developing aquatic-quantitative structure toxicity relationships (Aqua-QSTR). 2023 , 142,	0
373	Bismuth trichloride as a molecular precursor for silicon doping. 2023 , 122, 151601	O

372	Synthesis of pyrido-annelated [1,2,4,5]tetrazines, [1,2,4]triazepine, and [1,2,4,5]tetrazepines for anticancer, DFT, and molecular docking studies. 2023 , 13,	О
371	Transition metal-free synthesis of 2-aryl quinazolines via alcohol dehydrogenation. 2023, 542, 113110	O
370	Low-temperature NOx capture and reduction via NO oxidation by O3 on Cu-CHA. 2023 , 655, 119099	О
369	Performance of an anticonvulsant drug, expired gabapentin, on zinc corrosion in an acidic environment.	O
368	Remote substituent effects on catalytic activity of metal-organic frameworks: a linker orbital energy model. 2023 , 9,	O
367	Reaction mechanism and kinetics of H and Cl atom abstraction in Dichloromethane with OH radical. 2023 , 1223, 114082	0
366	A transfer-adsorption model for forward understanding the synergistic effects of additives in through-hole uniform copper thickening. 2023 , 936, 117373	0
365	Novel nanobuds from C20 with C30, C40, C50, C60 and C70 fullerene: Structural, electrical and optical properties and solvent effect. 2023 , 377, 121550	Ο
364	A bioinspired cobalt catalyst based on a tripodal imidazole/pyridine platform capable of water reduction and oxidation. 2023 , 242, 112162	Ο
363	Molecular modelling of ionic liquids: Perfluorinated anionic species with enlarged halogen substitutions. 2023 , 378, 121599	O
362	Biological determination, molecular docking and Hirshfeld surface analysis of rhoduim(I)-N-heterocyclic carbene complex: Synthesis, crystal structure, DFT calculations, optical and non linear optical properties. 2023 , 551, 121459	0
361	Heterojunction solar cell based on donor deceptor pi-conjugated naphthalene bisbenzimidazole, perylene bisbenzimidazole, and naphthalene imidazole: A spectroscopic, microscopic and DFT assessment. 2023 , 294, 122516	O
360	DFT and electrochemical study on some iron(III) complexes with 2-hydroxybenzophenones. 2023 , 550, 121445	0
359	Novel triphenylamine-based porphyrins: Synthesis, structural characterization, and theoretical investigation for dye-sensitized solar cell applications. 2023 , 1281, 135147	0
358	3-arylthioimidazo[1,2-a]pyridine derivatives: A theoretical and experimental study of its photophysical properties. 2023 , 440, 114675	0
357	Simulation and quantitative characterisation of polyvinyl alcohol grafted ethylenediamine tetraacetic acid chelating material. 2023 , 35, 105720	O
356	Theoretical study of lithium oxide clusters adsorbed on anatase TiO2 surface. 2023 , 38, 102856	O
355	Experimental and theoretical studies (DFT) on technetium extraction as HTcO4 using dicyclohexano-18-crown-6 in a blend of isodecyl alcohol and n-dodecane from acidic medium. 2023 , 160, 104684	O

354	DFT study of UVIIis-properties of thiophene-containing Cu(町iketonato)2 中 IApplication for DSSC. 2023 , 121, 108459	0
353	QSAR modeling, molecular docking and molecular dynamic simulation of phosphorus-substituted quinoline derivatives as topoisomerase I inhibitors. 2023 , 16, 104783	O
352	Efficient tuning of various coumarin based donor dyes with diketopyrrolopyrrole by forming D-A?-EA structure for high-efficiency solar cells: A DFT/TD-DFT study. 2023 , 45, 101017	О
351	Application of mesoporous CaO@g-C3N4 nanosorbent materials for high-efficiency removal of Pb (II) from aqueous solution. 2023 , 379, 121594	1
350	The interplay between spin states, geometries and biological activity of Fe(III) and Mn(II) complexes with thiosemicarbazone. 2023 , 237, 116389	О
349	Understanding of three different polyvinylpyrrolidone (PVP) based battery binders blends on graphene surfaces from first principles via DFT simulations. 2023 , 301, 127548	Ο
348	B12 and F430 models: Metal- versus ligand-centered redox in cobalt and nickel tetradehydrocorrin derivatives. 2023 , 243, 112199	0
347	DFT design of novel nano-bud from B12N12 and C60 fullerene. 2023 , 136, 109909	Ο
346	Structural evolution, electronic and magnetic properties investigation of V3Si[[n´=´14¶8) clusters based on photoelectron spectroscopy and density functional theory calculations. 2023 , 820, 140423	0
345	Nature and coordination geometry of geologically relevant aqueous Uranium(VI) complexes up to 400 °C: A review and new data. 2023 , 452, 131309	O
344	Synthesis, experimental, theoretical, and molecular dynamic studies of 1-(2,5-dimethoxy-4-methylphenyl)ethan-1-thiosemicarbazone as green inhibitor for carbon steel corrosion. 2023 , 1282, 135228	0
343	Ultra-low limit of luminescent detection of gossypol by terbium(III)-based metal-organic framework. 2023 , 452, 131289	O
342	New insights into the reactivity of the triscyclopentadienyl monothiolate uranium(IV) complexes: CS2 and CO2 insertion and redox properties. A DFT theoretical approach. 2023 , 992, 122692	0
341	Oxidative addition of halogens to a Dineophylplatinum(II) Complex: Halogen complexes and fluxional Platinum(IV) complexes. 2023 , 992, 122706	O
340	Performance enhancement of catechin-graphene quantum dot nanocomposites functionalized with carboxyl and doped/decorated with boron towards dye-sensitized solar cell applications: DFT and TD-DFT calculations. 2023 , 121, 108427	0
339	Spectroscopic, X-ray, mechanistic and DFT studies on formation of novel benzoimidazole-4-ones from cyclohexenyl carbothioamides. 2023 , 571, 111935	O
338	Experimental and theoretical investigation on piperazine-1,4-diium bis (2,5-dichlorophenoxyacetate) single crystal: A potential candidate for nonlinear optical applications. 2023 , 1285, 135520	O
337	DISSOLVE: Database of ionic solutesßolvation free energies. 2023 , 571, 113801	O

