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2236 Phase Segregation in Potassium-Doped Lead Halide Perovskites from 39K Solid-State NMR at 21.1 T.

2235 Synthesis of a Cyclic Co₂Sn₂ Cluster Using a Co Synthon.

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2231 Directed Hydroxylation of sp^2 and sp^3 CH Bonds Using Stoichiometric Amounts of Cu and H_2O_2 .

2230 Dipole, dipole-quadrupole, and dipole-octopole polarizability of adamantane, $\text{C}_{10}\text{H}_{16}$, from refractive index measurements, depolarized collision-induced light scattering, conventional ab initio and density functional theory calculations. **2001**, 115, 7957-7967 88

2229 pK(a) Calculations suggest storage of an excess proton in a hydrogen-bonded water network in bacteriorhodopsin. **2001**, 312, 203-19 105

2228 [2+2] versus [3+2] addition of metal oxides across C=C double bonds: toward an understanding of the surprising chemo- and periselectivity of transition-metal-oxide additions to ketene. **2001**, 123, 10085-94 44

2227 DFT studies on the copolymerization of alpha-olefins with polar monomers: ethylene-methyl acrylate copolymerization catalyzed by a Pd-based diimine catalyst. **2001**, 123, 12266-78 70

2226 Nickel dithiolenes revisited: structures and electron distribution from density functional theory for the three-member electron-transfer series $[\text{Ni}(\text{S}_2\text{C}_2\text{Me}_2)_2]_{0,1,-2}$. **2001**, 40, 4257-62 129

2225 Molecular and electronic structures of six-coordinate W complexes and polyanions containing tri-oxo groups. **2001**, 20, 3101-3111 13

2224 Understanding the nature of the bonding in transition metal complexes: from Dewar's molecular orbital model to an energy partitioning analysis of the metal-ligand bond. **2001**, 635, 9-23 134

2223 Base-induced 1,4-elimination: insights from theory and mass spectrometry. **2001**, 20, 347-61 24

2222 Iron bispentazole $\text{Fe}(\eta^5\text{-N}_5)_2$, a theoretically predicted high-energy compound: structure, bonding analysis, metal-ligand bond strength and a comparison with the isoelectronic ferrocene. **2001**, 7, 4155-63 147

2221 Excited state polarizabilities of conjugated molecules calculated using time dependent density functional theory. **2001**, 115, 10014-10021 84

2220 Collision effects in the nonlinear Raman response of liquid carbon disulfide. **2002**, 116, 3277-3285 25

2219 Improving Difficult Reaction barriers with self-interaction corrected density functional theory. **2002**, 116, 7806-7813 120

2218 Structural and electronic properties of $\text{Fe}^{3+} \text{-O}^{2-}$ Pairs in $\text{KM} \text{F}_3$ lattices ($\text{M}=\text{Mg}, \text{Zn}$): Is the superposition model valid?. **2002**, 157, 931-935 2

2217 Liquid xenon as an ideal probe for many-body effects in impulsive Raman scattering. **2002**, 117, 1181-1187 5

2216 RECENT ADVANCES IN ELECTRONIC STRUCTURE THEORY. **2002**, 01, 109-136 6

2215	Multiscale modeling of anisotropic wet chemical etching of crystalline silicon. 2002 , 60, 467-473	15
2214	Rules for Understanding and Designing Novel Molecule-Based Rare-Earth Magnetic Compounds. 2002 , 755, 1	4
2213	Response Properties of Furan Homologues by Time-Dependent Density Functional Theory. 2002 , 106, 10380-10390	9
2212	New Titanium Complexes Bearing Two IndolideImine Chelate Ligands for the Polymerization of Ethylene. 2002 , 35, 4880-4887	88
2211	Phosphorus NMR Chemical Shifts with Self-Interaction Free, Gradient-Corrected DFT. 2002 , 106, 1088-1099	46
2210	DFT Study of Olefin versus Nitrogen Bonding in the Coordination of Nitrogen-Containing Polar Monomers to Diimine and Salicylaldiminato Nickel(II) and Palladium(II) Complexes. Implications for Copolymerization of Olefins with Nitrogen-Containing Polar Monomers. 2002 , 21, 1603-1611	54
2209	Unified View of the Interaction of Tetrakis(carboxylato)dirhodium(II) with Axial Donor/Acceptor Ligands. 2002 , 21, 4303-4305	31
2208	On the competition of the purine bases, functionalities of peptide side chains, and protecting agents for the coordination sites of dicationic cisplatin derivatives. 2002 , 124, 5834-42	85
2207	Excited-State Dynamics of Cofacial Pacman Porphyrins. 2002 , 106, 11700-11708	58
2206	Density Functional Study of Benzene Adsorption on Pt(111). 2002 , 106, 7489-7498	147
2205	An ab Initio Study of the Interaction of SCN ⁻ with a Silver Electrode: The Prediction of Vibrational Frequencies. 2002 , 106, 1450-1457	37
2204	Orbital Interactions in Hydrogen Bonds Important for Cohesion in Molecular Crystals and Mismatched Pairs of DNA Bases. 2002 , 2, 239-245	49
2203	Molecular Structure and Bond Characterization of the Fischer-Type ChromiumCarbene Complexes (CO) ₅ Cr(X)R (X = H, OH, OCH ₃ , NH ₂ , NHCH ₃ and R = H, CH ₃ , CHCH ₂ , Ph, C≡CH). 2002 , 21, 4182-4191	71
2202	Nature of the Transition-Metal π -H ₂ Bond in TM(CO) ₃ X ₂ (π -H ₂) (TM = Cr, Mo, W; X = CO, PH ₃ , PCl ₃ , PMe ₃) Complexes 2002 , 21, 5803-5809	26
2201	Orbital symmetry as a tool for understanding the bonding in Krossing's cation. 2002 , 124, 12312-8	13
2200	Electronic structure of the alpha and beta isomers of [Mo(8)O(26)](4-). 2002 , 41, 3500-7	47
2199	The Electronic Structure and Stability of the Isomers of Octamolybdate. 2002 , 106, 12151-12160	54
2198	A structural model for the high-valent intermediate Q of methane monooxygenase from broken-symmetry density functional and electrostatics calculations. 2002 , 124, 5890-4	74

2197	Mössbauer quadrupole splittings and electronic structure in heme proteins and model systems: a density functional theory investigation. 2002 , 124, 13921-30	59
2196	The short N [bond] F bond in N(2)F(+) and how Pauli repulsion influences bond lengths. Theoretical study of N(2)X(+), NF(3)X(+), and NH(3)X(+) (X [double bond] F, H). 2002 , 124, 1500-5	43
2195	Isomorphous Substitution of Mn(II) into Aluminophosphate Zeotypes: A Combined High-Field ENDOR and DFT Study. 2002 , 106, 7509-7519	18
2194	Density functional study of the mechanism of a tyrosine phosphatase: I. Intermediate formation. 2002 , 124, 10225-35	41
2193	Do nonplanar distortions of porphyrins bring about strongly red-shifted electronic spectra? Controversy, consensus, new developments, and relevance to chelatases. 2002 , 124, 8099-103	122
2192	Chiroptical properties from time-dependent density functional theory. II. Optical rotations of small to medium sized organic molecules. 2002 , 117, 581-592	168
2191	Structure and Bonding in [W10O32]n- Isopolyanions. 2002 , 106, 6114-6120	19
2190	Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules. 2002 , 116, 6930-6940	346
2189	Catalytic Behavior of Bis(Pyrrolide-Imine) and Bis(Phenoxy-Imine) Titanium Complexes for the Copolymerization of Ethylene with Propylene, 1-Hexene, or Norbornene. 2002 , 42, 353-359	31
2188	Electronic absorption, resonance Raman, and electrochemical studies of planar and saddled copper(III) meso-triarylcorroles. Highly substituent-sensitive Soret bands as a distinctive feature of high-valent transition metal corroles. 2002 , 124, 8104-16	211
2187	Theoretical and experimental studies of the opto-electronic properties of positively charged oligo(phenylene vinylene)s: Effects of chain length and alkoxy substitution. 2002 , 117, 11366-11378	61
2186	Nature of the Metal-Ligand Bond in M(CO)5PX3 Complexes (M = Cr, Mo, W; X = H, Me, F, Cl): Synthesis, Molecular Structure, and Quantum-Chemical Calculations. 2002 , 21, 2921-2930	145
2185	Structure and bonding in [M(6)O(19)](n-) isopolyanions. 2002 , 41, 1761-70	52
2184	Validation study of meta-GGA functionals and of a model exchange-correlation potential in density functional calculations of EPR parameters. 2002 , 4, 5467-5474	63
2183	Challenge of the Copolymerization of Olefins with N-Containing Polar Monomers. Systematic Screening of Nickel(II) and Palladium(II) Catalysts with Brookhart and Grubbs Ligands. 2. Chain-Propagation Barriers, Intrinsic Regioselectivity, and Curtin-Hammett Reactivity 2002 , 21, 4432-4441	51
2182	Photophysics of trioxatriangulenium ion. electrophilic reactivity in the ground state and excited singlet state. 2002 , 1, 763-73	26
2181	A Density Functional Embedded Cluster Study of Proposed Active Sites in Heterogeneous Ziegler-Natta Catalysts. 2002 , 35, 7815-7829	95
2180	The Process of Mn(II) Incorporation into Aluminophosphate Zeotypes through High-Field ENDOR Spectroscopy and DFT Calculations. 2002 , 106, 9086-9097	22

2179	Structures, Metal-Ligand Bond Strength, and Bonding Analysis of Ferrocene Derivatives with Group-15 Heteroligands Fe(η -E5) ₂ and FeCp(η -E5) (E = N, P, As, Sb). A Theoretical Study 2002 , 21, 3351-3359	114
2178	Reinvestigation of Hydrogen Bond Effects on the Polarizability and Hyperpolarizability of Urea Molecular Clusters. 2002 , 106, 8954-8958	71
2177	Conformational changes of an oxovanadium complex probed by ENDOR spectroscopy and DFT calculations. 2002 , 4, 4937-4943	13
2176	Study of silver atoms in anionic position in KCl. 2002 , 157, 829-831	2
2175	Anaerobic enzyme-substrate structures provide insight into the reaction mechanism of the copper-dependent quercetin 2,3-dioxygenase. 2002 , 99, 16625-30	153
2174	Ultranonlocality in time-dependent current-density-functional theory: application to conjugated polymers. 2002 , 88, 186401	203
2173	A density functional study of S(N) ₂ substitution at square-planar platinum(II) complexes. 2002 , 41, 6614-22	224
2172	The Mechanism of Catalytic Enantioselective Fluorination: Computational and Experimental Studies. 2002 , 114, 1021-1024	23
2171	The mechanism of catalytic enantioselective fluorination: computational and experimental studies. 2002 , 41, 979-82	102
2170	Density functional studies of the ground- and excited-state potential-energy curves of stilbene cis-trans isomerization. 2002 , 3, 167-78	65
2169	Hole mobility in DNA: effects of static and dynamic structural fluctuations. 2002 , 3, 536-9	105
2168	A cylindrical polymer: a stack of discotic triphenylene within comblike polymethacrylate. 2002 , 3, 539-43	11
2167	Experimental Observation and Confirmation of Icosahedral W@Au ₁₂ and Mo@Au ₁₂ Molecules. 2002 , 114, 4980-4983	49
2166	Experimental observation and confirmation of icosahedral W@Au ₁₂ and Mo@Au ₁₂ molecules. 2002 , 41, 4786-9	299
2165	Hydrogenation kinetics of toluene on Pt/ZSM-22. 2002 , 90, 117-129	56
2164	Atomistic simulations of surface coverage effects in anisotropic wet chemical etching of crystalline silicon. 2002 , 202, 160-182	36
2163	The unique spectroscopic behavior of the Fe(III)-nitroprusside: a DFT study of the vibronic coupling in the ground and in the lowest excited state. 2002 , 592, 79-93	23
2162	Bonding in [W ₄ O ₁₆] ⁸⁻ isopolyanions. 2002 , 21, 2201-2206	15

2161	Density functional study of the vibrational frequencies of Lindqvist polyanions. 2002 , 279, 143-159	31
2160	Signal transduction in the photoactive yellow protein. II. Proton transfer initiates conformational changes. 2002 , 48, 212-9	36
2159	Signal transduction in the photoactive yellow protein. I. Photon absorption and the isomerization of the chromophore. 2002 , 48, 202-11	61
2158	Density functional study of the adsorption of 1,4-cyclohexadiene on Pt(111): origin of the C-H stretch red shift. 2002 , 513, 315-327	25
2157	The adsorption of nitrogen oxides and water on rare-earth ion-exchanged ZSM-5: a density functional study. 2002 , 202, 283-288	8
2156	A matrix isolation and DFT study of the generation and characterization of monomeric vapour phase platinum chlorides. 2002 , 351, 319-326	19
2155	Time-dependent density functional study of the static second hyperpolarizability of BB-, NN- and BN-substituted C60. 2002 , 359, 524-529	19
2154	Mechanism of ruthenium-catalyzed olefin metathesis reactions from a theoretical perspective. 2002 , 124, 8965-73	234
2153	Quantum-Chemical Calculation of Matrix Elements in a Basis of Functions with Polynomial Tails. 2003 , 44, 531-537	
2152	Numerically Integrable Confined Basis Functions for Band Structure Calculations. 2003 , 44, 911-917	1
2151	Supramolecular interactions between fullerenes and porphyrins. 2003 , 125, 6072-3	181
2150	L-edge X-ray absorption spectroscopy of non-heme iron sites: experimental determination of differential orbital covalency. 2003 , 125, 12894-906	173
2149	Accuracy of geometries: influence of basis set, exchange-correlation potential, inclusion of core electrons, and relativistic corrections. 2003 , 110, 34-41	96
2148	Relativistic DFT calculations of polyoxotungstate 183W NMR spectra: insight into their solution structure. 2003 , 4, 517-9	34
2147	Temperature-dependent behavior of protein-chromophore interactions: a theoretical study of a blue fluorescent antibody. 2003 , 4, 848-55	5
2146	A theoretical study of the UV/visible absorption and emission solvatochromic properties of solvent-sensitive dyes. 2003 , 4, 1084-94	75
2145	Optimized Slater-type basis sets for the elements 1-118. <i>Journal of Computational Chemistry</i> , 2003 , 24, 1142-56	3.5 1780
2144	Stereodiscrimination in Phosphanylthiolato Nickel(II) Complexes. 2003 , 2003, 4147-4151	14