336	Emerging Trends of Computational Chemistry and Molecular Modeling in Froth Flotation: A Review.	O
335	Molecular dynamics simulations, molecular docking study, and scaled quantum calculations of 5-hydroxy-2-nitrobenzaldehyde.	O
334	Decorated crown ethers as selective ion traps: Solvent role in crown preference towards a specific ion. 2023 , 121791	О
333	Transport properties in liquids from first-principles: The case of liquid water and liquid argon. 2023 , 158, 134503	O
332	Ultrasound assisted synthesis of spirooxindole analogs catalyzed by Fe3O4@PPCA NPs: Experimental, theoretical and in vitro biological studies. 2023 , 1284, 135363	O
331	Synthesis, characterization, quantum chemical calculation, Hirshfeld surface analysis and antibacterial activity of a co-crystal of 4-Aminopyridine: p-Hydroxybenzoic acid with a water molecule. 2023 , 1284, 135309	Ο
330	A density functional theory investigation on norepinephrine interaction with amino acids and alcohols. 2023 , 1283, 135305	0
329	Synthesis and molecular structure of V-shaped liquid crystalline compounds: Spectroscopic, mesomorphic, DFT investigations, electrochemical and fluorescence studies. 2023 , 1283, 135304	O
328	An electronic structure investigation of excited state intramolecular proton transfer in amino-benzazole derivatives: Relative energies and electron density descriptors. 2023 , 441, 114738	0
327	Switching the reaction mechanisms and pollutant degradation routes through active center size-dependent Fenton-like catalysis. 2023 , 329, 122569	Ο
326	Electronic effect of substituents regulates the photocatalytic activity of PhC2Cu. 2023, 949, 169885	O
325	Therapeutic potential of oxo-triarylmethyl (oxTAM) as a targeted drug delivery system for nitrosourea and fluorouracil anticancer drugs; A first principles insight. 2023 , 122, 108469	O
324	An overview process analysis of the aromatic-aliphatic separation by liquid []quid extraction with ionic liquids. 2023 , 316, 123848	0
323	Simulation of uranyl-biomolecule interaction using a cationic dummy atom model. 2023 , 822, 140479	O
322	Hydrogenation of NO into ammonia under ambient conditions: From mechanistic investigation to multiphase catalysis. 2023 , 329, 122548	О
321	A new view on the mechanism of UV photodegradation of the tricyclic antidepressant carbamazepine in aqueous solutions. 2023 , 329, 138652	O
320	CH Activation by Iron-Vanadium Bimetallic Oxide Cluster Anions FeV 3 O 10 Land FeV 5 O 15 LA Comparison with Scandium-Vanadium Oxide Clusters.	О
319	Maximized axial helicity in a Pd2L4 cage: inverse guest size-dependent compression and mesocate isomerism. 2023 , 14, 1524-1531	Ο

318	Projected Hybrid Density Functionals: Method and Application to Core Electron Ionization. 2023 , 19, 837-847	Ο
317	A method to capture the large relativistic and solvent effects on the UV-vis spectra of photo-activated metal complexes. 2023 , 25, 6153-6163	O
316	Boron-rich amorphous boron oxides from ab initio simulations. 2023 , 604, 122130	Ο
315	Insights into the CO 2 Capture Capacity of Covalent Organic Frameworks.	O
314	Phytochemical components of Allium Jesdianum flower as effective corrosion-resistant materials for Fe(1 1 0), Al(1 1 1), and Cu(1 1 1): DFT study. 2023 , 16, 104625	O
313	The adhesive energies between Poly(3-hexylthiophene) and Polyvinylpyrrolidone for organic electronic devices: Hybrid-exchange density-functional-theory studies.	O
312	Anion recognition using enhanced halogen bonding through intramolecular hydrogen bonds b computational insight. 2023 , 47, 4439-4447	Ο
311	New Dual Inhibitors of SARS-CoV-2 Based on Metal Complexes with Schiff-Base 4-Chloro-3-Methyl Phenyl Hydrazine: Synthesis, DFT, Antibacterial Properties and Molecular Docking Studies. 2023 , 11, 63	1
310	Recent progress of theoretical research on inorganic solid state electrolytes for Li metal batteries. 2023 , 561, 232720	1
309	Modeling of tenofovir disoproxil fumarate decontamination using sodium alginate-encapsulated activated carbon: Molecular dynamics, monte carlo and density functional theory. 2023 , 663, 131057	O
308	Reaction profiles for quantum chemistry-computed [3 + 2] cycloaddition reactions. 2023 , 10,	O
307	On the Trail of Molecular Hydrophilicity and Hydrophobicity at Aqueous Interfaces. 2023 , 14, 1301-1309	O
306	Exact Two-Component TDDFT with Simple Two-Electron Picture-Change Corrections: X-ray Absorption Spectra Near L- and M-Edges of Four-Component Quality at Two-Component Cost. 2023 , 127, 1360-1376	1
305	Hydroxide Diffusion in Functionalized Cylindrical Nanopores as Idealized Models of Anion Exchange Membrane Environments: An Ab Initio Molecular Dynamics Study. 2023 , 127, 2792-2804	O
304	Solvent Dynamics of Aqueous Halides before and after Photoionization. 2023 , 127, 1399-1413	Ο
303	Benchmark Structures and Conformational Landscapes of Amino Acids in the Gas Phase: A Joint Venture of Machine Learning, Quantum Chemistry, and Rotational Spectroscopy. 2023 , 19, 1243-1260	1
302	On the Cation-Lapabilities of infinitene (II Evaluation of bonding and circular dichroism properties for Infinitene-Ag(I)n (n´=´1II) complexes from relativistic DFT calculations. 2023 , 234, 116323	O
301	Palladium-catalyzed activation of HnAAHn bonds (AHn = CH3, NH2, OH, F). 2023 ,	Ο

300	Data-Efficient Machine Learning Potentials from Transfer Learning of Periodic Correlated Electronic Structure Methods: Liquid Water at AFQMC, CCSD, and CCSD(T) Accuracy.	0
299	Effects of dispersion corrections on the theoretical description of bulk metals. 2023, 107,	O
298	Derivatives of Pyridazine with Phenoxazine and 9,9-Dimethyl-9,10-dihydroacridine Donor Moieties Exhibiting Thermally Activated Delayed Fluorescence. 2023 , 16, 1294	O
297	Spectral analysis (FT-IR, FT-Raman, UV and NMR), molecular docking, ADMET properties and computational studies: 2-Hydroxy-5-nitrobenzaldehyde. 2023 , 100, 100927	O
296	Experimental and Theoretical Study of Tetrel Bonding and Noncovalent Interactions in Hemidirected Lead(II) Phosphorodithioates: An Implication on Crystal Engineering. 2023 , 23, 2138-2154	O
295	Pyridinecarboxaldehydes: Structures, Vibrational Assignments and Molecular Characteristics Using Experimental and Theoretical Methods. 2023 , 53,	O
294	Metallomimetic Chemistry of a Cationic, Geometrically Constrained Phosphine in the Catalytic Hydrodefluorination and Amination of Ar E Bonds. 2023 , 145, 3786-3794	О
293	Aromatic self-assembled monolayers with pentafluoro-B-sulfanyl (BF5) termination: Molecular organization and charge transport properties.	O
292	In-silico approaches towards development of model irreversible HIV-1 protease inhibitors.	O
291	Molecular dynamics simulation studies of 1,3-dimethyl imidazolium nitrate ionic liquid with water. 2023 , 158, 084505	O
290	Impact of the local atomic structure on the thermal conductivity of amorphous Ge2Sb2Te5. 2023 , 158, 084504	0
289	Copper(II) coordination polymer based on l-arginine as a supramolecular hybrid inorganicBrganic material: synthesis, structural, spectroscopic and magnetic properties.	O
288	Electronic Structure and Magneto-Structural Correlations Study of Cu2UL Trinuclear Schiff Base Complexes: A 3dBfBd Case. 2023 , 127, 1475-1490	O
287	Computational studies on anticancerous Camptothecin and it derivative Camp-10 by Density Functional Theory. 2023 , 5, 100837	O
286	Model Chemistry Recommendations for Scaled Harmonic Frequency Calculations: A Benchmark Study. 2023 , 127, 1715-1735	O
285	Theoretical Study on the Gas Phase and Gasliquid Interface Reaction Mechanism of Criegee Intermediates with Glycolic Acid Sulfate. 2023 , 24, 3355	1
284	Molecular Mechanism of Conformational Crossover of Mefenamic Acid Molecules in scCO2. 2023 , 16, 1403	О
283	An Oxytocin Sensor Based on an Organic Field-Effect Transistor Functionalized with a Molecularly Imprinted Polymer. 2022 ,	Ο

282	Theoretical simulations on metal nanocluster systems. 2023 , 201-231	О
281	Discrete Singular Metallophilic Interaction in Stable Large 12-Membered Binuclear Silver and Gold Metallamacrocycles of Amido-Functionalized Imidazole and 1,2,4-Triazole-Derived N-Heterocyclic Carbenes. 2023 , 8, 6439-6454	O
280	Unusual Square Pyramidal Chalcogenide Mo5 Cluster with Bridging Pyrazolate-Ligands. 2023 , 24, 3440	О
279	On the self-consistency of DFT-1/2. 2023 , 158, 094103	O
278	Mechanism of Calcium Permeation in a Glutamate Receptor Ion Channel. 2023 , 63, 1293-1300	1
277	Switching of Redox Levels Leads to High Reductive Stability in Water-in-Salt Electrolytes.	O
276	Protocol for extraction, characterization, and computational analysis of uranium from seawater. 2023 , 4, 102100	О
275	Benchmarking two-photon absorption strengths of rhodopsin chromophore models with CC3 and CCSD methodologies: An assessment of popular density functional approximations. 2023 , 158, 094106	О
274	The effects of experimentally obtained electron correlation and polarization on electron densities and exchange-correlation potentials. 2023 , 158, 124103	О
273	A Combined Experimental and Theoretical Study of ESR Hyperfine Coupling Constants for N,N,NINETetrasubstituted p-Phenylenediamine Radical Cations. 2023 , 24, 3447	O
272	Doping of Graphene Nanostructure with Iron, Nickel and Zinc as Selective Detector for the Toxic Gas Removal: A Density Functional Theory Study. 2023 , 9, 20	О
271	Electrochemical Properties of Ru Polypyridyl Phosphonates. 2023 , 26,	O
270	Structure, Vibrational Spectra, and Cryogenic MatrixPhotochemistry of 6-Bromopyridine-2-carbaldehyde: From the Single Molecule of the Compound to the Neat Crystalline Material. 2023 , 28, 1673	О
269	The Selection of the Best Derivatization Reagents for the Determination of Polyamines in Home-Made Wine Samples. 2023 , 16, 1474	O
268	Design, Synthesis, and Optical and Electrochemical Properties of DA Type Organic Dyes with Carbazole-Based Donor Units for Efficient Dye-Sensitized Solar Cells: Experimental and Theoretical Studies. 2023 , 52, 2525-2543	О
267	X-Ray Crystallography, Spectral Analysis, DFT Studies, and Molecular Docking of (C9H15N3)[CdCl4] Hybrid Material against Methicillin-Resistant Staphylococcus aureus (MRSA). 1-23	O
266	Intramolecular interactions (O-HD, C-HD, N-HD) in isomers of neutral, cation, and anion dopamine molecules: A DFT study on the influence of solvents (water and ethanol). 2023 , 29,	0
265	Resonance Raman and Visible Micro-Spectroscopy for the In-Vivo and In-Vitro Characterization of Anthocyanin-Based Pigments in Blue and Violet Flowers: A Comparison with HPLC-ESI- MS Analysis of the Extracts. 2023 , 28, 1709	O

(2023-2023)

264	Trihalide-included (I2, Br2 and IBrClpbambus[6]urils in halogenation and iodine-catalysed reactions. 2023 , 103, 81-87	O
263	Resonance-Enhanced Multiphoton Ionization Studies of the Lower Electronically Excited States of Flavone. 2023 , 127, 1649-1655	O
262	Revealing Structural and Physical Properties of Polylactide: What Simulation Can Do beyond the Experimental Methods. 1-39	О
261	Extending density functional theory with near chemical accuracy beyond pure water. 2023, 14,	O
260	Operando characterization of rhodium catalyst degradation in hydroformylation. 2023, 13, 1788-1801	1
259	Electronic structures and ligand effect on redox potential of iron and cobalt complexes: a computational insight.	O
258	BODIPY-Based Photothermal Agents with Excellent Phototoxic Indices for Cancer Treatment. 2023 , 145, 4534-4544	O
257	Position of Geminal Substitution of 瞬mino Acid Residues Modulates Their Ability to Form Isolated Non-Helical C 12 毗urn Mimics. 2023 , 8,	O
256	The effects of cation and halide anion on the stability, electronic and optical properties of double perovskite Cs2NaMX6 (M´=1n, Tl, Sb, bi; X´=´Cl, Br, I). 2023 , 220, 112058	O
255	Regeneration and Degradation in a Biomimetic Polyoxometalate Water Oxidation Catalyst. 2023 , 13, 3007-3019	O
254	Machine Learning-Guided Computational Screening of New Candidate Reactions with High Bioorthogonal Click Potential.	O
253	Theoretical NMR and IR spectroscopic analyses of the preferred conformers of the neurotransmitter anandamide.	O
252	Cell Survival Enabled by Leakage of a Labile Metabolic Intermediate. 2023 , 40,	O
251	Stable Silapyramidanes. 2023 , 145, 4757-4764	O
250	Dibenzyl-(1S*,2S*)-2,3-dihydro-1H-indene-1,2-dicarboxylate. 2023 , 2023, M1586	O
249	Scavenging of Superoxide in Aprotic Solvents of Four Isoflavones That Mimic Superoxide Dismutase. 2023 , 24, 3815	O
248	Rational Design to Activate Tetrafluoromethane by Two-Coordinate Borinium. 2023, 62, 3518-3524	O
247	A Trinuclear High-Spin Iron(III) Complex with a Geometrically Frustrated Spin Ground State Featuring Negligible Magnetic Anisotropy and Antisymmetric Exchange. 2023 , 62, 3420-3430	O

246	Characterizing the Self-Assembly Properties of Monoolein Lipid Isosteres. 2023, 127, 1771-1779	0
245	Slow Magnetic Relaxation and Modulated Photoluminescent Emission of Coordination Polymer Based on 3-Amino-4-hydroxybenzoate Zn and Co Metal Ions. 2023 , 28, 1846	O
244	Palbociclib (PD 0332991) Interaction with Kinases. Theoretical and Comparative Molecular Docking Study. 2023 , 20,	0
243	Environmentally benign synthesis of unsymmetrical ureas and their evaluation as potential HIV-1 protease inhibitors via a computational approach.	O
242	CO Inversion on a NaCl(100) Surface: A Multireference Quantum Embedding Study. 2023, 127, 1975-1987	0
241	TFE assisted mechanochemical synthesis of new pyrazolones from Meldrum acid carbothioamides-Experimental and theoretical studies. 2023 , 539, 113002	O
240	Endohedral group-14 clusters Au@X12 (X´=´Ge, Sn, Pb) and their anions: A first-principles study. 2023 , 376, 121477	0
239	USc2C2 and USc2NC Clusters with Ut Triple Bond Character Stabilized Inside Fullerene Cages. 2023 , 145, 5645-5654	O
238	A Self-Powered, Rechargeable, and Wearable Hydrogel Patch for Wireless Gas Detection with Extraordinary Performance. 2300046	0
237	Can Copper(I) and Silver(I) be Hydrogen Bond Acceptors?.	O
236	Synthesis and Biological Evaluation of Octahydroquinazolinones as Phospholipase A2, and Protease Inhibitors: Experimental and Theoretical Exploration. 2023 , 28, 1944	O
235	Adsorption of juglone on pure and boron-doped C24 fullerene-like nano-cage: A density functional theory investigation. 2023 , 1222, 114077	O
234	NHC-Stabilised Parent Tripentelyltrielanes.	0
233	Mechanistic Basis for a Connection between the Catalytic Step and Slow Opening Dynamics of Adenylate Kinase. 2023 , 63, 1556-1569	O
232	A Multifunctional Biomass Zinc Catalyst for Epoxy-Based Vitrimers and Composites. 2023, 188, 111936	0
231	Theoretical Investigation on 1-Ethyl-3-Methylimidazolium Fluoride: A Density Functional Theory Study. 2022 , 14, 1732-1740	O
	Advitor Selection of the Control of	
230	Mechanistic understanding of geopolymerization at the initial stage: Ab initio molecular dynamics simulations.	Ο