2143	Nuclear spin relaxation study of the solution reorientation of 3,5-dichlorophenyl- and phenylethynyl-mercury cyanide molecules and shielding tensors of nuclei forming the HgCN and C^1CHgCN groups: estimation of the heavy atom effect of mercury. 2003 , 41, 788-793	4
2142	Condensed polyhedral boranes and analogous organometallic clusters: a molecular orbital and density functional theory study on the $\text{cap}\cdots\text{cap}$ interactions. 2003 , 17, 480-492	9
2141	Electron pairing analysis of the Fischer-type chromium-carbene complexes $(\text{CO})_5\text{Cr}=\text{C}(\text{X})\text{R}$ ($\text{X}=\text{H}$, OH , OCH_3 , NH_2 , NHCH_3 and $\text{R}=\text{H}$, CH_3 , CH_2CH_2 , Ph , C_6H_5). 2003 , 294, 129-139	17
2140	Optical transitions of a D_{4h} complex with one electron in a $1g$ (B_{2g}): study of RhCl_6^{4-} . 2003 , 374, 151-156	17
2139	Structural, electronic, and magnetic properties of heterofullerene $\text{C}_{48}\text{B}_{12}$. 2003 , 375, 445-451	42
2138	Thermal versus electronic broadening in the density of states of liquid water. 2003 , 376, 68-74	56
2137	Metastable states in Au^{22+} : a density functional study. 2003 , 639, 203-211	3
2136	Density functional study of lanthanide complexes $(\text{Cp}^*-\text{C}_5\text{H}_5)_2\text{LnX}(\text{OC}_4\text{H}_8)$ ($\text{Ln}=\text{La}, \text{Lu}$; $\text{X}=\text{F}$, Cl , Br and I). 2003 , 679, 84-92	16
2135	Chemistry of the 1,3,5,7-octatetraynediyl carbon rod end-capped by two electron-rich $(\text{Cp}^*-\text{C}_5\text{Me}_5)(\text{P}^2\text{-dppe})\text{Fe}$ groups. 2003 , 683, 368-378	69
2134	Computational studies of the Brookhart's type catalysts for ethylene polymerisation. Part 2: ethylene insertion and chain transfer mechanisms. 2003 , 44, 2169-2176	19
2133	Density functional study of the vibrational frequencies of Keggin heteropolyanions. 2003 , 287, 55-69	95
2132	Theoretical investigation of mixed-ligand lanthanocene complexes, $(\text{Cp}^*-\text{C}_5\text{H}_5)_2\text{LnX}(\text{OC}_4\text{H}_8)$ ($\text{Ln}=\text{La}$, Gd , Lu ; $\text{X}=\text{F}$, Cl , Br , I). 2003 , 6, 1243-1245	11
2131	A computational and experimental study of anhydrous phosphotungstic acid and its interaction with water molecules. 2003 , 256, 51-68	92
2130	AddRemove: A new link model for use in QM/MM studies. 2003 , 91, 177-183	40
2129	Molecular structures, bond energies, and bonding analysis of group 11 cyanides $\text{TM}(\text{CN})$ and isocyanides $\text{TM}(\text{NC})$ ($\text{TM} = \text{Cu}$, Ag , Au). 2003 , 42, 4977-84	63
2128	Why is BCl_3 a stronger Lewis acid with respect to strong bases than BF_3 ?. 2003 , 42, 7990-4	114
2127	Representation of the exact relativistic electronic Hamiltonian within the regular approximation. 2003 , 119, 11526-11540	37
2126	A Combined Experimental and Theoretical Study Examining the Binding of N-Heterocyclic Carbenes (NHC) to the Cp^*RuCl ($\text{Cp}^* = \text{Cp}^*-\text{C}_5\text{Me}_5$) Moiety: Insight into Stereoelectronic Differences between Unsaturated and Saturated NHC Ligands. 2003 , 22, 4322-4326	354

2125	A facile and novel route to unprecedented manganese C4 cumulenyl complexes. 2003 , 2006-8	23
2124	A Comparative Investigation of Structure and Bonding in Mo and W [TeM6O24]6- and [PM12O40]3- Heteropolyanions. 2003 , 107, 6613-6621	37
2123	Energy Partitioning Analysis of the Bonding in L2TM(C2H2) and L2TM(C2H4) (TM = Ni, Pd, Pt; L2 = (PH3)2, (PMe3)2, H2PCH2PH2, H2P(CH2)2PH2) 2003 , 22, 2758-2765	82
2122	A discrete solvent reaction field model within density functional theory. 2003 , 118, 514-521	83
2121	Jahn-Teller Ions in Cubic Crystals Explored Through DFT Calculations. 2003 , 445-459	23
2120	A Quantum Molecular Dynamics Simulation Study of the Initial Hydrolysis Step in Sol-Gel Process. 2003 , 107, 1518-1524	106
2119	Charge transport in columnar stacked triphenylenes: Effects of conformational fluctuations on charge transfer integrals and site energies. 2003 , 119, 9809-9817	346
2118	Energy decomposition analysis of the chemical bond in main group and transition metal compounds. 2003 , 124, 365-78; discussion 393-403, 453-5	129
2117	Solid-state structure dependence of the molecular distortion and spectroscopic properties of the Cu(I) bis(2,9-dimethyl-1,10-phenanthroline) ion. 2003 , 42, 8794-802	63
2116	Spectroscopic and Computational Assessment of the Rotational Barrier of a Ferrocenyl-Stabilized Cyclopentadienyl Cation: Evidence for the First Hydroxyfulvalene Ligand. 2003 , 22, 663-669	24
2115	A theoretical study of the NMR spin-spin coupling constants of the complexes [(NC)(5)Pt-Tl(CN)(n)](n-) (n = 0-3) and [(NC)(5)Pt-Tl-Pt(CN)(5)](3-): a lesson on environmental effects. 2003 , 125, 13585-93	41
2114	Predicting 13C NMR Spectra by DFT Calculations. 2003 , 107, 9964-9973	108
2113	Molybdenum-phosphorus triple bond stabilization by ancillary alkoxide ligation: synthesis and structure of a terminal phosphide tris-1-methylcyclohexanoxide complex. 2003 , 125, 9264-5	31
2112	Analytic and Variational X ⁿ in the Slater-Boothaan Method. 2003 , 107, 10082-10089	18
2111	Electronic and Structural Evolution of Monoiron Sulfur Clusters, FeSn- and FeSn (n = 1-8), from Anion Photoelectron Spectroscopy. 2003 , 107, 2821-2828	38
2110	The Smallest Possible Nanocrystals of Semiconducting Oxides. 2003 , 107, 3336-3339	63
2109	A theoretical study of the large Hg-Hg spin-spin coupling constants in Hg(2)(2+), Hg(3)(2+), and Hg(2)(2+)-crown ether complexes. 2003 , 125, 4937-42	31
2108	Influence of the ligand on the coupling between the metal-based electrons in face-shared [M2X9]3- (M = Mo, W; X = F, Cl, Br, I) systems. 2003 , 42, 5252-8	9

2107	Terminal Phosphinidene Complexes CpR(L)MPAr of the Group 9 Transition Metals Cobalt, Rhodium, and Iridium. Synthesis, Structures, and Properties. 2003 , 22, 1827-1834	67
2106	Finite Temperature Structure and Dynamics of Zinc Dialkyldithiophosphate Wear Inhibitors: A Density Functional Theory and ab Initio Molecular Dynamics Study. 2003 , 107, 5058-5070	32
2105	Electronic structure contributions to electron-transfer reactivity in iron-sulfur active sites: 2. Reduction potentials. 2003 , 42, 689-95	36
2104	Mapping the sites for selective oxidation of guanines in DNA. 2003 , 125, 13658-9	86
2103	[(Cp*Me2Flu)2Ln]-[Li(ether)n]+ (Ln = Y, La): Complexes with Unusual Coordination Modes of the Fluorenyl Ligand and the First Examples of Bis-Ansa Lanthanidocenes. 2003 , 22, 4038-4046	30
2102	Single crystal EPR studies of the reduced active site of [NiFe] hydrogenase from <i>Desulfovibrio vulgaris</i> Miyazaki F. 2003 , 125, 83-93	166
2101	Propensity of Different AgBr Surfaces for Photoinduced Silver Cluster Formation: A Molecular Orbital Analysis 2003 , 107, 8184-8190	12
2100	Uranium tris-aryloxide derivatives supported by triazacyclononane: engendering a reactive uranium(III) center with a single pocket for reactivity. 2003 , 125, 4565-71	186
2099	Theoretical study of cisplatin binding to purine bases: why does cisplatin prefer guanine over adenine?. 2003 , 125, 14082-92	229
2098	Ring Opening of Methylenecyclopropane over Lanthanocene Catalyst: A Quantum-Chemical Molecular Dynamics Simulation Study. 2003 , 22, 2181-2183	31
2097	Photoisomerization and proton transfer in photoactive yellow protein. 2003 , 125, 8186-94	54
2096	Unusual geometries and questions of oxidation state in potential Sn(III) chemistry. 2003 , 42, 8161-70	2
2095	Electron Distribution, Bonding, and $J(\text{SiH})$ NMR Coupling Constant in $(\eta\text{-C}_5\text{H}_5)(\text{CO})_2\text{MnHSiCl}_3$: The Molecular Orbital View. 2003 , 22, 1599-1602	38
2094	$\text{Cl}(\mu\text{-S}(\text{CH}_3)_2)_3\text{VCl}_3(2)^{-}$: a first-row, face-shared bioctahedral complex with multiple metal-metal bonding. 2003 , 42, 4417-24	4
2093	Dinuclear copper(I) complexes with hexaaza macrocyclic dinucleating ligands: structure and dynamic properties. 2003 , 42, 4456-68	19
2092	Electronic structure contributions to electron-transfer reactivity in iron-sulfur active sites: 3. Kinetics of electron transfer. 2003 , 42, 696-708	41
2091	MLCT state structure and dynamics of a copper(I) diimine complex characterized by pump-probe X-ray and laser spectroscopies and DFT calculations. 2003 , 125, 7022-34	283
2090	Molybdenum chalcogenobenzimidato complexes: radical synthesis and nitrile extrusion via beta-EPh (E = S, Se, and Te) elimination. 2003 , 42, 8621-3	16

2089	Theoretical investigation of the apparently irregular behavior of pt-pt nuclear spin-spin coupling constants. 2003 , 125, 1028-32	37
2088	Density Functional Theory Analysis of Benzene (De)hydrogenation on Pt(111): Addition and Removal of the First Two H-Atoms. 2003 , 107, 3844-3855	65
2087	On the origin of the optical activity in the d-d transition region of tris-bidentate Co(III) and Rh(III) complexes. 2003 , 42, 8902-10	45
2086	Nickel complexes of o-amidochalcogenophenolate(2-)/o-iminochalcogenobenzosemiquinonate(1-) pi-radical: synthesis, structures, electron spin resonance, and x-ray absorption spectroscopic evidence. 2003 , 42, 3925-33	27
2085	Combinatorial Computational Chemistry Approach to the High-Throughput Screening of Metal Sulfide Catalysts for CO Hydrogenation Process. 2003 , 17, 857-861	9
2084	DFT calculations of isomer shifts and quadrupole splitting parameters in synthetic iron-oxo complexes: applications to methane monooxygenase and ribonucleotide reductase. 2003 , 42, 5244-51	40
2083	Chemistry in Stringland: One-Dimensional Complexes of Main-Group Metal Ions with the Ligands NC _{2n} X (X = N, CH; n = 0, 1, 2, 3). 2003 , 107, 10441-10449	15
2082	An Investigation of the Unusual ⁵⁷ Fe Mössbauer Quadrupole Splittings and Isomer Shifts in 2 and 3-Coordinate Fe(II) Complexes. 2003 , 107, 7180-7188	25
2081	Relativistic DFT Calculations of Copper Hyperfine Coupling Constants: Effect of Spin-Orbit Coupling. 2003 , 107, 5583-5587	14
2080	Electronic structure contributions to electron-transfer reactivity in iron-sulfur active sites: 1. Photoelectron spectroscopic determination of electronic relaxation. 2003 , 42, 679-88	34
2079	The Pacman effect: a supramolecular strategy for controlling the excited-state dynamics of pillared cofacial bisporphyrins. 2003 , 42, 8262-9	35
2078	Density Functional Theory. 2003 , 491-510	18
2077	Reactions of Organic Nitriles with a Three-Coordinate Molybdenum(III) Complex and with a Related Molybdaziridine-Hydride. 2003 , 22, 2902-2913	59
2076	Surface complexation of arsenic(V) to iron(III) (hydr)oxides: structural mechanism from ab initio molecular geometries and EXAFS spectroscopy. 2003 , 67, 4223-4230	545
2075	Density functional calculations on electronic circular dichroism spectra of chiral transition metal complexes. 2003 , 42, 2867-77	86
2074	NWChem for materials science. 2003 , 28, 209-221	20
2073	Thermodynamic properties of PaCl ₅ and PaF ₅ based on quantum chemical calculations. 2003 , 353, 128-132	8
2072	Bis(benzene)chromium Is a π -Bonded Molecule and Ferrocene Is a σ -Bonded Molecule 2003 , 22, 3304-3308	104

2071	Structures and bonding of the sandwich complexes [Ti(eta5-E5)2]2- (E = CH, N, P, As, Sb): a theoretical study. 2003 , 42, 2504-11	84
2070	Noble gas-actinide complexes of the CUO molecule with multiple Ar, Kr, and Xe atoms in noble-gas matrices. 2003 , 125, 3126-39	117
2069	Time-dependent density-functional calculations for the optical spectra of molecules, clusters, and nanocrystals. 2003 , 15, R1517-R1547	56
2068	Ab initio molecular dynamics study of aqueous solvation of ethanol and ethylene. 2003 , 118, 8831-8840	55
2067	Big off-center displacements of ions in insulators: The Jahn-Teller ion Ni ⁺ in CaF ₂ . 2003 , 67,	18
2066	Analysis of Aromatic Delocalization: Individual Molecular Orbital Contributions to Nucleus-Independent Chemical Shifts. 2003 , 107, 6470-6475	141
2065	Copper complexes of nitrogen-anchored tripodal N-heterocyclic carbene ligands. 2003 , 125, 12237-45	135
2064	Computational Analysis of Mo and W Oxoanions through Bond Order and Bonding Energy Approaches. 2003 , 107, 4568-4577	24
2063	Structure and dynamics of copper complexes with 2,2':6',2''-terpyridines in glassy matrices. 2003 , 5, 3959-3967	18
2062	On the physical meaning of the ZORA Hamiltonian. 2003 , 101, 2295-2302	39
2061	¹³ C- ⁷⁷ Se and ⁷⁷ Se- ⁷⁷ Se spin-spin coupling tensors in carbon diselenide: NMR experiments and ZORA DFT calculations. 2003 , 5, 4551-4555	15
2060	Relativistic Density-Functional Computations of the Chemical Shift of ¹²⁹ Xe in 60. 2003 , 107, 4967-4972	59
2059	Connecting terminal carboxylate groups in nine-coordinate lanthanide podates: consequences on the thermodynamic, structural, electronic, and photophysical properties. 2003 , 42, 4680-95	60
2058	A discrete solvent reaction field model for calculating molecular linear response properties in solution. 2003 , 119, 3800-3809	66
2057	A theoretical analysis of the conformational behaviour of substituted methylenecyclohexanes. 2003 , 81, 1101-1107	2
2056	On the nature of the short Pt-Tl bonds in model compounds [H5Pt-TlHn] ⁿ⁻ . 2003 , 124, 41-51; discussion 53-6, 453-5	13
2055	An experimental and theoretical study of [RhCl(PF ₃) ₂] ₂ fragmentation. 2003 , 5, 268-274	17
2054	Ag ₃ Born-Oppenheimer potential hypersurfaces. 2003 , 118, 9241-9246	10

2053	First-principles calculations of structural, electronic, vibrational, and magnetic properties of C60 and C48N12: A comparative study. 2003 , 118, 8621-8635	64
2052	Analysis of the bonding and reactivity of H and the Al13 cluster using density functional concepts. 2003 , 119, 5128-5141	53
2051	Tuning of the excited state properties of phenylenevinylene oligomers: A time-dependent density functional theory study. 2003 , 118, 9441-9446	19
2050	A discrete solvent reaction field model for calculating frequency-dependent hyperpolarizabilities of molecules in solution. 2003 , 119, 12998-13006	41
2049	Calculation of electric properties using regular approximations to relativistic effects: The polarizabilities of RuO4, OsO4, and HsO4 (Z=108). 2003 , 119, 1412-1420	29
2048	Density functional theory based molecular-dynamics study of aqueous chloride solvation. 2003 , 119, 11788-11791	115
2047	Investigation of metal-dithiolate fold angle effects: implications for molybdenum and tungsten enzymes. 2003 , 100, 3719-24	72
2046	Time-dependent density functional theory study of the electronic states of Bi. 2003 , 36, 2283-2290	3
2045	Polarizabilities of amino acid residues. 2004 , 4, 419-425	16
2044	Estimation of Electron Spectra Transitions of Free-Based Porphin and Mg-Porphin Using Various Quantum Chemical Approaches. 2004 , 5, 196-213	9
2043	Saturated adsorption of CO and coadsorption of CO and O2 on AuN- (N=2-7) clusters. 2004 , 120, 6574-84	71
2042	Vibronic coupling and double excitations in linear response time-dependent density functional calculations: dipole-allowed states of N2. 2004 , 121, 6155-66	71
2041	Between geometry, stability, and polarizability: density functional theory studies of silicon clusters Sin (n = 3-10). 2004 , 121, 4628-34	95
2040	Calculation of EPR g-Tensors with Density Functional Theory. 2004 , 505-532	20
2039	Recent Developments in Computational Bioinorganic Chemistry. 2004 , 37-70	12
2038	Pentadienyls vs cyclopentadienyls and reversal of metal-ligand bonding affinity with metal oxidation state: synthesis, molecular structures, and electronic structures of high-valent zirconium pentadienyl complexes. 2004 , 126, 14105-16	22
2037	Methods and Implementation of Robust, High-Precision Gaussian Basis DFT Calculations for Periodic Systems: the GTOFF Code. 2004 , 171-228	9
2036	Time-dependent density functional theory based on a noncollinear formulation of the exchange-correlation potential. 2004 , 121, 12191-6	215

2035	Charge transport properties in discotic liquid crystals: a quantum-chemical insight into structure-property relationships. 2004 , 126, 3271-9	432
2034	Oxidative Addition of Aryl Halides to Palladium(0) Complexes: A Density-Functional Study Including Solvation. 2004 , 23, 2980-2988	193
2033	Quantum Chemical Analysis of the Chemical Bonds in Tris(8-hydroxyquinolino)aluminum as a Key Emitting Material for OLED. 2004 , 108, 10296-10301	64
2032	Hydrogen bonds of RNA are stronger than those of DNA, but NMR monitors only presence of methyl substituent in uracil/thymine. 2004 , 126, 16718-9	81
2031	Active site modeling in copper azurin molecular dynamics simulations. 2004 , 10, 25-31	18
2030	Density functional theory and tight-binding quantum chemical molecular dynamics calculations on Ce η^5 Cu η^2 O η^2 catalyst and the adsorptions of CH $_3$ OH and CH $_3$ O on Ce η^5 Cu η^2 O η^2 . 2004 , 384, 30-34	16
2029	Are LCAO-MO Models Useful Estimators for Electric Field Gradients in Simple Molecules?. 2004 , 158, 71-78	
2028	The Electric Field Gradient of ^{111}Ag in Macrocyclic Crown Thioethers. 2004 , 158, 79-88	3
2027	Density Functional Theory and Low-Temperature Matrix Investigations of CO-Loss Photochemistry from [(C $_5$ R $_5$)Ru(CO) $_2$] $_2$ (R = H, Me) Complexes. 2004 , 15, 469-487	3
2026	Calculation of NMR parameters in van der Waals complexes involving organic systems and xenon. 2004 , 17, 945-950	8
2025	Choice of atomic orbitals to evaluate sensitive properties of molecules: An example of NMR chemical shifts. 2004 , 100, 214-220	3
2024	Green oxidation catalysts: computational design of high-efficiency models of galactose oxidase. 2004 , 43, 3286-9	24
2023	Green Oxidation Catalysts: Computational Design of High-Efficiency Models of Galactose Oxidase. 2004 , 116, 3348-3351	14
2022	Strongly Nucleophilic RhI Centre in Square-Planar Complexes with Terdentate (β) 2,2':6',2''-Terpyridine Ligands: Crystallographic, Electrochemical and Density Functional Theoretical Studies. 2004 , 2004, 1675-1686	19
2021	Electronic Structure of Transition Metal β ocorrole Complexes: A First Quantum Chemical Study. 2004 , 2004, 2442-2445	18
2020	EPR Insensitivity of the Metal-Nitrosyl Spin-Bearing Moiety in Complexes [LnRuII-NO] $_k$. 2004 , 2004, 2902-2907	35
2019	Conformational Analysis of Saturated trans-Fused 1,3,2-Benzoxazaphosphinine 2-Oxides [DFT Calculation of NMR J(P,H) Coupling Constants. 2004 , 2004, 4921-4930	11
2018	Voronoi deformation density (VDD) charges: Assessment of the Mulliken, Bader, Hirshfeld, Weinhold, and VDD methods for charge analysis. <i>Journal of Computational Chemistry</i> , 2004 , 25, 189-210	3-5 782

2017	QM/MM study of aqueous solvation of the uranyl fluoride [UO ₂ F ₄ (2-)] complex. <i>Journal of Computational Chemistry</i> , 2004 , 25, 386-92	3.5	34
2016	Calculation of electrostatic interaction energies in molecular dimers from atomic multipole moments obtained by different methods of electron density partitioning. <i>Journal of Computational Chemistry</i> , 2004 , 25, 921-34	3.5	71
2015	The performance of nonhybrid density functionals for calculating the structures and spin states of Fe(II) and Fe(III) complexes. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1840-8	3.5	82
2014	Solvent effects on ¹⁹⁵ Pt and ²⁰⁵ Tl NMR chemical shifts of the complexes [(NC) ₅ Pt–Tl(CN) _n] _n (n=0-3), and [(NC) ₅ Pt–Tl–Pt(CN) ₅] ₃ studied by relativistic density functional theory. 2004 , 10, 2581-9		45
2013	A theoretical study on the cyclopropane adsorption onto the copper surfaces by density functional theory and quantum chemical molecular dynamics methods. 2004 , 220, 189-198		16
2012	The photohydrochlorination of platinum(IV) chloride in chloroform. 2004 , 357, 639-643		10
2011	Spectroscopic constants of gallium monohalides: a DFT study. 2004 , 668, 209-215		1
2010	Decomposition of intermolecular interactions: comparison between SAPT and density-functional decompositions. 2004 , 685, 43-56		14
2009	Theoretical study of UX ₆ and UO ₂ X ₂ (X=F, Cl, Br, I). 2004 , 684, 35-42		29
2008	ESR/UV-Vis/IR cyclovoltammetry of macrocyclic complex [CuI(bite)]BF ₄ at different temperatures. 2004 , 566, 123-129		6
2007	Relativistic DFT calculation of the reaction cycle intermediates of [NiFe] hydrogenase: a contribution to understanding the enzymatic mechanism. 2004 , 98, 862-77		79
2006	Theoretical investigation of the metal-metal interaction in dimolybdenum complexes with bridging hydride and methyl ligands. 2004 , 23, 2879-2900		47
2005	Theoretical studies of 18-electron M(CnHn)(C10H10) (M=Fe, Ru, Os; n=3, 4, 5) sandwich complexes. 2004 , 23, 2993-3002		8
2004	A quantitative study of the charge-transfer between conjugated thiophene rings in vibrationally excited states. 2004 , 350, 220-223		7
2003	Ligand effect on the periodic properties of trivalent organolanthanide complexes: a density functional study. 2004 , 7, 566-568		6
2002	Efficient symmetry treatment for the nonrelativistic and relativistic molecular Kohn-Sham problem. The symmetry module of the program ParaGauss. 2004 , 160, 91-119		17
2001	A circular dichroism and structural study of the inclusion complex artemisinin- β -cyclodextrin. 2004 , 383, 566-571		29
2000	Jahn-Teller impurities in tetragonal lattices: Why is the ligand octahedron of Cu ²⁺ in layered perovskites compressed?. 2004 , 385, 286-291		34

- 1999 Combination of the exact potential and multipole methods (EP/MM) for evaluation of intermolecular electrostatic interaction energies with pseudoatom representation of molecular electron densities. **2004**, 391, 170-175 97
- 1998 Quantum chemical analysis of the chemical bonds in Mq_3 ($M=Al, Ga$) as emitting material for OLED. **2004**, 394, 120-125 37
- 1997 An interesting property of the Perdew-Wang 91 density functional. **2004**, 396, 10-15 10
- 1996 Size-scaling of the polarizability of tubular fullerenes investigated with time-dependent (current)-density-functional theory. **2004**, 395, 274-278 30
- 1995 Density functional theory studies of correlations between structure, binding energy, and dipole polarizability in Si_9 and Si_{12} . **2004**, 398, 283-286 19
- 1994 Calculation of nuclear magnetic resonance shielding constants using potential-based methods. **2004**, 399, 84-88 24
- 1993 The calculation of ESR parameters by density functional theory: the g- and A-tensors of Co(acac)₃. **2004**, 399, 433-439 46
- 1992 Atomic-silicon cryptates in siloxanic networks. **2004**, 400, 179-184 3
- 1991 Design of new catalysts for ecological high-quality transportation fuels by combinatorial computational chemistry and tight-binding quantum chemical molecular dynamics approaches. **2004**, 89, 479-493 12
- 1990 Darmstadtium carbonyl and carbide resemble platinum carbonyl and carbide. **2004**, 1982-3 25
- 1989 Organogermanium reactive intermediates. The direct detection and characterization of transient germynes and digermenes in solution. **2004**, 126, 16105-16 68
- 1988 On the role of the conserved aspartate in the hydrolysis of the phosphocysteine intermediate of the low molecular weight tyrosine phosphatase. **2004**, 126, 12677-84 19
- 1987 Organometallic derivatives of fullerenes: a DFT study of $(\eta^2-C_x)[Pt(PH_3)_2]_n$ ($x = 60, 70, 84$; $n = 1-6$). **2004**, 43, 6815-21 11
- 1986 Activation and cleavage of dinitrogen by three-coordinate metal complexes involving Mo(III) and Nb(II/III). **2004**, 2492-5 19
- 1985 Systematic discrepancy of theoretical predictions of NMR chemical shifts for chlorinated aromatic carbons using the GIAO DFT method. **2004**, 102, 1903-1908 12
- 1984 Excitation energies of some d1 systems calculated using time-dependent density functional theory: an implementation of open-shell TDDFT theory for doublet-doublet excitations. **2004**, 102, 2585-2595 54
- 1983 Properties of WAu₁₂. **2004**, 6, 11-22 93
- 1982 Carbonyl analogues? Analysis of Fe-E (E=B, Al, Ga) bonding in cationic terminal diyl complexes by density functional theory. **2004**, 2649-54 62

1981	Theoretical analysis of the $[\text{Mn}_2(\text{Ebxo})_2(\text{Ecarboxylato})_2]^+$ core. 2004 , 6, 4871-4877	9
1980	Structural analysis of porphyrin molecular squares using molecular mechanics and density-functional methods. 2004 , 121, 7228-36	13
1979	Ab initio benchmark study for the oxidative addition of CH_4 to Pd: importance of basis-set flexibility and polarization. 2004 , 121, 9982-92	66
1978	Organometallics versus P_4 Complexes of Group 11 Cations: Periodic Trends and Relativistic Effects in the Involvement of $(n-1)d, ns, \text{ and } np$ Orbitals in Metal-Ligand Interactions. 2004 , 23, 2343-2349	55
1977	Electronic structure of bent titanocene complexes with chelated dithiolate ligands. 2004 , 43, 8110-8	24
1976	Can Cu^+ -Exchanged Zeolites Store Molecular Hydrogen? An Ab-Initio Periodic Study Compared with Low-Temperature FTIR. 2004 , 108, 8278-8286	83
1975	A Computational Study of Ligand Interactions with Hafnium and Zirconium Metal Complexes in the Liquid-Liquid Extraction Process. 2004 , 108, 6112-6120	13
1974	Electronic Structure of Thienylene Vinylene Oligomers: Singlet Excited States, Triplet Excited States, Cations, and Dications. 2004 , 108, 16139-16146	35
1973	Where Are the Hydrogen Atoms in $[(\text{E}-\text{C}_5\text{H}_5)(\text{PH}_3)_2\text{W}(\text{H}_2\text{SiMe}_2)]^+$? A Theoretical Study. 2004 , 23, 2944-2948	13
1972	Chemistry of C-Trimethylsilyl-Substituted Heterocarboranes. 30. Synthetic and Structural Studies on Oxide Ion Encapsulating Tetralanthanide Tetrahedra Surrounded by Carbons Apart C ₂ B ₄ -Carborane Ligands (Ln(III) = La, Nd, Gd, Tb, Ho, Lu). 2004 , 23, 4621-4629	15
1971	Sulfuric Acid and Sulfuric Acid Hydrates in the Gas Phase: A DFT Investigation. 2004 , 108, 8914-8929	76
1970	Hydrogen-bonding-induced shifts of the excitation energies in nucleic acid bases: an interplay between electrostatic and electron density overlap effects. 2004 , 126, 11444-5	115
1969	Hydrogen Transfer between Ligands: A Density Functional Study of the Rearrangement of $\text{M}(\text{E}-\text{C}_7\text{H}_8)_2$ into $\text{M}(\text{E}'-\text{C}_7\text{H}_7)(\text{E}-\text{C}_7\text{H}_9)$ [$\text{M} = \text{Mo}, \text{Mo}^+, \text{Zr}$]. 2004 , 23, 2658-2669	7
1968	Polyene Cyclization by a Double Intramolecular Heck Reaction. A DFT Study. 2004 , 23, 2784-2796	31
1967	A DFT Study of the Interstitial Chemical Shifts in Main Group Element Centered Hexazirconium Halide Clusters. 2004 , 108, 350-357	3
1966	Multielectron chemistry of zinc porphyrinogen: a ligand-based platform for two-electron mixed valency. 2004 , 126, 2829-37	44
1965	Density functional investigation of metal-metal interactions in mixed-valence d_2d_3 (Cr, Mo, W) and d_3d_4 (Mn, Tc, Re) face-shared $[\text{M}_2\text{Cl}_9]^{2-}$ systems. 2004 , 43, 6734-44	14
1964	Targeted proton delivery in the catalyzed reduction of oxygen to water by bimetallic pacman porphyrins. 2004 , 126, 10013-20	227