228	Gas-phase molecular formation mechanisms of cyanamide (NH2CN) and its tautomer carbodiimide (HNCNH) under Sgr B2(N) astrophysical conditions. 2023 , 672, A49	0
227	Naphthalene Carboxylation in the Sulfate-Reducing Enrichment Culture N47 Is Proposed to Proceed via 1,3-Dipolar Cycloaddition to the Cofactor Prenylated Flavin Mononucleotide. 2023 , 89,	O
226	Mechanism and Selectivity of Copper-Catalyzed Bromination of Distal C(sp3)⊞ Bonds.	0
225	Theoretically Revealing the Response of Intermolecular Vibration Energy Transfer and Decomposition Process of the DNTF System to Electric Fields Using Two-Dimensional Infrared Spectra. 2023 , 24, 4352	o
224	Machine Learning-Boosted Design of Ionic Liquids for CO2 Absorption and Experimental Verification. 2023 , 127, 2022-2027	О
223	DFT calculation, a practical tool to predict the electrochemical behaviour of organic electrolytes in aqueous redox flow batteries. 2023 , 564, 232817	O
222	Histidine oxidation in lytic polysaccharide monooxygenase. 2023 , 28, 317-328	О
221	Quantum-Chemical Insight into Self-Organization of Complex Molecules from Acetylene and Anilines Catalyzed by Superbase KOH/DMSO: One-Pot Cascade Assembly of 1,3-Bis(arylamines). 2023 , 12,	0
220	Impedimetric sensor for iron (III) detection based on small molecule (E)-2-((phenylimino)methyl) phenol-modified platinum electrode.	0
219	Not antiaromaticity gain, but increased asynchronicity enhances the DielsAlder reactivity of tropone. 2023 , 59, 3703-3706	O
218	A quantum chemical study of the mechanism of thermal decomposition of N?-methoxy-N-methyldiazene N-oxide. 2022 , 71, 2595-2604	О
217	Application of Quantumthemical Methods in the Forensic Prediction of Psychedelic Drugs Spectra (IR, NMR, UVI/IS, and MS): A Case Study of LSD and Its Analogs. 2023 , 13, 2984	O
216	Catalytic activity of OH functionalized N-doped graphene in oxygen reduction reaction for fuel cell applications: a DFT study. 2023 , 129,	О
215	Newly Synthesized Aminothiazole Based Disazo Dyes and Their Theoretical Calculations. 1-23	O
214	NIR Absorbing Aromatic E-Ethylene Bridged Hexaphyrins (2.1.1.2.1.1): Synthesis, Characterization, and Protonation Studies. 2023 , 25, 1491-1496	0
213	Excellent Optoelectronic Properties and Low Contact Resistance of Graphene/MoS2 Heterostructure Optoelectronic Devices: First-Principles Calculation and Experimental Verification. 2023 , 5, 1676-1687	o
212	Molecular Orbitals. 2023,	O
211	Ladderphane copolymers for high-temperature capacitive energy storage. 2023 , 615, 62-66	0

210	Ein Kooperatives Rhodium/Sekund Ees Phosphinoxid [Rh/P(O) n Bu 2]-Template zur Katalytischen Hydrodefluorierung von Perfluoroarenen.	О
209	Antioxidant Properties of Thymoquinone, Thymohydroquinone and Black Cumin (Nigella sativa L.) Seed Oil: Scavenging of Superoxide Radical Studied Using Cyclic Voltammetry, DFT and Single Crystal X-ray Diffraction. 2023 , 12, 607	O
208	Exploring the Interaction Between the Newly Designed Antitumor Zn(II) Complex and CT-DNA/BSA: Spectroscopic Methods, DFT Computational Analysis, and Docking Simulation.	О
207	Entrainer selection for the extractive distillation of acrylic acid and propionic acid. 2023 , 192, 653-663	О
206	Synthesis, characterization, photophysical, and magnetic studies of mixed-ligand thorium(IV) complex of 2-hydroxy-5-sulfobenzoic acid and 1,10-phenanthroline. 2023 , 37,	0
205	A Cooperative Rhodium/Secondary Phosphine Oxide [Rh/P(O) n Bu 2] Template for Catalytic Hydrodefluorination of Perfluoroarenes.	О
204	Reactivity and Selectivity of the DielsAlder Reaction of Anthracene in [Pd6L4]12+ Supramolecular Cages: A Computational Study. 2023 , 62, 4330-4340	0
203	Computation Study on Copper-Catalyzed Aerobic Intramolecular Aminooxygenative C?C Bond Cleavage to Imides: Different Roles of Mononuclear and Dinuclear Copper Complexes. 2023 , 13, 3815-3829	О
202	Mechanistic insights into H3B•NMeH2 dehydrogenation by Co-based complexes: a DFT perspective. 2023 , 47, 6661-6672	0
2 01	Fine Tuning of Quantum Dots Photocatalysts for the Synthesis of Tropane Alkaloid Skeletons**.	Ο
200	Reactivity of Cytosine with Alkylmercury Ions in the Gas Phase: the Critical Role of the Alkyl Chain.	0
199	Isostructural coordination polymers of the tethering naphthalene anchored bis(2-methylpyridinecarboxamide) ligand: single crystal, XPS, EDS and theoretical studies. 2023 , 47, 5477-5487	,0
198	Triterpene Derivatives as Potential Inhibitors of the RBD Spike Protein from SARS-CoV-2: An In Silico Approach. 2023 , 28, 2333	0
197	Influence of Group 15 elements on the $[3 + 2]$ cycloaddition reactivity of G15 = G15 \square 15-based 1,3-dipoles with cyclooctyne. 2023 , 52, 4796-4807	O
196	Theoretical descriptions of novel silicon analogs of cyclo[18]carbon.	О
195	Mononuclear mononitrosyl iron complex with 8-mercaptoquinoline. Synthesis, structure and properties. 2023 , 1284, 135285	O
194	The Electronic Structures and Energies of the Lowest Excited States of the Ns0, Ns+, Nsland Ns-H Defects in Diamond. 2023 , 16, 1979	О
193	Synthesis of Ester-Containing Chroman-4-Ones via Cascade Radical Annulation of 2-(Allyloxy)Arylaldehydes with Oxalates under Metal Free Conditions. 2023 , 24, 5028	О