1963	Living copolymerization of ethylene with norbornene catalyzed by bis(pyrrolide-imine) titanium complexes with MAO. 2004 , 126, 12023-32	176
1962	Improved Description of Chemical Barriers with Generalized Gradient Approximations (GGAs) and Meta-GGAs. 2004 , 108, 4459-4469	46
1961	A homoleptic molybdenum(IV) enolate complex: synthesis, molecular and electronic structure, and NCN group transfer to form a terminal cyanoimide of molybdenum(VI). 2004 , 126, 11370-6	32
1960	Preparation, characterization, and magnetic behavior of the Ln derivatives (Ln = Nd, La) of a 2,6-diiminepyridine ligand and corresponding dianion. 2004 , 43, 5771-9	71
1959	Density functional study of a micro-1,1-carboxylate bridged Fe(III)-O-Fe(IV) model complex. 2. Comparison with ribonucleotide reductase intermediate X. 2004 , 43, 613-21	21
1958	Structure and dynamics of a dihydrogen/hydride ansa molybdenocene complex. 2004 , 43, 3475-83	35
1957	Synthesis, photophysics, electrochemistry, theoretical, and transient absorption studies of luminescent copper(I) and silver(I) diyne complexes. X-ray crystal structures of [Cu3(micro-dppm)3(micro3-eta1-C triple bond CC triple bond CPh)2]PF6 and [Cu3(micro-dppm)3(micro3-eta1-C triple bond CC triple bond CH)2]PF6. 2004 , 126, 7300-10	77
1956	VIS/NIR Absorption Spectra of Positively Charged Oligo(phenylenevinylene)s and Comparison with Time-Dependent Density Functional Theory Calculations. 2004 , 108, 19967-19975	13
1955	Photochemically induced dynamic nuclear polarization in photosystem I of plants observed by ¹³ C magic-angle spinning NMR. 2004 , 126, 12819-26	52
1954	Eclipsed M2X6 compounds exhibiting very short metal-metal triple bonds. 2004 , 43, 3618-24	34
1953	Synthesis of a Base-Free Titanium Imido and a Transient Alkylidene from a Titanocene Dinitrogen Complex. Studies on TiNR Hydrogenation, Nitrene Group Transfer, and Comparison of 1,2-Addition Rates. 2004 , 23, 3448-3458	119
1952	Quantum chemical studies of intermediates and reaction pathways in selected enzymes and catalytic synthetic systems. 2004 , 104, 459-508	331
1951	Stable room-temperature molecular negative differential resistance based on molecule-electrode interface chemistry. 2004 , 126, 11648-57	65
1950	Cisplatin Binding to DNA Oligomers from Hybrid Car-Parrinello/Molecular Dynamics Simulations. 2004 , 108, 2699-2707	101
1949	Why Does Disubstituted Hexamolybdate with Arylimido Prefer to Form an Orthogonal Derivative? Analysis of Stability, Bonding Character, and Electronic Properties on Molybdate Derivatives by Density Functional Theory (DFT) Study. 2004 , 108, 17337-17343	36
1948	A Molecular Mechanics Study of Copper(II)-Catalyzed Asymmetric Diels-Alder Reactions. 2004 , 23, 1042-1054	17
1947	Zirconium sandwich complexes with eta(9) indenyl ligands: well-defined precursors for zirconocene-mediated coupling reactions. 2004 , 126, 16937-50	64
1946	On the mechanism of dioxygen formation from a di-mu-oxo-bridged manganese dinuclear complex. 2004 , 43, 5237-44	9

1945	Divalent molybdenum complexes of the dipyrroliide ligand system. Isolation of a Mo ₂ unit with a 45 degree twist angle. 2004 , 43, 1108-15	16
1944	Origin of enantioselectivity in the asymmetric Ru-catalyzed metathesis of olefins. 2004 , 126, 9592-600	111
1943	Activation of H-H, C-H, C-C, and C-Cl Bonds by Pd(0). Insight from the Activation Strain Model. 2004 , 108, 8460-8466	111
1942	Density functional investigation of metal-metal interactions in d ₄ d ₄ face-shared [M ₂ Cl ₉] ³⁻ (M = Mn, Tc, Re) systems. 2004 , 43, 2368-78	13
1941	Excitations, optical absorption spectra, and optical excitonic gaps of heterofullerenes. I. C ₆₀ , C ₅₉ N ⁺ , and C ₄₈ N ₁₂ : theory and experiment. 2004 , 120, 5133-47	44
1940	Electronic structures of metal sites in proteins and models: contributions to function in blue copper proteins. 2004 , 104, 419-58	708
1939	DFT and metal-metal bonding: a dys-functional treatment for multiply charged complexes?. 2004 , 43, 2597-610	46
1938	Raman under nitrogen. The high-resolution Raman spectroscopy of crystalline uranocene, thorocene, and ferrocene. 2004 , 120, 2708-18	26
1937	Carbon-Carbon Bonds of Manganese Half-Sandwich Complexes for Electron Reservoir Functions. 2004 , 23, 1183-1186	34
1936	Observation of proton-coupled electron transfer by transient absorption spectroscopy in a hydrogen-bonded, porphyrin donor-acceptor assembly. 2004 , 108, 6315-21	72
1935	Performance of the OPBE exchange-correlation functional. 2004 , 102, 2467-2474	330
1934	Quantum Chemistry Study of Actinide(III) and Lanthanide(III) Complexes with Tridentate Nitrogen Ligands. 2004 , 108, 6893-6900	97
1933	Cu ²⁺ impurities in fluorite-type crystals: Mechanisms favoring an off-center motion. 2004 , 69,	22
1932	Calculation of the A term of magnetic circular dichroism based on time dependent-density functional theory I. Formulation and implementation. 2004 , 120, 10942-54	50
1931	Spectroscopic and computational studies of the azide-adduct of manganese superoxide dismutase: definitive assignment of the ligand responsible for the low-temperature thermochromism. 2004 , 126, 12477-91	49
1930	Energy Partitioning Analysis of the Bonding in Ethylene and Acetylene Complexes of Group 6, 8, and 11 Metals: (CO) ₅ TM-η ² H ₂ and Cl ₄ TM-η ² H ₂ (TM = Cr, Mo, W), (CO) ₄ TM-η ² H ₂ (TM = Fe, Ru, Os), and TM-η ² H ₂ (TM = Cu, Ag, Au). 2004 , 108, 3134-3142	134
1929	FeB Double Bonds: Synthetic, Structural, and Reaction Chemistry of Cationic Terminal Borylene Complexes. 2004 , 23, 2911-2926	117
1928	Validation of Exchange-Correlation Functionals for Spin States of Iron Complexes. 2004 , 108, 5479-5483	353

1927	Theoretical analysis of singlet and triplet excited states of nickel porphyrins. 2004 , 121, 1317-24	31
1926	Proton as the simplest of all catalysts for [2 + 2] cycloadditions: DFT study of acid-catalyzed imine metathesis. 2004 , 69, 6173-84	9
1925	Quantum chemical investigations and bonding analysis of iron complexes with mixed cyano and carbonyl ligands. 2004 , 43, 778-84	32
1924	Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes. 2004 , 108, 3545-3555	38
1923	Investigating the M*He exciplexes, M={Li,Na,K,Rb,Cs,Fr}: density functional approach. 2004 , 121, 11625-8	25
1922	Nickel complexes of carboxylate-containing polydentate ligands as models for the active site of urease. 2004 , 43, 8252-62	81
1921	Discrete bridging and terminal copper carbenes in copper-catalyzed cyclopropanation. 2004 , 126, 10085-94	165
1920	Kinetic models for catalytic reactions from first principles: benzene hydrogenation. 2004 , 102, 267-272	15
1919	Dynamics, Site Binding, and Distribution of Counterions in Polyelectrolyte Solutions Studied by Electron Paramagnetic Resonance Spectroscopy \square 2004 , 108, 3698-3704	51
1918	Synthesis and characterization of a novel tantalum chalcogen-rich molecular cluster with square planar metal core. 2004 , 43, 7966-8	14
1917	Small-Molecule Activation by Molybdaziridine Hydride Complexes: Mechanistic Sequence of the Small-Molecule Binding and Molybdaziridine Ring-Opening Steps. 2004 , 23, 3126-3138	26
1916	Density functional calculations of the ^{13}C NMR chemical shifts in (9,0) single-walled carbon nanotubes. 2004 , 126, 13079-88	148
1915	Synthesis and characterization of hypoelectronic rhenaboranes. Analysis of the geometric and electronic structures of species following neither borane nor metal cluster electron-counting paradigms. 2004 , 126, 3203-17	129
1914	X-ray magnetic circular dichroism of <i>Pseudomonas aeruginosa</i> nickel(II) azurin. 2004 , 126, 5859-66	13
1913	Calculating the electron paramagnetic resonance parameters of exchange coupled transition metal complexes using broken symmetry density functional theory: application to a MnIII/MnIV model compound. 2004 , 126, 2613-22	176
1912	Icosahedral gold cage clusters: M@Au $_{12}$ - (M=V, Nb, and Ta). 2004 , 121, 8369-74	127
1911	Theoretical Study of the Copolymerization of Ethylene and Propylene by a Heterogeneous Ziegler-Natta Catalyst. 2004 , 37, 9191-9200	31
1910	Relativistic Effects on NMR Chemical Shifts. 2004 , 14, 552-597	47

1909	Calculation of Free Energy Profiles for Elementary Bimolecular Reactions by ab Initio Molecular Dynamics: Sampling Methods and Thermostat Considerations. 2004 , 108, 2167-2180	50
1908	Embracing ligands. Synthesis, characterisation and the correlation between ⁵⁹ Co NMR and ligand field parameters of Co(III) complexes with a new class of nitrogen-thioether multidentate ligand. 2004 , 767-77	7
1907	Vanadium(V) adsorption onto goethite (FeOOH) at pH 1.5 to 12: a surface complexation model based on ab initio molecular geometries and EXAFS spectroscopy. 2004 , 68, 1723-1733	193
1906	Copper(II) sorption onto goethite, hematite and lepidocrocite: a surface complexation model based on ab initio molecular geometries and EXAFS spectroscopy. 2004 , 68, 2623-2637	171
1905	The influence of a transmembrane pH gradient on protonation probabilities of bacteriorhodopsin: the structural basis of the back-pressure effect. 2004 , 339, 571-89	31
1904	Simulation of the substrate cavity dynamics of quercetinase. 2004 , 344, 725-38	9
1903	g-Factor calculations for the species occurring in borate glasses. 2004 , 343, 159-162	3
1902	FT-EPR spectroscopy in the borate system. 2004 , 345-346, 45-49	3
1901	The Significance of π Interactions in Group 11 Complexes with N-Heterocyclic Carbenes 2004 , 23, 3640-3646	274
1900	Group 11 Metal Complexes of N-Heterocyclic Carbene Ligands: Nature of the Metal-Carbene Bond. 2004 , 23, 755-764	341
1899	Ab Initio Quality Electrostatic Atomic and Molecular Properties Including Intermolecular Energies from a Transferable Theoretical Pseudoatom Databank. 2004 , 108, 4283-4300	144
1898	Density-functional generalized-gradient and hybrid calculations of electromagnetic properties using Slater basis sets. 2004 , 120, 7252-61	25
1897	The importance of spin-orbit coupling and electron correlation in the rationalization of the ground state of the CUO molecule. 2004 , 121, 5783-8	32
1896	Theoretical Study of Stable Intermolecular Complexes of Furan with Hydrogen Halides. 2004 , 108, 11375-11380	4
1895	Temperature and isotope substitution effects on the structure and NMR properties of the pertechnetate ion in water. 2004 , 126, 11583-8	17
1894	Preparation and molecular and electronic structures of iron(0) dinitrogen and silane complexes and their application to catalytic hydrogenation and hydrosilation. 2004 , 126, 13794-807	707
1893	Organic nitriles from acid chlorides: an isovalent N for (O)CL exchange reaction mediated by a tungsten nitride complex. 2004 , 126, 7742-3	43
1892	Synthesis and structural characterization of some selenoruthenates and telluroruthenates. 2005 , 44, 3441-8	13

1891	Electronic structure analysis of iron(III)-porphyrin complexes by X-ray absorption spectra at the C, N and Fe K-edges. 2005 , 21, 309-14	13
1890	Local structure of nitrogen atoms in a porphine ring of mesophenyl substituted porphyrin with an electron-withdrawing group using X-ray photoelectron spectroscopy and X-ray absorption spectroscopy. 2005 , 21, 635-9	28
1889	Activation of C-H, C=C and C≡C bonds by Pd and cis-Pd(CO) ₂ Cl ₂ . Catalyst-substrate adaptation. 2005 , 690, 2191-2199	24
1888	Toward the catalytic synthesis of phosphiranes. A computational study. 2005 , 690, 5517-5524	10
1887	Bonding aspects of P-heterocyclic carbene transition metal complexes. A computational assessment. 2005 , 690, 6068-6078	36
1886	Chemical bonding in transition metal carbene complexes. 2005 , 690, 6178-6204	180
1885	The existence of atomic-like states of silicon in siloxanic networks: A DFT approach. 2005 , 81, 448-460	
1884	Theoretical investigation of the exciplexes. 2005 , 341, 170-176	5
1883	Theoretical investigation of adsorption of organic molecules onto Fe(110) surface. 2005 , 716, 45-60	20
1882	DFT studies of copper complexes with biphenyldiimino dithioether. 2005 , 718, 175-181	3
1881	TD-DFT studies on the electronic structure of imidazole bound vanadate in vanadium containing haloperoxidases (VHPO). 2005 , 725, 163-175	29
1880	Molecular geometry, electronic structure and optical properties study of meridional tris(8-hydroxyquinolinato)gallium(III) with ab initio and DFT methods. 2005 , 755, 19-30	16
1879	The actinide-imide bonding revisited: A relativistic DFT study. 2005 , 757, 155-164	18
1878	The NMR response of boroxol rings: a density functional theory study. 2005 , 27, 5-9	25
1877	Chemisorption of NCO on Cu(100): A density functional theory study. 2005 , 598, 57-67	17
1876	DFT calculations of EPR parameters of transition metal complexes: Implications for catalysis. 2005 , 105, 122-133	63
1875	Electronic structures and spectral properties of endohedral fullerenes. 2005 , 249, 1111-1132	131
1874	DFT benchmark study for the oxidative addition of CH ₄ to Pd. Performance of various density functionals. 2005 , 313, 261-270	87