192	Performance of Density Functionals and Semiempirical 3c Methods for Small GoldII hiolate Clusters. 2023 , 127, 2242-2257	О
191	Solvation Effects on Polarizability of Aromatic Fluids. 2023 , 127, 2237-2249	O
190	Carbene Cross-Linking in Gas-Phase Peptide Ion Scaffolds. 2023 , 34, 763-774	O
189	Retrosynthesis from transforms to predictive sustainable chemistry and nanotechnology: a brief tutorial review.	O
188	New Diacetic Acids Containing Quinazolin-4(3 H)-one: Synthesis, Characterization, Anticholinergic Properties, DFT Analysis and Molecular Docking Studies. 2023 , 8,	O
187	Heteronuclear Dual Single-Atom Catalysts for Ambient Conversion of CO2 from Air to Formate. 2023 , 13, 3915-3924	O
186	Efficient Synthesis of 1H-Benzo[4,5]imidazo[1,2-c][1,3]oxazin-1-one Derivatives Using Ag2CO3/TFA-Catalyzed 6-endo-dig Cyclization: Reaction Scope and Mechanistic Study. 2023 , 28, 2403	O
185	Stabilisation and reactivity studies of donor-base ligand-supported gallium-phosphides with stronger binding energy: a theoretical approach. 2023 , 13, 7738-7751	O
184	Quantum-Chemical Prediction of Molecular and Electronic Structure of Carbon-Nitrogen Chemical Compound with Unusual Ratio Atoms: C(N20). 2023 , 24, 5172	Ο
183	A comparative study of the potential of [Os{(NHCH 2 CH 2) 3 X}] catalysts (X?N, P) for the reduction of dinitrogen to ammonia and hydrazine using FLP-H 2 as a co-catalyst by density functional theory. 2023 , 37,	O
182	Quest of Quadruple Bonding Between Two Main-Group Atoms in AeB Land AeC (Ae=Ca, Sr, Ba) and the Role of d Orbitals of Heavier Alkaline-Earth Atoms in Covalent Interactions.	Ο
181	DELTA50: A Highly Accurate Database of Experimental 1H and 13C NMR Chemical Shifts Applied to DFT Benchmarking. 2023 , 28, 2449	O
180	A Multiple Proton Transfer Mechanism for the Charging Step of the Aminoacylation Reaction at the Active Site of Aspartyl tRNA Synthetase. 2023 , 63, 1819-1832	O
179	Evaluating performance of the approximate 3D-RISM-KH molecular solvation theory for solvation free energies in alkanes and alkane-water partition coefficients. 2023 , 378, 121597	O
178	Understanding the solvation structures of glyme-based electrolytes by machine learning molecular dynamics. 2023 , 100061	0
177	Photodehydration of Ethanol Mediated by CuCl2 E thanol Complex. 2023 , 14, 2750-2757	O
176	Facile Synthesis, Crystal Structure, Hirshfeld Surface Analysis, DFT Calculation and in vitro Antifungal Evaluation of 4-Arylidene-1H-pyrazol-5(4H)-ones. 1-15	O
175	Hydrothiolation of alkynes with thioldatechol derivatives catalysed by CuNPs/TiO2: exploring the reaction mechanism by DFT calculations. 2023 , 13, 8025-8033	O

174	Disturbance of intermolecular forces: eutectics as a new tool for the preparation of vapor-phase deposition precursors. 2023 , 25, 8336-8340	О
173	Controlled Shell and Kernel Modifications of Atomically Precise Pd/Ag Superatomic Nanoclusters.	O
172	Self-Assembled Encapsulation of CuX2[(X = Br, Cl) in a Gold Phosphine Box-like Cavity with Metallophilic Autu Interactions. 2023 , 62, 4467-4475	O
171	Halogen-Bonded Mono-, Di-, and Tritopic N-Alkyl-3-iodopyridinium Salts. 2023 , 23, 2361-2374	O
170	Stereochemical Properties of Two Schiff-Base Transition Metal Complexes and Their Ligand by Using Multiple Chiroptical Spectroscopic Tools and DFT Calculations. 2023 , 28, 2571	0
169	Comparative study of the gas phase reaction of SiCl4, SiHCl3, SiH2Cl2, and SiH3Cl by thermodynamic analysis. 2023 , 62, 048002	O
168	Solvation Shell Structures of Ammonia in Reline and Ethaline Deep Eutectic Solvents. 2023 , 127, 2499-2510	О
167	Theoretical Study on the Gas-Phase and Aqueous Interface Reaction Mechanism of Criegee Intermediates with 2-Methylglyceric Acid and the Nucleation of Products. 2023 , 24, 5400	O
166	Low-Temperature Observation of the Excited-State Decay of Ruthenium-(Mono-2,2?:6?,2?-Terpyridine) lons with Innocent Ligands: DFT Modeling of an 3MLCTBMC Intersystem Crossing Pathway. 2023 , 8, 11623-11633	О
165	Assessments of DFT-based energy decomposition analysis methods for intermolecular interactions. 2023 , 158, 124116	O
164	Synergistic Catalysis in Heterobimetallic Complexes for Homogeneous Carbon Dioxide Hydrogenation. 2023 , 28, 2574	0
163	Surface-Enhanced Raman Spectroscopic Analysis of Flavoenzyme Cofactors: Guidance for Flavin-Related Bio- and Chemo- Sensors. 2023 , 11, 190	O
162	Controlling doping efficiency in organic semiconductors by tuning short-range overscreening. 2023 , 14,	O
161	Target State Optimized Density Functional Theory for Electronic Excited and Diabatic States. 2023 , 19, 1777-1789	O
160	Theoretical Research Methods Involved in This Book. 2023 , 19-43	0
159	A Comprehensive Ab Initio Study of Halogenated A ⁴⁴⁴ U and G ⁴⁴⁴ C Base Pair Geometries and Energies. 2023 , 24, 5530	О
158	Classification of doubly excited molecular electronic states. 2023 , 14, 4012-4026	0
157	Practical Aspects of Thermal Dissociation and Recombination Reactions: the Reaction Systems CF 3 $X(+M)<-EF$ 3 +X (+M) with X=F, Cl, Br, and I.	O

156	Modeling the Effect of Disorder in the Two-Dimensional Electronic Spectroscopy of Poly-3-hexyltiophene in an Organic Photovoltaic Blend: A Combined Quantum/Classical Approach. 2023 , 127, 6793-6801	О
155	Co-Catalyzed Asymmetric Hydrogenation. The Same Enantioselection Pattern for Different Mechanisms. 2023 , 24, 5568	O
154	Room-Temperature Cu-Catalyzed Amination of Aryl Bromides Enabled by DFT-Guided Ligand Design. 2023 , 145, 6966-6975	O
153	Molecular Structure of M(N13) Compounds with 12-Membered Nitrogen-Containing Cycle and Axial Nitrogen Atom (M = Mn, Fe): Quantum-Chemical Design by DFT Method. 2023 , 5, 282-293	O
152	Molecular Basis of RNA-Driven ATP Hydrolysis in DExH-Box Helicases. 2023 , 145, 6691-6701	О
151	Mechanistic aspect for the atom transfer radical polymerization of itaconimide monomers with methyl methacrylate: a computational study. 2023 ,	O
150	Experimental-Theoretical Approach for the Chemical Detection of Glyphosate and Its Potential Interferents Using a Copper Complex Fluorescent Probe. 2023 , 11, 194	O
149	Excited-State Intramolecular Proton Transfer in Salicylidene-Hydroxy Carboxylate Derivatives: Direct Detection of the Triplet Excited State of the cis-Keto Tautomer. 2023 , 127, 2765-2778	O
148	DFT Method Used for Prediction of Molecular and Electronic Structures of Mn(VI) Macrocyclic Complexes with Porhyrazine/Phthalocyanine and Two Oxo Ligands. 2023 , 16, 2394	О
147	In Silico Prediction of Stratum Corneum Partition Coefficients via COSMOmic and Molecular Dynamics Simulations. 2023 , 127, 2719-2728	O
146	Molecular Structure, Electronic Properties, Reactivity (ELF, LOL, and Fukui), and NCI-RDG Studies of the Binary Mixture of Water and Essential Oil of Phlomis bruguieri. 2023 , 28, 2684	О
145	Determination of tilt angle and its behavior in chiral smectic phases by exploring molecular conformations using complementary methods. 2023 , 107,	O
144	Unraveling Binding Mechanism and Stability of Urease Inhibitors: A QM/MM MD Study. 2023 , 28, 2697	O
143	Origin and Quantitative Description of the NESSIAS Effect at Si Nanostructures. 2200065	О
142	Chemistry in Fungal Bioluminescence: Theoretical Studies on Biosynthesis of Luciferin from Caffeic Acid and Regeneration of Caffeic Acid from Oxidized Luciferin. 2023 , 9, 369	O
141	Solvent effect on adsorption of benzylidene oxindole to C 20 nanocage: A DFT approach.	О
140	Reducing Exact Two-Component Theory for NMR Couplings to a One-Component Approach: Efficiency and Accuracy. 2023 , 19, 2010-2028	О
139	Electronic Born Dppenheimer approximation in nuclear-electronic orbital dynamics. 2023, 158, 114118	O