1873	AFMM: A molecular mechanics force field vibrational parametrization program. 2005 , 167, 34-42		35
1872	Substrate binding in the active site of cytochrome P450cam. 2005 , 403, 35-41		9
1871	Magnetic exchange of trinuclear spin frustration system: CASPT2 and density functional theory study on hydroxo-bridged chromium complex [Cr ₃ (NH ₃) ₁₀ (OH) ₄] ³⁺ Br ⁻ . 2005 , 407, 147-152		12
1870	Structure and stability of thiophene-hydrogen halide complexes: An ab initio molecular orbital study. 2005 , 407, 222-226		10
1869	Modeling properties of molecules with open d-shells using density functional theory. 2005 , 8, 1421-1433		25
1868	Structural and spectroscopic studies on mercury(II) tribenzylphosphine complexes. 2005 , 1602-12		12
1867	Multicomponent synthesis of 2-imidazolines. 2005 , 70, 3542-53		141
1866	Density functional studies of actinyl aquo complexes studied using small-core effective core potentials and a scalar four-component relativistic method. 2005 , 109, 10961-74		194
1865	Density functional calculation of the electronic circular dichroism spectra of the transition metal complexes [M(phen) ₃] ²⁺ (M = Fe, Ru, Os). 2005 , 109, 4836-46		53
1864	Absolute rates of hole transfer in DNA. 2005 , 127, 14894-903		303
1863	The nature of the supramolecular association of 1,2,5-chalcogenadiazoles. 2005 , 127, 3184-90		229
1862	A sparse algorithm for the evaluation of the local energy in quantum Monte Carlo. <i>Journal of Computational Chemistry</i> , 2005 , 26, 708-15	3.5	23
1861	Zori 1.0: a parallel quantum Monte Carlo electronic structure package. <i>Journal of Computational Chemistry</i> , 2005 , 26, 856-62	3.5	24
1860	Oxidative addition of the ethane C-C bond to Pd. An ab initio benchmark and DFT validation study. <i>Journal of Computational Chemistry</i> , 2005 , 26, 1006-20	3.5	63
1859	Ab initio and DFT benchmark study for nucleophilic substitution at carbon (S _N 2@C) and silicon (S _N 2@Si). <i>Journal of Computational Chemistry</i> , 2005 , 26, 1497-504	3.5	120
1858	EPR, ENDOR, and DFT Studies on (η ⁵ -Octahalo-meso-tetraarylporphyrin)copper Complexes: Characterization of the Metal(d)Porphyrin(a _{2u}) Orbital Interaction. 2005 , 2005, 1609-1615		21
1857	Lanthanide(III)-Induced Conversion of 12-Metallacrown-4 to 5-Metallacrown-5 Complexes in Solution. 2005 , 2005, 3303-3310		29
1856	On the Borderline between cis and trans in Organometallic(Phosphane)platinum(II) Complexes. 2005 , 2005, 4056-4063		18

1855	Extending the NHC Concept: $\text{C}\equiv\text{C}$ Coupling Catalysis by a PdII Carbene (rNHC) Complex with Remote Heteroatoms. 2005 , 2005, 2973-2977	59
1854	Norcorrole and Dihydronorcorrole: A Predictive Quantum Chemical Study. 2005 , 2005, 4479-4485	33
1853	Vicinal tungsten-tungsten coupling constants in polyoxotungstates: DFT calculations challenge an empirical rule. 2005 , 44, 2023-6	34
1852	Heterobimetallic main-group-transition-metal paddle-wheel carboxylates. 2005 , 44, 1721-4	61
1851	Direct estimate of the conjugative and hyperconjugative stabilization in diynes, dienes, and related compounds. 2005 , 44, 3617-20	85
1850	$[\text{Re}_{12}\text{CS}_{17}(\text{CN})_6]_n$ (n=6, 8): a sulfido-cyanide rhenium cluster with an interstitial carbon atom. 2005 , 44, 6867-71	39
1849	Experimental evidence for a Jahn-Teller distortion in AuCl_3 . 2005 , 44, 6746-50	21
1848	Vicinal Tungsten-Tungsten Coupling Constants in Polyoxotungstates: DFT Calculations Challenge an Empirical Rule. 2005 , 117, 2059-2062	10
1847	Heterobimetallic Main-Group-Transition-Metal Paddle-Wheel Carboxylates. 2005 , 117, 1749-1752	13
1846	Direkte Bestimmung der konjugativen und hyperkonjugativen Stabilisierung in Diinen, Dienen und verwandten Verbindungen. 2005 , 117, 3683-3686	29
1845	$[\text{Re}_{12}\text{CS}_{17}(\text{CN})_6]_n$ (n=6, 8): A Sulfido-Cyanide Rhenium Cluster with an Interstitial Carbon Atom. 2005 , 117, 7027-7031	4
1844	Experimental Evidence for a Jahn-Teller Distortion in AuCl_3 . 2005 , 117, 6904-6908	8
1843	Hyperolactone C: determination of its absolute configuration by comparison of experimental and calculated CD spectra. 2005 , 17, 250-6	18
1842	Calculation of the redox potential of the protein azurin and some mutants. 2005 , 6, 738-46	46
1841	The "invisible" ^{13}C NMR chemical shift of the central carbon atom in $[(\text{Ph}_3\text{PAu})_6\text{C}]^{2+}$: a theoretical investigation. 2005 , 11, 1677-86	12
1840	The nature of the chemical bond revisited: an energy-partitioning analysis of nonpolar bonds. 2005 , 11, 1813-25	124
1839	$\text{C}_5\text{H}_4\text{-BR}_2$ bending in ferrocenylboranes: a delocalized through-space interaction between iron and boron. 2005 , 11, 584-603	123
1838	Metallophilicity versus pi-pi interactions: ligand-unsupported argentophilicity/cuprophilicity in oligomers-of-dimers $[\text{M}_2\text{L}_2]_n$ (M=CuI or AgI, L=tridentate ligand). 2005 , 11, 552-61	124

1837	Regioselective intramolecular Pauson-Khand reactions of C60: an electrochemical study and theoretical underpinning. 2005 , 11, 2716-29	52
1836	Syntheses, structures, photoluminescence and theoretical studies of xanthone in crystalline resorcinarene-based inclusion complexes. 2005 , 11, 3583-90	24
1835	Fine-tuning the electronic properties of highly stable organometallic Cu(III) complexes containing monoanionic macrocyclic ligands. 2005 , 11, 5146-56	97
1834	Theoretical search for atomic-like states of silicon at the surface of thermally grown SiO ₂ films on silicon surfaces. 2005 , 80, 1617-1623	3
1833	A theoretical investigation of the photo-induced intramolecular charge transfer excitation of cuprous (I) bis-phenanthroline by density functional theory. 2005 , 690, 187-192	8
1832	Electronic structure and electrophilic reactivity of discrete copper diphenylcarbenes. 2005 , 690, 5989-6000	55
1831	DFT studies on isomerization reactions in the copolymerization of ethylene and methyl acrylate catalyzed by Ni-diimine and Pd-diimine complexes. 2005 , 11, 341-50	21
1830	Interconverting WW Triple Bonds and W ₄ Clusters: Structures of W ₄ (OPrn) ₁₆ and [Li ₂ W ₂ (OPrn) ₈ (DME)] ₂ *. 2005 , 16, 231-249	1
1829	DFT Study of HFI in Halogen-Containing Gold, Silver and Copper Complexes. 2005 , 159, 293-304	2
1828	The structure of short-lived excited states of molecular complexes by time-resolved X-ray diffraction. 2005 , 61, 162-72	79
1827	Complexes of 1,3-Bis(diphenylphosphano)propane (dppp) with Dichloroplatinum(II) and Bis(chlorogold(I)): Intramolecular versus Intermolecular AuI⋯AuI Association of [(Edppp)(AuCl) ₂] in catena and cyclo Forms. 2005 , 631, 1355-1358	9
1826	Trichloropalladate(II) Complexes with Pyridine Ligands [Molecular Structure and Conformational Analysis of [K(18C6)][PdCl ₃ (py)]. 2005 , 631, 1456-1462	6
1825	Organoplatinum Complexes of the N,N-Diisopropyl-diazabutadiene Ligand: A Structural and Spectroscopic Study. 2005 , 631, 2669-2676	3
1824	Theoretical Studies of Inorganic Compounds. 341) Energy Decomposition Analysis of EE Bonding in Planar and Perpendicular X ₂ EE ₂ (E = B, Al, Ga, In, Tl; X = H, F, Cl, Br, I). 2005 , 631, 1803-1809	35
1823	DFT study of mixed-valent Mn(II/III) hexacyanide clusters. 2005 , 101, 753-760	9
1822	Molecular impurities in crystals: (ReO ₄) ₂ ⊂Jahn-Teller ion in KCl. 2005 , 101, 802-806	
1821	Energy analysis of the chemical bond in group IV and V complexes: A density functional theory study. 2005 , 101, 869-877	22
1820	Density functional calculations of ¹⁹ F and ²³⁵ U NMR chemical shifts in uranium (VI) chloride fluorides UF ₆ Cl _n : Influence of the relativistic approximation and role of the exchange-correlation functional. 2005 , 101, 372-380	27

1819	Calculation of spin-orbit coupling within the LFDFT: Applications to $[\text{NiX}_4]_2$ ($X = \text{F}, \text{Cl}, \text{Br}, \text{I}$) 2005 , 102, 119-131	45
1818	Refractive index and third-order nonlinear susceptibility of C60 in the condensed phase calculated with the discrete solvent reaction field model. 2005 , 102, 612-619	21
1817	Analytical second derivatives in the Amsterdam density functional package. 2005 , 104, 645-659	152
1816	Electronic properties of Strandberg anions: A DFT study of $[\text{X}_2\text{Mo}_5\text{O}_{23}]_n$ ($X = \text{PV}, \text{SVI}, \text{AsV}, \text{SeVI}$), and $[(\text{RP})_2\text{Mo}_5\text{O}_{21}]_4$ ($R = \text{H}, \text{CH}_3, \text{C}_2\text{H}_5$). 2005 , 105, 37-42	12
1815	The nature of the chemical bond in the light of an energy decomposition analysis. 2005 , 291-372	57
1814	Applied density functional theory and the deMon codes 1964-2004. 2005 , 1079-1097	4
1813	Circular dichroism in the angle-resolved C 1s photoemission spectra of gas-phase carvone enantiomers. 2005 , 123, 234310	33
1812	Geometric, electronic, and bonding properties of AuNM ($N = 1-7$, $M = \text{Ni}, \text{Pd}, \text{Pt}$) clusters. 2005 , 122, 114310	153
1811	Analysis of the viscoelastic coefficients in the Vignale-Kohn functional: The cases of one- and three-dimensional polyacetylene. 2005 , 71,	18
1810	Coherent tunneling in Cu^{2+} - and Ag^{2+} -doped MgO and $\text{CaO}:\text{Cu}^{2+}$ explored through ab initio calculations. 2005 , 72,	26
1809	A density-functional study on the formation of $\text{Mo}(2)_2^+$. 2005 , 123, 134313	5
1808	Critical examination of the supermolecule density functional theory calculations of intermolecular interactions. 2005 , 122, 14117	47
1807	Gauge invariance of the spin-other-orbit contribution to the g-tensors of electron paramagnetic resonance. 2005 , 122, 214101	26
1806	Ab initio calculation of the C/D ratio of magnetic circular dichroism. 2005 , 122, 094112	29
1805	High-resolution infrared spectroscopy of the charge-transfer complex $[\text{Ar-N}_2]^+$: a combined experimental/theoretical study. 2005 , 123, 144305	8
1804	Time-dependent current-density-functional theory for the metallic response of solids. 2005 , 71,	40
1803	Origin of warping in the E \otimes e Jahn-Teller problem: Quadratic vibronic coupling versus anharmonicity and application to $\text{NaCl}:\text{Rh}^{2+}$ and triangular molecules. 2005 , 71,	62
1802	Theory and method for calculating resonance Raman scattering from resonance polarizability derivatives. 2005 , 123, 174110	155

1801	Investigation of chromophore-chromophore interaction by electro-optic measurements, linear dichroism, x-ray scattering, and density-functional calculations. 2005 , 72, 036610	35
1800	Importance of vibronic effects on the circular dichroism spectrum of dimethyloxirane. 2005 , 122, 234305	52
1799	Origin of the different color of ruby and emerald. 2005 , 72,	42
1798	The merits of the frozen-density embedding scheme to model solvatochromic shifts. 2005 , 122, 094115	187
1797	Applications of quantum chemical methods in zeolite science. 2005 , 243-262	7
1796	A physical model for the longitudinal polarizabilities of polymer chains. 2005 , 123, 174910	12
1795	Charging mechanism for the bond elongation observed in suspended chains of gold atoms. 2005 , 72,	12
1794	The uranyl ion revisited: the electric field gradient at U as a probe of environmental effects. 2005 , 103, 775-787	10
1793	Microscopic and macroscopic polarization within a combined quantum mechanics and molecular mechanics model. 2005 , 122, 34103	36
1792	Controlling ligand substitution reactions of organometallic complexes: tuning cancer cell cytotoxicity. 2005 , 102, 18269-74	262
1791	Nanocones \square a different form of carbon with unique properties. 2005 , 901, 1	2
1790	Ligand rotation in $[\text{Ar}(\text{R})\text{N}]_3\text{M}-\text{N}_2-\text{M}'[\text{N}(\text{R})\text{Ar}]_3$ ($\text{M}, \text{M}' = \text{MoIII}, \text{NbIII}$; $\text{R} = \text{iPr}$ and tBu) dimers. 2005 , 962-8	21
1789	Orbital-free embedding applied to the calculation of induced dipole moments in $\text{CO}_2\cdots\text{X}$ ($\text{X} = \text{He}, \text{Ne}, \text{Ar}, \text{Kr}, \text{Xe}, \text{Hg}$) van der Waals complexes. 2005 , 123, 174104	55
1788	Density functional theory study on the first hyperpolarizabilities of organoimido derivatives of hexamolybdates. 2005 , 109, 22332-6	57
1787	The first hyperpolarizability of p-nitroaniline in 1,4-dioxane: a quantum mechanical/molecular mechanics study. 2005 , 123, 074307	62
1786	Comparison of various Franck-Condon and vibronic coupling approaches for simulating electronic spectra: the case of the lowest photoelectron band of ethylene. 2005 , 7, 1759-71	52
1785	Metal-metal interactions in mixed-valence $[\text{M}_2\text{Cl}_9]^{2-}$ species: electronic structure of d_1d_2 ($\text{V}, \text{Nb}, \text{Ta}$) and d_4d_5 ($\text{Fe}, \text{Ru}, \text{Os}$) face-shared systems. 2005 , 44, 5081-91	11
1784	Activation of H-H, C-H, C-C and C-Cl Bonds by Pd and PdCl(-). Understanding Anion Assistance in C-X Bond Activation. 2005 , 1, 286-98	129

1783	Effect of self-interaction error in the evaluation of the bond length alternation in trans-polyacetylene using density-functional theory. 2005 , 123, 121102	30
1782	Large hyperpolarizabilities of trinuclear transition metal clusters [M ₂ Ag ₂ X ₄ (C ₅ H ₅ NS)(PPh ₃) ₂][CH ₂ Cl ₂ (M = Mo, W; X = S, Se): a DFT study. 2005 , 29, 362-365	11
1781	A chemically intuitive proposal for the structure of n-diamond. 2005 , 103, 2707-2715	23
1780	Core spin-polarization correction in pseudopotential-based electronic structure calculations. 2005 , 71,	30
1779	Oxidative addition of iodo-acetonitrile and of elemental halogens to [Pt ₃ (μ-CO) ₃ (PCy ₃) ₃]. 2005 , 315-25	17
1778	Synthesis of a four-coordinate titanium(IV) oxoanion via deprotonation and decarbonylation of complexed formate. 2005 , 3403-5	22
1777	Experimental and theoretical study of intramolecular exchange in Ir ₂ Rh ₂ (CO) ₁₂ and Ir ₄ (CO) ₁₁ (micro-SO ₂). 2005 , 310-4	3
1776	NMR and EPR studies of the bis(pyridine) and bis(tert-butyl isocyanide) complexes of iron(III) octaethylchlorin. 2005 , 44, 1890-903	15
1775	Magnetic field dependence of photo-CIDNP MAS NMR on photosynthetic reaction centers of Rhodobacter sphaeroides WT. 2005 , 127, 14290-8	65
1774	Combined theoretical and experimental deep-UV resonance raman studies of substituted pyrenes. 2005 , 109, 2100-6	56
1773	Ab initio and microcalorimetric investigations of alkene adsorption on phosphotungstic acid. 2005 , 21, 4738-45	25
1772	Electronic properties and stability of dititanium(IV) substituted alpha-Keggin polyoxotungstate with heteroatom phosphorus by DFT. 2005 , 44, 100-7	52
1771	Density Functional Study of H-D Coupling Constants in Heavy Metal Dihydrogen and Dihydride Complexes: The Role of Geometry, Spin-Orbit Coupling, and Gradient Corrections in the Exchange-Correlation Kernel. 2005 , 1, 601-11	20
1770	Unprecedented eta ³ -M ₃ coordination mode in a terpyridine ligand. 2005 , 3355-6	20
1769	Fragment-oriented design of catalysts based on the activation strain model. 2005 , 103, 995-998	32
1768	Paramagnetic NMR spectroscopy and density functional calculations in the analysis of the geometric and electronic structures of iron-sulfur proteins. 2005 , 44, 779-97	57
1767	The Asymmetric Schrock Olefin Metathesis Catalyst. A Computational Study. 2005 , 24, 3200-3206	41
1766	Calculation of excitation energies of open-shell molecules with spatially degenerate ground states. I. Transformed reference via an intermediate configuration Kohn-Sham density-functional theory and applications to d ¹ and d ² systems with octahedral and tetrahedral symmetries. 2005 , 123, 144105	29

- 1765 On the origin of optical activity in tris-diamine complexes of Co(III) and Rh(III): a simple model based on time-dependent density function theory. **2005**, 127, 975-85 71
- 1764 Effects of peripheral substituents and axial ligands on the electronic structure and properties of cobalt porphyrins. **2005**, 109, 11996-2005 26
- 1763 Crystal chemistry of mercury oxo- and chalcogenides. **2005**, 11, 87-123 12
- 1762 Metal π -olefin Interactions in $M(CO)_5(\text{cycloolefin})$ ($M = \text{Cr, Mo, W}$; Cycloolefin = Cyclopropene to Cyclooctene): Strain Relief and Metal π -olefin Bond Strength. **2005**, 24, 3882-3890 21
- 1761 Combined charge and spin density experimental study of the yttrium(III) semiquinonato complex $Y(\text{HBPz3})_2(\text{DTBSQ})$ and DFT calculations. **2005**, 109, 2723-32 23
- 1760 Solution calorimetric and stopped-flow kinetic studies of the reaction of $^*Cr(CO)_3C_5Me_5$ with PhSe-SePh and PhTe-TePh . Experimental and theoretical estimates of the Se-Se, Te-Te, H-Se, and H-Te bond strengths. **2005**, 44, 3127-36 25
- 1759 C-H Bond Activation Reactions with Ligand Adducts of a π -Diimine Iridium Dihydride. **2005**, 24, 4367-4373 24
- 1758 Atomic silicon in siloxanic networks: the nature of the oxo-oxygen-silicon bond. **2005**, 44, 1381-90 4
- 1757 Experimental and theoretical studies of carbodiphosphorane-CX₂ adducts with unusual bonding situations: preparation, crystal structures, and bonding analyses of $S_2CC(\text{PPh}_3)_2$, $O_2CC(\text{PPh}_3)_2$, and $[(CO)_4MS_2CC(\text{PPh}_3)_2]$ ($M = \text{Cr, Mo, W}$). **2005**, 44, 1263-74 86
- 1756 Ground states, excited states, and metal-ligand bonding in rare earth hexachloro complexes: a DFT-based ligand field study. **2005**, 44, 2954-63 61
- 1755 Active site structure of class I ribonucleotide reductase intermediate X: a density functional theory analysis of structure, energetics, and spectroscopy. **2005**, 127, 15778-90 62
- 1754 Optical properties and delocalization of excess negative charges on oligo(phenylenevinylene)s: a quantum chemical study. **2005**, 109, 5644-52 21
- 1753 Coordination of nitroxide and nitronyl-nitroxide organic radicals to trimeric perfluoro-o-phenylene mercury. **2005**, 44, 6248-55 29
- 1752 Spectroscopy of non-heme iron thiolate complexes: insight into the electronic structure of the low-spin active site of nitrile hydratase. **2005**, 44, 1826-36 35
- 1751 Molecular Modeling of Stereo- and Regioselectivity of Group 4 Heterocenes in the Polymerization of Propene. **2005**, 38, 3973-3976 14
- 1750 Multiple Isomerism (cis/trans; syn/anti) in $[(\text{dmsO})_2\text{Pt}(\text{aryl})_2]$ Complexes: A Combined Structural, Spectroscopic, and Theoretical Investigation. **2005**, 24, 4125-4131 29
- 1749 DFT Study of Ethylene and Propylene Copolymerization over a Heterogeneous Catalyst with a Coordinating Lewis Base. **2005**, 38, 9865-9872 42
- 1748 Geometrical and electronic structures of dinuclear complex ions $\{(\mu\text{-bpym})[\text{Cu}(\text{EAR}_3)_2]_2\}^{2+}$ with intramolecular "organic sandwich" formation ($E = \text{P or As}$; $\text{Ar} = \text{Aryl}$; $\text{bpym} = 2,2'$ -bipyrimidine). **2005**, 44, 4637-43 22

1747	Spectroscopic and computational studies of the ATP:corrinoid adenosyltransferase (CobA) from <i>Salmonella enterica</i> : insights into the mechanism of adenosylcobalamin biosynthesis. 2005 , 127, 8710-9	77
1746	Intramolecular Coupling of α -Iminoacyls on Zirconium Bis(aryloxides) and Calix[4]arenes: Revised Mechanism by DFT Calculations and CarParrinello Molecular Dynamics Simulations. 2005 , 24, 1867-1875	9
1745	Possible side reactions due to water in emulsion polymerization by late transition metal complexes. 1. Water complexation and hydrolysis of the growing chain. 2005 , 44, 7806-18	24
1744	Interaction of a bulky N-heterocyclic carbene ligand with Rh(I) and Ir(I). Double C-H activation and isolation of bare 14-electron Rh(III) and Ir(III) complexes. 2005 , 127, 3516-26	264
1743	Experimental and Computational Study of the [2 + 2] Dissociation of Rhenaioxetanes in the Gas Phase. 2005 , 24, 3040-3042	15
1742	Co-C bond activation in methylmalonyl-CoA mutase by stabilization of the post-homolysis product Co ²⁺ cobalamin. 2005 , 127, 16522-8	33
1741	Study of Hg ²⁺ and complexes of NpO ²⁺ and UO ²⁺ in solution. examples of cation-cation interactions. 2005 , 44, 6975-82	31
1740	Mechanism of white phosphorus activation by three-coordinate molybdenum(III) complexes: a thermochemical, kinetic, and quantum chemical investigation. 2005 , 127, 15191-200	41
1739	Electronic structure studies of the adenosylcobalamin cofactor in glutamate mutase. 2005 , 44, 15167-81	20
1738	Probing the geometric and electronic structures of the low-temperature azide adduct and the product-inhibited form of oxidized manganese superoxide dismutase. 2005 , 44, 1504-20	56
1737	Designing Molecules for Metal-Metal Electronic Communication: Synthesis and Molecular Structure of the Couple of Heterobimetallic Isomers [η^6 -(2-Ferrocenyl)indene]-Cr(CO) ₃ and [η^6 -(3-Ferrocenyl)indene]-Cr(CO) ₃ . 2005 , 24, 4691-4694	18
1736	Density functional theory study of the Jahn-Teller effect and spin-orbit coupling for copper and gold trimers. 2005 , 109, 512-9	22
1735	NLO properties of metallabenzene-based chromophores: a time-dependent density functional study. 2005 , 109, 5454-62	43
1734	Ab initio reaction path analysis of benzene hydrogenation to cyclohexane on Pt(111). 2005 , 109, 2064-73	72
1733	3H-benzophosphepine complexes: versatile phosphinidene precursors. 2005 , 127, 16985-99	45
1732	Oxidative addition of the fluoromethane C-F bond to Pd. An ab initio benchmark and DFT validation study. 2005 , 109, 9685-99	57
1731	Spectroscopic and density functional studies of the red copper site in nitrosocyanin: role of the protein in determining active site geometric and electronic structure. 2005 , 127, 3531-44	90
1730	An explicit quantum chemical method for modeling large solvation shells applied to aminocoumarin C151. 2005 , 109, 7805-14	120

1729	Energetics of binuclear spin transition complexes. 2005 , 127, 16197-201	78
1728	The performance of time-dependent density functional theory based on a noncollinear exchange-correlation potential in the calculations of excitation energies. 2005 , 122, 074109	115
1727	Vibronic structure of the permanganate absorption spectrum from time-dependent density functional calculations. 2005 , 109, 1168-79	58
1726	Influence of pi-stacking on the resonant enhancement of the second-order nonlinear optical response of dipolar chromophores. 2005 , 109, 18378-84	6
1725	Ab initio quantum chemical and mixed quantum mechanics/molecular mechanics (QM/MM) methods for studying enzymatic catalysis. 2005 , 56, 389-427	447
1724	The calculation of excitation energies based on the relativistic two-component zeroth-order regular approximation and time-dependent density-functional with full use of symmetry. 2005 , 122, 204103	214
1723	Surface complexation model for multisite adsorption of copper(II) onto kaolinite. 2005 , 69, 3733-3745	66
1722	Modeling solvent effects on electron-spin-resonance hyperfine couplings by frozen-density embedding. 2005 , 123, 114101	57
1721	Steric and electronic properties of N-heterocyclic carbenes (NHC): a detailed study on their interaction with Ni(CO) ₄ . 2005 , 127, 2485-95	512
1720	Quantum mechanical continuum solvation models. 2005 , 105, 2999-3093	11786
1719	Finite lifetime effects on the polarizability within time-dependent density-functional theory. 2005 , 122, 224115	146
1718	High-field EPR spectroscopy applied to biological systems: characterization of molecular switches for electron and ion transfer. 2005 , 7, 19-42	88
1717	Carbon-Carbon Bonds of Dinuclear Manganese Half-Sandwich Complexes as Electron Reservoirs. 2005 , 24, 920-932	46
1716	Structural, optical, and photophysical properties of nickel(II) alkylthioporphyryns: insights from experimental and DFT/TDDFT studies. 2005 , 44, 6609-22	45
1715	Distance measurements between paramagnetic centers and a planar object by matrix Mims electron nuclear double resonance. 2005 , 122, 024515	20
1714	Molecular modelling for coordination compounds: Cu(II)-amine complexes. 2005 , 3638-45	31
1713	Why do the heavy-atom analogues of acetylene E ₂ H ₂ (E = Si-Pb) exhibit unusual structures?. 2005 , 127, 6290-9	157
1712	Theoretical study of the adsorption and dissociation of oxygen on Pt(111) in the presence of homogeneous electric fields. 2005 , 109, 6304-10	112

1711	Calculation of the birefringences of nematic liquid crystals at optical and infrared wavelengths. 2005 , 123, 134904	13
1710	Reductive Elimination of Organic Molecules from PalladiumDiphosphine Complexes. 2005 , 24, 3703-3710	83
1709	Lanthanide(III)/Actinide(III) Differentiation in Mixed Cyclopentadienyl/Dithiolene Compounds from X-ray Diffraction and Density Functional Theory Analysis. 2005 , 24, 4940-4952	62
1708	DFT Study of the Tetranuclear Lutetium and Yttrium Polyhydride Cluster Complexes [(C5Me4SiMe3)4Ln4H8] (Ln = Lu, Y) that Contain a Four-Coordinate Hydrogen Atom. 2005 , 24, 4362-4366	66
1707	Thermodynamic study of the complexation of trivalent actinide and lanthanide cations by ADPTZ, a tridentate N-donor ligand. 2005 , 44, 1404-12	105
1706	Density Functional Methods for Excited States: Equilibrium Structure and Electronic Spectra. 2005 , 16, 93-128	169
1705	Spectroscopic and theoretical evidence for the elusive intermediate of the photoinitiated and thermal rearrangements of photochromic spiropyrans. 2005 , 109, 9605-16	32
1704	Relativistic density functional calculations of EPR g tensor for eta1{CuNO}(11) species in discrete and zeolite-embedded states. 2005 , 109, 10571-81	21
1703	Iron versus Ruthenium: Dramatic Changes in Electronic Structure Result from Replacement of One Fe by Ru in [{Cp*(dppe)Fe}-CC-CC-{Fe(dppe)Cp*}]n+ (n = 0, 1, 2). 2005 , 24, 3864-3881	110
1702	Electron Transfer and Electron Exchange between [Cp*(dppe)Fe]n+ (n = 0, 1) Building Blocks Mediated by the 9,10-Bis(ethynyl)anthracene Bridge. 2005 , 24, 4558-4572	102
1701	Electronic ground states of iron porphyrin and of the first species in the catalytic reaction cycle of cytochrome P450s. 2005 , 109, 3411-7	95
1700	Relativistic two-component calculations of electronic g-tensors that include spin polarization. 2005 , 123, 244103	65
1699	Metal and ligand K-edge XAS of organotitanium complexes: metal 4p and 3d contributions to pre-edge intensity and their contributions to bonding. 2005 , 127, 667-74	110
1698	Electronic structure of M(BH4)4, M = Zr, Hf, and U, by variable photon-energy photoelectron spectroscopy and density functional calculations. 2005 , 44, 7781-93	15
1697	A simplified relativistic time-dependent density-functional theory formalism for the calculations of excitation energies including spin-orbit coupling effect. 2005 , 123, 154102	180
1696	Charge transport in self-organized pi-stacks of p-phenylene vinylene oligomers. 2005 , 109, 18267-74	89
1695	Multielectron redox chemistry of iron porphyrinogens. 2005 , 127, 4730-43	68
1694	The unexpected similar second-order NLO response for nearly planar and largely twisted push-pull stilbazole chromophores: EFISH and theoretical TD-DFT evidence. 2005 , 5405-7	12