138	Control of Molecular Packing in Crystal and Electron Communication of Two Ferrocenyl Moieties across Chiral Isomannide or Isosorbide Bridge. 2023 , 13, 520	0
137	Expanding the Chemical Space of Arsenicin A-C Related Polyarsenicals and Evaluation of Some Analogs as Inhibitors of Glioblastoma Stem Cell Growth. 2023 , 21, 186	О
136	On the energetic and magnetic stability of neutral and charged lithium clusters doped with one and two yttrium atoms. 2023 , 25, 9656-9668	О
135	DFT Treatment of Some Cantharidine Isomers and Some Radicals from Them. 77-91	О
134	Nucleolar Essential Protein 1 (Nep1): Elucidation of Enzymatic Catalysis Mechanism by Combined Molecular Dynamics Simulation and Quantum Chemical Calculations.	0
133	Hirshfeld Atom Refinement of Metal©rganic Complexes: Treatment of Hydrogen Atoms Bonded to Transition Metals. 2023 , 127, 3020-3035	O
132	Mechanistic insight into the carboxylic derivatives formation from CO2 and ethylene over iron(0)-based catalyst. 2023 , 541, 113084	0
131	Calculated Physicochemical Properties of Glycerol-Derived Solvents to Drive Plastic Waste Recycling.	О
130	Diplomeroterpenoid G: An unusual meroterpenoid from Mimosa pudica Linn. (Mimosaceae). 2023 , 120, 154451	0
129	Ab Initio Dynamics of Graphene and Graphyne Electrodes in Vacuum and in the Presence of Electrolytes. 2023 , 127, 6515-6523	O
128	Understanding the fundamentals of TiO2 surfacesPart II. Reactivity and surface chemistry of TiO2 single crystals. 2022 , 38, 846-906	0
127	Exciton states in ultrathin crystalline films of 3,4,9,10-perylene tetracarboxyl dianhydride and their optical properties. 2023 ,	О
126	Development of AMBER Parameters for Molecular Simulations of Selected Boron-Based Covalent Ligands. 2023 , 28, 2866	О
125	Electrostatic Potential for Exploring Electron Delocalization in Infinitenes, Circulenes, and Nanobelts. 2023 , 88, 4123-4133	o
124	Process Development for a 1H-Indazole Synthesis Using an Intramolecular Ullmann-Type Reaction. 2023 , 88, 4209-4223	0
123	Electric-field induced entropic effects in liquid water.	o
122	The essential role of symmetry in understanding 3He chemical shifts in endohedral helium fullerenes. 2023 , 25, 10620-10627	0
121	Size Limiting Elemental Ferroelectricity in Bi Nanoribbons: Observation, Mechanism, and Opportunity. 2023 , 14, 3160-3167	О

120	Diffusion Monte Carlo calculations on the low-lying states of LaX ($X'=Ge$, As, Te).	О
119	Supramolecular Structure of Tris(1,10-phenanthroline)zinc(II)-Cation and N,N?,N?-tris(carboxymethyl)-1,3,5-benzenetricarboxamide-Anion: Synthesis, Crystal Structure, Vibrational Spectra, and Theoretical Investigations. 2023 , 13, 569	O
118	Noncollinear and Spin-Flip TDDFT in Multicollinear Approach.	O
117	Propane Oxidative Dehydrogenation on Nanosized Boron Carbide: Effect of Boron Content and Its Oxidation Implicated by DFT Calculations. 2023 , 127, 6280-6293	O
116	Syntheses, Characterizations, Crystal Structures, and Protonation Reactions of Dinitrogen Chromium Complexes Supported with Triamidoamine Ligands. 2023 , 62, 5320-5333	0
115	A first glance into mixed phosphinestibine moieties as protecting ligands for gold clusters. 2023 , 15, 6934-6940	O
114	Improved Elastic Image Pair Method for Finding Transition States.	О
113	Enhanced Stability of Rhombic Dodecahedron Nb15Iwith Well-Organized Superatomic States. 2023 , 127, 2912-2920	O
112	Fractional Charge Density Functional Theory and Its Application to the Electro-inductive Effect. 2023 , 14, 3329-3334	О
111	Effects of Solvents on Reaction Products: Synthesis of Endohedral Metallofullerene Oxazoline and Epoxide. 2023 , 88, 4234-4243	O
110	Transition metal (X = Mn, Fe, Co, Ni, Cu, Zn)-doped graphene as gas sensor for CO2 and NO2 detection: a molecular modeling framework by DFT perspective. 2023 , 29,	0
109	meso-Carbazole decorated BODIPYs Ian electron donor acceptor system with excellent fluorosolvato/vapochromic behavior, aggregation-induced emission, and antileishmanial activity.	O
108	Spectroscopy, docking and molecular dynamics studies on the interaction between cis and trans palladium-alanine complexes with calf-thymus DNA and antitumor activities. 1-24	О
107	Heteroligand Iron(V) Complexes Containing Porphyrazine, trans-Di[benzo]porphyrazine or Tetra[benzo]porphyrazine, Oxo and Fluoro Ligands: DFT Quantum-Chemical Study. 2023 , 24, 6442	O
106	Diastereoselective Synthesis of cis-2,6-Disubstituted Dihydropyrane Derivatives through a Competitive Silyl-Prins Cyclization versus Alternative Reaction Pathways. 2023 , 28, 3080	0
105	Rhodium-catalyzed double hydroboration of pyridine: the origin of the chemo- and regioselectivities.	O
104	Identifying novel therapeutic inhibitors to target FMS-like tyrosine kinase-3 (FLT3) against acute myeloid leukemia: a molecular docking, molecular dynamics, and DFT study. 1-19	О
103	A General Picture of Cucurbit[8]uril Host G uest Binding: Recalibrating Bonded Interactions. 2023 , 28, 3124	O