- 1693 On the spectral similarity of bridging and nonbridging oxygen in tellurites. **2005**, 109, 7636-41 16
- 1692 Spectroscopy and computations of supported metal adducts. 1. DFT Study of CO and NO adsorption and coadsorption on Cu/SiO₂. **2005**, 109, 10291-303 18
- 1691 Theoretical study of the electronic spectra of square-planar platinum (II) complexes based on the two-component relativistic time-dependent density-functional theory. **2005**, 123, 194102 40
- 1690 A computational and experimental study of the structures and Raman and ⁷⁷Se NMR spectra of SeX₃⁺ and SeX₂ (X = Cl, Br, I): FT-Raman spectrum of (SeI₃)[AsF₆]. **2005**, 44, 1904-13 16
- 1689 Effect of the f-Orbital Delocalization on the Ligand-Field Splitting Energies in Lanthanide-Containing Elpasolites. **2006**, 2, 1106-11 29
- 1688 Tuning the photoinduced O₂-evolving reactivity of Mn₄O₄⁷⁺, Mn₄O₄⁶⁺, and Mn₄O₃(OH)₆⁺ manganese-oxo cubane complexes. **2006**, 45, 189-95 54
- 1687 Surface-enhanced raman scattering of pyrazine at the junction between two Ag₂₀ nanoclusters. **2006**, 6, 1229-34 196
- 1686 Experimental and density functional theoretical investigations of linkage isomerism in six-coordinate FeNO(6) iron porphyrins with axial nitrosyl and nitro ligands. **2006**, 128, 2093-104 68
- 1685 Adenine tautomers: relative stabilities, ionization energies, and mismatch with cytosine. **2006**, 110, 4012-20 111
- 1684 DFT/TDDFT study of lanthanide(III) mono- and bisporphyrin complexes. **2006**, 110, 13089-98 25
- 1683 Dependence of the Intermolecular Electrostatic Interaction Energy on the Level of Theory and the Basis Set. **2006**, 2, 81-9 35
- 1682 Prediction of second-order optical nonlinearity of trisorganotin-substituted beta-Keggin polyoxotungstate. **2006**, 45, 7864-8 42
- 1681 Copper(II) complexes of salen analogues with two differently substituted (push-pull) salicylaldehyde moieties. A study on the modulation of electronic asymmetry and nonlinear optical properties. **2006**, 45, 10976-89 122
- 1680 Metal-metal bonding in molecular actinide compounds: electronic structure of [M₂X₈]⁽²⁻⁾ (M = U, Np, Pu; X = Cl, Br, I) complexes and comparison with d-block analogues. **2006**, 5476-83 35
- 1679 Catalytic mechanism of glycosyltransferases: hybrid quantum mechanical/molecular mechanical study of the inverting N-acetylglucosaminyltransferase I. **2006**, 128, 16921-7 37
- 1678 ON THE STRUCTURE OF i-CARBON. **2006**, 05, 175-185 13
- 1677 Efficient charge transport along phenylene-vinylene molecular wires. **2006**, 110, 14659-66 54
- 1676 Influence of the membrane potential on the protonation of bacteriorhodopsin: insights from electrostatic calculations into the regulation of proton pumping. **2006**, 128, 12129-39 23

1675	Optical properties of Cr ³⁺ doped oxides: Different behavior of two centers in alexandrite. 2006 , 74,	32
1674	Investigation of the Dithiolene Ligand Conformation in Analogous U(IV)/U(V) Complexes: X-ray Diffraction and Density Functional Theory Analysis of the U π (CC) Interaction. 2006 , 25, 2782-2795	20
1673	Mechanism of bleomycin suicide: a Car-Parrinello molecular dynamics investigation. 2006 , 110, 21245-50	2
1672	Optical and vibrational properties of MnF ₆ ⁴⁻ complexes in cubic fluoroperovskites: insight through embedding calculations using Kohn-Sham equations with constrained electron density. 2006 , 18, 1519-1534	26
1671	Efficient green-blue-light-emitting cationic iridium complex for light-emitting electrochemical cells. 2006 , 45, 9245-50	183
1670	Group 11 complexes with the bis(3,5-dimethylpyrazol-1-yl)methane ligand. How secondary bonds can influence the coordination environment of Ag(I): the role of coordinated water in [Ag ₂ (μ -L) ₂ (OH ₂) ₂](OTf) ₂ . 2006 , 4104-13	32
1669	Magnetic coupling in dinuclear Gd complexes. 2006 , 128, 568-75	148
1668	Resonance Raman scattering of rhodamine 6G as calculated using time-dependent density functional theory. 2006 , 110, 5973-7	303
1667	Density functional investigation of the adsorption of a methane monolayer on an MgO(100) surface. 2006 , 73,	13
1666	Pyridine-Ag ₂₀ cluster: a model system for studying surface-enhanced Raman scattering. 2006 , 128, 2911-9	430
1665	Acetylenic carbon-13 chemical shift tensors for diphenylacetylene and (η^2 -Diphenylacetylene)Pt(PPh ₃) ₂ : a solid-state NMR and theoretical study. 2006 , 45, 2461-73	17
1664	Copper(II) hexaaza macrocyclic binuclear complexes obtained from the reaction of their copper(I) derivatives and molecular dioxygen. 2006 , 45, 3569-81	56
1663	A first structural and theoretical comparison of pyridinylidene-type rNHC (remote N-heterocyclic carbene) and NHC complexes of Ni(II) obtained by oxidative substitution. 2006 , 1226-33	74
1662	First hyperpolarizability of a sesquifulvalene transition metal complex by time-dependent density-functional theory. 2006 , 110, 1014-21	26
1661	Migratory insertion in N-heterocyclic carbene-containing Fe carbonyl complexes: an experimental and theoretical study. 2006 , 2535-41	31
1660	Tuning the Palladium-Silicon Bond: Bond Analysis of Bisphosphine Silyl Palladium Hydrides. 2006 , 25, 1945-1952	6
1659	"Dormant" secondary metal-alkyl complexes are not omnipresent. 2006 , 103, 15338-42	21
1658	Electronic spectra of uranyl chloride complexes in acetone: a CASSCF/CASPT2 investigation. 2006 , 8, 4311-9	28

1657	Magnetostructural correlations in the cyano-bridged CrNi, Cr ₂ Ni and CrNi ₆ complexes: density functional theory calculations. 2006 , 16, 4657	9
1656	Comparison of frozen-density embedding and discrete reaction field solvent models for molecular properties. 2006 , 8, 2349-59	80
1655	SPANphos: trans-spanning diphosphines as cis chelating ligands!. 2006 , 268-78	46
1654	¹⁹⁵ Pt NMR and DFT computational methods as tools towards the understanding of speciation and hydration/solvation of [PtX ₆] ²⁻ (X = Cl-, Br-) anions in solution. 2006 , 3277-84	40
1653	Molecular modelling of Jahn-Teller distortions in Cu(II)N ₆ complexes: elongations, compressions and the pathways in between. 2006 , 1092-100	44
1652	Density functional theory investigation of the geometric and electronic structures of [UO ₂ (H ₂ O) _m (OH) _n] ⁽²⁻ⁿ⁾ (n + m = 5). 2006 , 2403-14	56
1651	Periodic trends in metal-metal interactions in face-shared [M ₂ Cl ₉] ^{z-} systems. 2006 , 2017-25	13
1650	Density-Functional Theory Investigation of the Geometric, Energetic, and Optical Properties of the Cobalt(II)tris(2,2'-bipyridine) Complex in the High-Spin and the Jahn-Teller Active Low-Spin States. 2006 , 2, 1342-59	49
1649	Molecular Squares, Rectangles, and Corners: Ground-State Electronic Structure and Configurational Properties. 2006 , 18, 620-628	1
1648	Photochemistry of Methyltrioxorhenium Revisited: A DFT/TD-DFT and CASSCF/MS-CASPT2 Theoretical Study. 2006 , 25, 5235-5241	11
1647	Structural and electronic analysis of lanthanide complexes: reactivity may not necessarily be independent of the identity of the lanthanide atom—a DFT study. 2006 , 110, 11324-31	46
1646	Photo-CIDNP MAS NMR in intact cells of Rhodobacter sphaeroides R26: molecular and atomic resolution at nanomolar concentration. 2006 , 128, 12794-9	52
1645	An NMR and relativistic DFT investigation of one-bond nuclear spin-spin coupling in solid triphenyl group-14 chlorides. 2006 , 8, 2733-43	15
1644	Pi-conjugation in donor-substituted cyanoethynylethenes: an EDA study. 2006 , 5030-2	32
1643	A trinuclear Pt(II) compound with short Pt-Pt-Pt contacts. An analysis of the influence of pi-pi stacking interactions on the strength and length of the Pt-Pt bond. 2006 , 1188-96	62
1642	Energy partitioning schemes. 2006 , 8, 4630-46	25
1641	Vibrational and electron paramagnetic resonance properties of free and MgO supported AuCO complexes. 2006 , 124, 174709	25
1640	Quantum Chemical Calculations of the Influence of Anchor-Cum-Spacer Groups on Femtosecond Electron Transfer Times in Dye-Sensitized Semiconductor Nanocrystals. 2006 , 2, 441-51	238

1639	Anion- π interactions as controlling elements in self-assembly reactions of Ag(I) complexes with π -acidic aromatic rings. 2006 , 128, 5895-912	281
1638	Interactions study between the copper II ion and constitutive elements of chitosan structure by DFT calculation. 2006 , 7, 31-7	47
1637	Ion binding to cucurbit[6]uril: structure and dynamics. 2006 , 110, 14463-8	11
1636	Preparation, properties, and reactivities of unprecedented oxo-sulfido Nb(IV) aqua ions and crystal structure of (Me ₂ NH ₂) ₆ [Nb ₅ (μ ₃ -S) ₂ (μ ₃ -O) ₂ (μ ₂ -O) ₂ (NCS) ₁₄].3.5H ₂ O. 2006 , 45, 5008-17	4
1635	Spherical harmonic expansion of short-range screened Coulomb interactions. 2006 , 39, 8613-8630	12
1634	Theoretical study of the relationship between the nearest-neighbor exchange coupling interactions and the number of peripheral complexes in the cyano-bridged CrMn ₆ (CN) ₆ and CrMn ₂ (CN) ₂ clusters. 2006 , 110, 5096-101	12
1633	DFT Study on 3-Substituted Tetrahydropyran-2-yl Radicals. 2006 , 71, 1453-1469	2
1632	Synergism of porphyrin-core saddling and twisting of meso-aryl substituents. 2006 , 110, 5180-90	73
1631	Spectroscopic studies of the corrinoid/iron-sulfur protein from Moorella thermoacetica. 2006 , 128, 5010-20	43
1630	Vibrational spectroscopy of mass-selected [UO ₂ (ligand) _n] ²⁺ complexes in the gas phase: comparison with theory. 2006 , 128, 4802-13	91
1629	Crystallographic evidence of theoretically novel anion- π interactions. 2006 , 30, 1561-1566	55
1628	Correlation between Hammett substituent constants and directly calculated π -conjugation strength. 2006 , 71, 2251-6	82
1627	Synthesis, structure, and photophysical properties of luminescent platinum(II) complexes containing cyclometalated 4-styryl-functionalized 2-phenylpyridine ligands. 2006 , 45, 8584-96	100
1626	Synthesis, structural studies, theoretical calculations, and linear and nonlinear optical properties of terpyridyl lanthanide complexes: new evidence for the contribution of f electrons to the NLO activity. 2006 , 128, 12243-55	107
1625	Relativistic DFT Calculation of (119)Sn Chemical Shifts and Coupling Constants in Tin Compounds. 2006 , 2, 37-46	76
1624	Chemical bonding in phosphane and amine complexes of main group elements and transition metals. 2006 , 45, 6956-64	74
1623	Self-consistent combination of the three-dimensional RISM theory of molecular solvation with analytical gradients and the Amsterdam density functional package. 2006 , 110, 6083-90	75
1622	¹⁷ O nuclear quadrupole coupling constants of water bound to a metal ion: a gadolinium(III) case study. 2006 , 125, 054503	20

1621	Spectral and structural characterization of amidate-bridged platinum-thallium complexes with strong metal-metal bonds. 2006 , 45, 4526-36	50
1620	Electronic structures and absorption spectra of linkage isomers of trithiocyanato (4,4',4' '-tricarboxy-2,2':6,2' '-terpyridine) ruthenium(II) complexes: a DFT study. 2006 , 45, 7600-11	93
1619	Relativistic density functional theory study of dioxoactinide(VI) and -(V) complexation with alaskaphyrin and related Schiff-base macrocyclic ligands. 2006 , 110, 9486-99	68
1618	Theoretical and spectroscopic study of the effect of ring substitution on the adsorption of anisole on platinum. 2006 , 110, 9956-65	24
1617	Temperature Dependence of Three-Terminal Molecular Junctions with Sulfur End-Functionalized Tercyclohexylidenes. 2006 , 6, 1031-1035	105
1616	Titanium(IV) Alkoxy-N-heterocyclic Carbenes: Structural Preferences of Alkoxide and Bromide Adducts. 2006 , 25, 1861-1867	42
1615	Spectroscopic determination of proton position in the proton-coupled electron transfer pathways of donor-acceptor supramolecule assemblies. 2006 , 128, 10474-83	77
1614	Mixed-metal cluster chemistry. 29. Core expansion and ligand-driven metal exchange at group 6-iridium clusters. 2006 , 45, 10859-72	7
1613	Nucleophilic substitution at phosphorus (S(N)2@P): disappearance and reappearance of reaction barriers. 2006 , 128, 10738-44	126
1612	Electronic transitions in [Re6S8X6](4-) (X = Cl, Br, I): results from time-dependent density functional theory and solid-state calculations. 2006 , 45, 8273-82	12
1611	Density functional theory study of Fe(IV) d-d optical transitions in active-site models of class I ribonucleotide reductase intermediate X with vertical self-consistent reaction field methods. 2006 , 45, 8533-42	26
1610	Fries rearrangement of aryl formates: a mechanistic study by means of 1H, 2H, and 11B NMR spectroscopy and DFT calculations. 2006 , 71, 9331-40	25
1609	Electrochemical oxidation of CoCp(CO)2: radical-substrate reaction of a 17 e-/18 e- pair and production of a unique dimer radical. 2006 , 128, 16587-99	50
1608	Unsaturated Cyclopentadienyl-Molybdenum and Tungsten Carbonyl Cluster Complexes Containing Pd- and Pt(PBut3) Groups. 2006 , 25, 2673-2682	6
1607	Optimizing small molecule activation and cleavage in three-coordinate M[N(R)Ar]3 complexes. 2006 , 45, 6851-9	25
1606	The chromophore of asFP595: a theoretical study. 2006 , 110, 9348-53	20
1605	Exohedral reactivity of trimetallic nitride template (TNT) endohedral metallofullerenes. 2006 , 71, 46-54	72
1604	Divinylphenylene-Bridged Diruthenium Complexes Bearing Ru(CO)Cl(PiPr3)2 Entities \square 2006 , 25, 3701-3712	98