102	A Density Functional Study on Ethylene Trimerization and Tetramerization Using Real Sasol Cr-PNP Catalysts. 2023 , 28, 3101	О
101	Investigating the Thermodynamics and Kinetics of Catechin Pyrolysis for Environmentally Friendly Binders. 2023 , 8, 12693-12701	O
100	How Metal Nuclearity Impacts Electrocatalytic H2 Production in Thiocarbohydrazone-Based Complexes. 2023 , 11, 149	0
99	Novel asymmetrical azines appending 1,3,4-thiadiazole sulfonamide: synthesis, molecular structure analyses, in silico ADME, and cytotoxic effect. 2023 , 13, 10353-10366	0
98	First principles terahertz spectroscopy of molecular crystals: the crucial role of periodic boundary conditions benchmarked with experimental l-ascorbic acid spectra.	O
97	Computer-Aided and Experimental Studies of Conjugation Effect in Azobenzene-Based Compounds towards Nonlinear Optic Application. 2023 , 8,	O
96	Photoinduced Long-Distance Hydrogen-Atom Transfer in Molecules with a 7-Hydroxyquinoline Frame and a Carbaldehyde or Aldoxime Group as the Intramolecular Hydrogen Transporting Crane. 2023 , 127, 3104-3113	О
95	A metal Lewis base activation model for Pd-catalyzed hydroamination of amines and 1,3-dienes.	O
94	Energy level alignments between organic and inorganic layers in 2D layered perovskites: conjugation vs. substituent.	0
93	Exploring Antimicrobial Features for New Imidazo[4,5-b]pyridine Derivatives Based on Experimental and Theoretical Study. 2023 , 28, 3197	O
92	Propane Dehydrogenation Using Platinum Supported on Gallium-Doped Silica.	0
91	Genuine quadruple bonds between two main-group atoms. Chemical bonding in $AeF[Ae = BeBa]$ and isoelectronic EF (E = BII) and the particular role of d orbitals in covalent interactions of heavier alkaline-earth atoms.	O
90	Regulating the photophysical properties of ESIPT-based fluorescent probes by functional group substitution: a DFT/TDDFT study. 2023 , 29,	0
89	DFT+U-type functional derived to explicitly address the flat plane condition. 2023, 107,	O
88	Photoelectrocatalytic Dioxygen Reduction Based on a Novel Thiophene-Functionalized Tricarbonylchloro(1,10-phenanthroline)rhenium(I). 2023 , 28, 3229	0
87	Cost-Effective Simulations of Vibrationally-Resolved Absorption Spectra of Fluorophores with Machine-Learning-Based Inhomogeneous Broadening.	O
86	Density functional theory (DFT) simulation and approach to property-driven investigations in ceramic and composites materials. 2023 , 461-490	0
85	Ultrafast Quantum Processes at the Nanoscale: Insights from Modeling. 2023 , 139-171	O

84	A Tetraiodomanganate(II) Compound with P,P?-Diprotonated Bis(2-Diphenylphosphinophenyl)Ether Manifesting Unexpected Short Luminescence Lifetime. 2023 , 64, 398-409	О
83	ETS-NOCV and molecular electrostatic potential-based picture of chemical bonding. 2023,	О
82	The activity of Fe/Co/Ni multi-metal doped electrocatalysts for oxygen reduction reaction.	O
81	Quantum Chemical Study of the Mechanism of (E,Z)-1,3-Diphenyl-2-Aza-1,3-Diene Stereoselective Formation from N-Benzyl-1-Phenylethane-1-Imine and Acetylene in the KOt-Bu/DMSO Superbasic Environment. 2023 , 64, 386-397	0
80	Separation of phenolic compounds from water by using monoterpenoid and fatty acid based hydrophobic deep eutectic solvents. 2023 , 381, 121806	O
79	In silico and in vitro investigation of bile salts as coformers for edaravone coamorphous dispersion-Part I. 2023 , 253, 105302	O
78	A computational investigation of galactopyranoside esters as antimicrobial agents through antiviral, molecular docking, molecular dynamics, pharmacokinetics, and bioactivity prediction. 1-16	0
77	Two Shared Icosahedral Metallacarboranes through Iron: A Joint Experimental and Theoretical Refinement of MI Ssbauer Spectrum in [Fe(1,2-C2B9H11)2]Cs. 2023 , 8, 13993-14004	O
76	Accurate Interaction Energies of CO2 with the 20 Naturally Occurring Amino Acids.	O
75	DFT Study on the Mechanisms of Iron-Catalyzed Ortho CH Homoallylation of Aromatic Ketones with Methylenecyclopropanes.	O
74	Design of a minimal di-nickel hydrogenase peptide. 2023 , 9,	O
73	High-density frustrated Lewis pairs based on Lamellar Nb2O5 for photocatalytic non-oxidative methane coupling. 2023 , 14,	O
72	Cytotoxic properties of fac-Re(CO)3 complexes with quinoline Coligands: Insights on the mode of cell death and DNA fragmentation. 2023 , 121521	0
71	Performance of Common Density Functionals for Excited States of Tetraphenyldibenzoperiflanthene. 2023 , 127, 3265-3273	O
70	Gas-phase detection of oxirene. 2023 , 9,	0
69	Molecular Engineering to Tune Functionality: The Case of Cl-Substituted [Fe(terpy)2]2+.	O
68	Synergy of Magnetic Anisotropy and Ferromagnetic Interaction Triggering a Dimeric Cr(II) Zero-Field Single-Molecule Magnet.	О
67	Understanding the Stability of an Unprecedented Si B e Bond within Quantum Confinement.	O

66	Interactions between curcumin and human salt-induced kinase 3 elucidated from computational tools and experimental methods. 14,	O
65	Reimagining the Wave Function in Density Functional Theory: Exploring Strongly Correlated States in Pancake-Bonded Radical Dimers.	O
64	A conserved hymenopteran-specific family of cytochrome P450s protects bee pollinators from toxic nectar alkaloids. 2023 , 9,	0
63	The role of ETFS amino acids on the stability and inhibition of p53-MDM2 complex of anticancer p53-derivatives peptides: Density functional theory and molecular docking studies. 2023 , 122, 108472	O
62	Accurate Structures and Spectroscopic Parameters of Phenylalanine and Tyrosine in the Gas Phase: A Joint Venture of DFT and Composite Wave-Function Methods.	0
61	First-Principles Simulations of Salt-Concentrated Electrolytes for Li-Based Batteries: How Solvents Tune Solvation Structures and Li-Ion Conductivity.	O
60	Antioxidant Activity via Free Radical Scavenging of Pitavastatin and Its Hydroxylated Metabolites. A Quantum Chemical Attempt Aiming to Assist Drug Development.	O
59	Peroxo-Diiron(III/III) as the Reactive Intermediate for N-Hydroxylation Reactions in the Multidomain Metalloenzyme SznF: Evidence from Molecular Dynamics and Quantum Mechanical/Molecular Mechanical Calculations. 5808-5818	O
58	A Bifunctional NHC-Aryloxido Titanium Catalyst for the Ring-Opening Polymerization of Caprolactone and an Unusual Fragmentation of Its Ligand Backbone.	0
57	COSMO-RS Exploration of Highly CO2-Selective Hydrogen-Bonded Binary Liquid Absorbents under Humid Conditions: Role of Trace Ionic Species.	O
56	Theoretical Study on the Interaction between Cis-2 Bis(benzofuro) [60]fullerene Derivative and NO Dominated Double Gas Molecule. 2023 ,	O
55	Phototunable Cell Killing by Photochromic Diarylethene of Thiazoyl and Thienyl Derivatives.	O
54	Photoinduced Dynamics of 13,13?-Diphenylpropyl-tarotene. 2023 , 28, 3505	0
53	Cobalt and Iron Phthalocyanine Derivatives: Effect of Substituents on the Structure of Thin Films and Their Sensor Response to Nitric Oxide. 2023 , 13, 484	O
52	Structural, electronic properties and optical absorption of oxygen vacancy cluster defects in KDP crystals: hybrid density functional theory investigation.	O
51	Electronic effects of the substituted dopants on stability and reactivity of difuranosilapyridine-4-ylidenes: DFT approach.	O
50	Clay-supported acidic ionic liquid as an efficient catalyst for conversion of carbohydrates to 5-hydroxymethylfurfural. 2023 , 121847	0
49	Catalytic production of ammonia from dinitrogen employing molybdenum complexes bearing N-heterocyclic carbene-based PCP-type pincer ligands.	O

48	Exploring the Potential of Anthracene Derivatives as Fluorescence Emitters for Biomedical Applications.	О
47	Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins. 2023 , 28, 3487	O
46	Some Isomers of Nevirapine - A DFT Study. 93-109	0
45	Synthesis, Photophysical, and (Spectro)Electrochemical Properties of New Benzo[1,2-c][1,2,5]thiadiazoles and Benzo[1,2-d][1,2,3]triazoles Fused with Two Thiazole Rings.	O
44	Defect formation energy for various charge states of point defects in CdGa2S4.	0
43	Control and regulation of the performance of fullerene-based dye-sensitized solar cells with D-D-A structure by external electric fields.	O
42	High photovoltaic performance (23.75) of triazatruxene-based dye-sensitized solar cells containing different [bridges: computational investigation.	0
41	Adsorption-Controlled Wettability and Self-Cleaning of TiO2.	O
40	Lysosome directed red light photodynamic therapy using glycosylated iron(III) conjugates of boron-dipyrromethene. 2023 , 112226	0
39	Molecular modeling and DFT studies on the antioxidant activity of Centaurea scoparia flavonoids and molecular dynamics simulation of their interaction with ¶actoglobulin. 2023 , 13, 12361-12374	O
38	Thermochemistry of the Smallest Hyperbolic Paraboloid Hydrocarbon: A High-Level Quantum Chemical Perspective. 2023 , 9, 41	0
37	Constrained density functional theory calculations for estimation of forward and backward intermolecular charge transfer energy.	O
36	Structural Features of 4-VP-HEMA-SiO2 Hybrid Membranes and Their Proton Conductivity. 2023, 5, 92-97	О
35	SYNTHESIS, STRUCTURE, DNA/BSA BINDING, ANTIBACTERIAL AND MOLECULAR DOCKING STUDIES OF TETRADENTATE ONNO SCHIFF BASE METAL COMPLEXES. 2023 , 135570	O
34	Tailoring the Bystem of benzimidazole ligands towards stable light-harvesting cyclometalated iridium(III) complexes.	O
33	Computational Study on a Transfer Hydrogenation Catalysed by a Ru(II) Bis-Pyrazolyl Pyridine Complex.	О
32	Concerted Proton-Coupled Electron Transfer to a Graphite Adsorbed Metalloporphyrin Occurs by Band to Bond Electron Redistribution.	О
31	Magneto®tructural maps and bridged-ligand effect for dichloro-bridged dinuclear copper(ii) complexes: a theoretical perspective. 2023 , 13, 12430-12437	О

30	Design and computational studies on energetic compounds composing bridged bis triazolo-triazine framework. 2023 , 111939	O
29	Computational Methods in the Drug Delivery of Carbon Nanocarriers onto Several Compounds in Sarraceniaceae Medicinal Plant as Monkeypox Therapy. 2023 , 11, 84	O
28	Sensitized Singlet Fission in Rigidly Linked Axial and Peripheral Pentacene-Subphthalocyanine Conjugates.	O
27	Probing Superatomic Orbitals of Sc-Doped and Undoped Silver Cluster Anions via Photoelectron Angular Anisotropy. 4011-4018	O
26	Density functional theory-based molecular modeling. 2023 , 95-113	O
25	Transient and general synthesis of high-density and ultrasmall nanoparticles on two-dimensional porous carbon via coordinated carbothermal shock. 2023 , 14,	O
24	Search for a Grotthuss mechanism through the observation of proton transfer. 2023, 6,	O
23	Meta-GGA Density Functional Calculations on Atoms with Spherically Symmetric Densities in the Finite Element Formalism.	O
22	The gas-phase pyrolysis of cyclopropylamine. A computational study on the kinetics and reaction mechanism. 2023 , 253, 112774	O
21	Hydrogen-Bonding Receptor substituted BODIPYs as Selective ON-OFF Fluorimetric Sensors for Fluoride Ions in Polar Aprotic Organic Solvents - A Molecular-level Understanding based on Experimental and Theoretical Studies. 2023 , 114780	O
20	A molecular electron density theory study of mechanism and selectivity of the intramolecular [3+2] cycloaddition reaction of a nitronelinylphosphonate adduct.	О
19	Vibrational circular dichroism spectra of natural products by means of the nuclear velocity perturbation theory. 2023 , 122769	O
18	Design and synthesis of uracil/thiouracil based quinoline scaffolds as topoisomerases I&II inhibitors for chemotherapy: A new hybrid navigator with DFT calculation. 2023 , 106560	O
17	Dative quadruple bonds between d 10 transition metals and beryllium in BeM (PMe 3) 2 and BeM (CO) 2 (M $=$ Ni, Pd , and Pt.	O
16	Indotricarbocyanine dyes relevant for photodynamic therapy and their radicals: Substituent effects studied by optical and electrochemical methods. 2023 , 216, 111344	O
15	An organic (4-nitrophenyl) methionine single crystal: growth, optical properties and quantum chemical investigations for NLO device fabrication.	O
14	Experimental and Theoretical Investigation of Inclusion Complexes of 红yclodextrin with Fingolimod. 2023 , 97, 469-476	O
13	Intramolecular Hiyama Coupling: Synthesis of 1,8,13-Trisubstituted Chiral Triptycenes with Three Different Substituents by Intramolecular Substituent Transfer.	O

CITATION REPORT

12	Reactivity of a Free Aluminylene towards Boron Lewis Acids: Accessing Aluminum-Boron-Bonded Species.	О
11	Arylazo under Extreme Conditions: [2 + 2] Cycloaddition and Azo Metathesis. 2023 , 127, 8482-8492	0
10	Pyrene-Based Polyimide Covalent Organic Framework with Temperature-Dependent Fluorescence.	0
9	A semilocal machine-learning correction to density functional approximations. 2023, 158,	O
8	Computational Study of the Fe(II) and Eketoglutarate-Dependent Aryloxyalkanoate Dioxygenase (AAD-1) in the Degradation of the Herbicide 2,4-Dichlorophenoxyacetic Acid. 2023 , 63, 2759-2768	0
7	Including vibrational effects in magnetic circular dichroism spectrum calculations in the framework of excited state dynamics. 2023 , 158,	o
6	Ab Initio Molecular Dynamics: A Guide to Applications. 2023,	O
5	Ab Initio Molecular Dynamics: A Guide to Applications. 2023, Mono-nuclear ruthenium catalyst for hydrogen evolution. 2023,	0
5	Mono-nuclear ruthenium catalyst for hydrogen evolution. 2023,	0
5	Mono-nuclear ruthenium catalyst for hydrogen evolution. 2023 , Optical properties of in-plane chemically ordered i-MAX structures. 2023 , 25, 13665-13672 Insights into the carbonization mechanism of PAN-derived carbon precursor fibers and	0