1603	Theoretical study on the optoelectronic properties of electron-withdrawing substituted diethynylfluorenyl gold(I) complexes. 2006 , 110, 13036-44	21
1602	Multinuclear high-resolution NMR study of compounds from the ternary system NaF-CaF ₂ -AlF ₃ : from determination to modeling of NMR parameters. 2006 , 45, 10215-23	27
1601	Arene Coordination in Bis(imino)pyridine Iron Complexes: Identification of Catalyst Deactivation Pathways in Iron-Catalyzed Hydrogenation and Hydrosilylation. 2006 , 25, 4269-4278	179
1600	Oxidative Addition versus Dehydrogenation of Methane, Silane, and Heavier AH ₄ Congeners Reacting with Palladium. 2006 , 25, 4260-4268	37
1599	Noncovalent interactions between organometallic metallocene complexes and single-walled carbon nanotubes. 2006 , 125, 154704	41
1598	Covalency in Highly Polar Bonds. Structure and Bonding of Methylalkalimetal Oligomers (CH ₃ M) _n (M = Li-Rb; n = 1, 4). 2006 , 2, 965-80	43
1597	Exploring the ability of frozen-density embedding to model induced circular dichroism. 2006 , 110, 8786-96	49
1596	Oxidative addition of hydrogen halides and dihalogens to Pd. Trends in reactivity and relativistic effects. 2006 , 110, 7943-51	9
1595	Planar tetracoordinated silicon in silicon carbonyl complexes: a DFT approach. 2006 , 110, 4582-91	15
1594	2004, Volume 108A Sulfuric Acid and Sulfuric Acid Hydrates in the Gas Phase: A DFT Investigation. 2006 , 110, 7982-7984	10
1593	Density functional theory-based prediction of some aqueous-phase chemistry of superheavy element 111. Roentgenium(I) is the "softest" metal ion. 2006 , 45, 10780-5	19
1592	The origin of chemo- and enantioselectivity in the hydrogenation of diketones on platinum. 2006 , 128, 4048-57	46
1591	On the interplay between CH...O and OH...O interactions in determining crystal packing and molecular conformation: an experimental and theoretical charge density study of the fungal secondary metabolite austdiol (C ₁₂ H ₁₂ O ₅). 2006 , 110, 6405-14	42
1590	Hangman salen platforms containing two xanthene scaffolds. 2006 , 71, 8706-14	32
1589	Oxidative Addition of the Chloromethane C-Cl Bond to Pd, an ab Initio Benchmark and DFT Validation Study. 2006 , 2, 322-35	77
1588	Analysis of Electron Paramagnetic Resonance Spectra with Very Large Quadrupole Couplings. 2006 , 110, 7984-7984	
1587	Oxidative addition of dihydrogen to (eta ⁶ -arene)Mo(PMe ₃) ₃ complexes: origin of the naphthalene and anthracene effects. 2006 , 128, 5452-61	48
1586	A nitridoniobium(V) reagent that effects acid chloride to organic nitrile conversion: synthesis via heterodinuclear (Nb/Mo) dinitrogen cleavage, mechanistic insights, and recycling. 2006 , 128, 940-50	133

1585	Reactions of gadolinium atoms and dimers with CO: formation of gadolinium carbonyls and photoconversion to CO activated molecules. 2006 , 110, 12585-91	30
1584	Electronic structure and stability of pentaorganosilicates. 2006 , 128, 13634-9	53
1583	Linear and nonlinear optical response of aromatic amino acids: a time-dependent density functional investigation. 2006 , 110, 9967-73	22
1582	The influence of amine/amide versus bisamide coordination in nickel superoxide dismutase. 2006 , 45, 10552-66	47
1581	Chiroptical and computational studies of a bridled chiorporphyrin and of its nickel(II), copper(II), and zinc(II) complexes. 2006 , 128, 6347-56	15
1580	Reactions of tBuC ⁺ P with Cyclooctatetraene-Supported Titanium Imido Complexes. 2006 , 25, 3688-3700	14
1579	Molecular structures of arachno-decaborane derivatives 6,9-X ₂ B ₈ H ₁₀ (X = CH ₂ , NH, Se) including a gas-phase electron-diffraction study of 6,9-C ₂ B ₈ H ₁₄ . 2006 , 45, 6014-9	14
1578	Synthesis, structural characterization, and theoretical studies of gold(I) and gold(I)-gold(III) thiolate complexes: quenching of gold(I) thiolate luminescence. 2006 , 45, 1059-68	58
1577	Spectroscopic and computational studies of Co ¹⁺ cobalamin: spectral and electronic properties of the "superreduced" B ₁₂ cofactor. 2006 , 128, 9144-56	75
1576	DFT studies on the magnetic exchange across the cyanide bridge. 2006 , 110, 13332-40	50
1575	Thalophilic interactions in aryloxide compounds: the [Tl ₂ (μ ₂ -OAr) ₄] structural motif in (TlOAr) ₄ and Tl ₂ Cu(OAr) ₄ compounds. 2006 , 45, 3864-77	45
1574	Charge transfer in polypeptides: effect of secondary structures on charge-transfer integral and site energies. 2006 , 110, 11551-6	15
1573	Molecular structure and bonding of copper cluster monocarbonyls Cu _n CO (n = 1-9). 2006 , 110, 6526-36	88
1572	On the paucity of molecular actinide complexes with unsupported metal-metal bonds: a comparative investigation of the electronic structure and metal-metal bonding in U ₂ X ₆ (X = Cl, F, OH, NH ₂ , CH ₃) complexes and d-block analogues. 2006 , 45, 6828-39	39
1571	Photoelectron spectroscopy and DFT calculations of easily ionized quadruply bonded Mo ₂ (4+) compounds and their bicyclic guanidinate precursors. 2006 , 110, 19793-8	22
1570	Effect of hydration on coordination properties of uranyl(VI) complexes. A first-principles molecular dynamics study. 2006 , 128, 6357-68	103
1569	Iodine Substituted Tetrathiafulvalene Radical Cation Salts with [M(isoq) ₂ (NCS) ₄] ⁻ Anions where M = Cr ^{III} , Ga ^{III} : Role of I _π S and S _π S Contacts on Structural and Magnetic Properties. 2006 , 18, 790-797	41
1568	Theoretical study on the electronic spectrum and the origin of remarkably large third-order nonlinear optical properties of organoimide derivatives of hexamolybdates. 2006 , 110, 23092-8	81

1567	Neutral high-potential nickel triad bisdithiolenes: structure and solid-state NMR properties of Pt[S ₂ C ₂ (CF ₃) ₂] ₂ . 2006 , 45, 8850-2	19
1566	Proton Affinities of Anionic Bases: Trends Across the Periodic Table, Structural Effects, and DFT Validation. 2006 , 2, 281-7	46
1565	Fe L-edge XAS studies of K ₄ [Fe(CN) ₆] and K ₃ [Fe(CN) ₆]: a direct probe of back-bonding. 2006 , 128, 10442-51	168
1564	Mono-, di-, tri-, and tetra-substituted fluorotyrosines: new probes for enzymes that use tyrosyl radicals in catalysis. 2006 , 128, 1569-79	115
1563	Electronic structure and optical properties of charged oligofluorenes studied by VIS/NIR spectroscopy and time-dependent density functional theory. 2006 , 110, 5984-93	39
1562	Metal and ligand K-edge XAS of titanium-TEMPO complexes: determination of oxidation states and insights into Ti-O bond homolysis. 2006 , 45, 4468-77	30
1561	Origin of the photoinduced optical second harmonic generation arising in N-phenyl microcrystalline films. 2006 , 110, 6492-8	16
1560	Computational Studies of Structures and Properties of Metallaboranes. 2. Transition-Metal Dicarbolide Complexes. 2006 , 25, 2173-2181	45
1559	Redox non-innocence of thioether macrocycles: elucidation of the electronic structures of mononuclear complexes of gold(II) and silver(II). 2006 , 128, 13827-39	45
1558	Piano-Stool Iron(II) Complexes as Probes for the Bonding of N-Heterocyclic Carbenes: Indications for σ -Acceptor Ability. 2006 , 25, 5648-5656	174
1557	A quantum chemical study of the decomposition of Keggin-structured heteropolyacids. 2006 , 110, 4170-8	34
1556	Homolytic dissociation of the vulcanization accelerator tetramethylthiuram disulfide (TMTD) and structures and stabilities of the related radicals Me ₂ NCSn* (n = 1-4). 2006 , 71, 9302-11	14
1555	High hydride count rhodium octahedra, [Rh ₆ (PR ₃) ₆ H ₁₂][BARF ₄] ₂ : synthesis, structures, and reversible hydrogen uptake under mild conditions. 2006 , 128, 6247-63	63
1554	Density Functional Theoretical Studies of the Re-Xe Bonds in Re(Cp)(CO)(PF ₃)Xe and Re(Cp)(CO) ₂ Xe. 2006 , 25, 5242-5248	11
1553	Tertiary Arsine Adducts of Iodoarsines: A Structural and Theoretical Investigation. 2006 , 25, 164-171	6
1552	Computational studies of the coordination stereochemistry, bonding, and metal selectivity of mercury. 2006 , 110, 452-62	41
1551	Competition between metal-amido and metal-imido chemistries in the alkaline earth series: an experimental and theoretical study of BaNH. 2006 , 128, 1109-18	11
1550	Electronic structure and molecular properties of the heptacyanorhenate [Re(CN) ₇] ³⁻ and [Re(CN) ₇] ⁴⁻ complexes. 2006 , 110, 1072-7	7

1549	Sensitivity enhancement and heteronuclear distance measurements in biological ^{17}O solid-state NMR. 2006 , 110, 16089-101	58
1548	1,3 Geminal interactions as the possible trend setting factors for C-H and C-C bond energies in alkanes. Support from a density functional theory based bond energy decomposition study. 2006 , 71, 9208-11	38
1547	Density functional investigation of high-spin XY (X = Cr, Mo, W and Y = C, N, O) molecules. 2006 , 110, 4846-53	19
1546	Two-Dimensional Charge Delocalization in X-Shaped Phenylenevinylene Oligomers. 2006 , 18, 2118-2129	23
1545	TDDFT studies of absorption and SERS spectra of pyridine interacting with Au_{20} . 2006 , 110, 13317-24	150
1544	C7 and C9 carbon-rich bridges in diruthenium systems: synthesis, spectroscopic, and theoretical investigations of different oxidation States. 2006 , 128, 5859-76	93
1543	Combinatorial computational chemistry: first principles quantum methods as a tool for industrial innovations. 2006 , 159, 9-16	
1542	Guest Atom Displacements in Silicon Cluster $\text{Na}_2@_{\text{Si}}50\text{H}_{44}$. 2006 , 47, 63-66	2
1541	The Binding Properties of Terminal and Bridging Fluoride and of Aqua Ligands in Semiempirical Vibronic Coupling and DFT Study of Mixed-Ligand Manganese(III) Complexes. 2006 , 632, 1375-1398	23
1540	On the calculation of the electrostatic potential, electric field and electric field gradient from the aspherical pseudoatom model. 2006 , 62, 400-8	46
1539	6-Nitro-1-deazapurine. 2006 , 62, o223-o225	4
1538	Time-dependent density functional theory simulation of hyper-Raman spectra. 2006 , 106, 599-608	18
1537	Theoretical study of the magnetic exchange coupling behavior substituting Cr(III) with Mo(III) in cyano-bridged transition metal complexes. 2006 , 106, 1551-1560	12
1536	Density functional study of protonation sites of Keggin isopolyanions. 2006 , 106, 1860-1864	21
1535	Orbital interactions and charge redistribution in weak hydrogen bonds: Watson-Crick GC mimic involving C-H proton donor and F proton acceptor groups. 2006 , 106, 2428-2443	8
1534	Optimization of strong and weak coordinates. 2006 , 106, 2536-2544	92
1533	DFT study of bare and dye-sensitized TiO_2 clusters and nanocrystals. 2006 , 106, 3214-3234	212
1532	Catalytic dehydrogenation of ethane over mononuclear Cr(III) silica surface sites. Part 2: C-H activation by oxidative addition. 2006 , 19, 25-33	19

1531	EPR and DFT study of NO interaction with Ni/SiO ₂ catalyst: Insight into mechanistic steps of disproportionation process promoted by tripodal surface nickel complex. 2006 , 114, 154-161	16
1530	Low-temperature lifetimes of metastable high-spin states in spin-crossover and in low-spin iron(II) compounds: The rule and exceptions to the rule. 2006 , 250, 1642-1652	157
1529	The preparation of substitution-inert ⁹⁹ Tc metal-fragments: Promising candidates for the design of new ^{99m} Tc radiopharmaceuticals. 2006 , 250, 2034-2045	45
1528	Ab initio molecular dynamics simulations of organometallic reactivity. 2006 , 250, 1497-1513	24
1527	Free tetra- and hexa-coordinated platinum-cyanide dianions, and : A combined photodetachment photoelectron spectroscopic and theoretical study. 2006 , 329, 230-238	21
1526	Reactivity of silicon carbonyl with ethylene. 2006 , 418, 383-385	1
1525	Scalar relativistic correction to nucleus-independent chemical shifts of coinage-metal compounds: How does the pseudopotential approximation perform?. 2006 , 418, 437-441	10
1524	The Rh- π bond: RhX (X=C, N, O, F, P and Cl) molecules. 2006 , 421, 281-286	18
1523	Electronic structure and molecular properties of the octacyanorhenate [Re(CN) ₈] ³⁻ and [Re(CN) ₈] ²⁻ complexes. 2006 , 422, 89-94	5
1522	A computational study on electron transfer mechanism between alkaline earth metal atoms and cyclooctatetraene to form cation- π bonded complexes. 2006 , 423, 339-343	10
1521	A density functional theory study of Ti-doped NaAlH ₄ clusters. 2006 , 426, 180-186	25
1520	Ab initio and DFT study of the exchange coupling in the highly reduced polyoxoanion [PMo ₁₂ O ₄₀ (VO) ₂] ⁵⁻ . 2006 , 428, 88-92	10
1519	Performance of various density functionals for the hydrogen bonds in DNA base pairs. 2006 , 426, 415-421	141
1518	A DFT based ligand field study of the EPR spectra of Co(II) and Cu(II) porphyrins. 2006 , 427, 449-454	16
1517	Oxygen influence on the dissociative chemisorption of methane on nickel: A quantum chemical cluster model study. 2006 , 432, 94-99	3
1516	Theoretical study of structure, pK _a , lipophilicity, solubility, absorption, and polar surface area of some centrally acting antihypertensives. 2006 , 14, 1715-28	70
1515	Combined EPR and DFT study of the copper(II) complexes with N-phosphoryl thioureas. 2006 , 320, 59-74	17
1514	Density functional theory calculation of 2p core-electron binding energies of Si, P, S, Cl, and Ar in gas-phase molecules. 2006 , 151, 9-13	28

1513	Synthesis, crystal structure and quantum study of organoammonium polyoxomolybdate with one-dimension chain containing face-shared molybdenum oxygen octahedra. 2006 , 359, 2550-2554	12
1512	Kinetic studies on the first dihydrogen aquacomplex, [Ru(H ₂)(H ₂ O) ₅] ²⁺ : Formation under H ₂ pressure and catalytic H/D isotope exchange in water. 2006 , 359, 1795-1806	27
1511	Asymmetric η -1,1-azido bridged copper(II) complex: Synthesis, X-ray structure, magnetic study and DFT calculations. 2006 , 359, 1193-1199	63
1510	A DFT and MP2 study of luminescence of gold(I) complexes. 2006 , 359, 3617-3624	17
1509	Theoretical studies of loading and structural diversity in Cp ₃ MX (M=Zr, Hf; X=H, CH ₃ , OR, NR ₂) compounds. 2006 , 25, 575-584	10
1508	DFT studies of copper complexes with biphenyldiimino dithioether II. Mechanical strain. 2006 , 25, 2559-2564	2
1507	Investigation of charge transfer and structural distortions during photo-induced excitation of cuprous bis-2,9-dimethyl-1,10-phenanthroline complex by density functional theory. 2006 , 691, 551-556	13
1506	Acidity and basicity of N-heterocyclic carbene ligands. A computational assessment. 2006 , 691, 4350-4358	171
1505	A theoretical study of the original Shilov reaction involving methane activation by platinum tetrachloride in an acidic aqueous solution. 2006 , 691, 4486-4497	40
1504	Formation of pyridine from acetylenes and nitriles catalyzed by RuCpCl, CoCp, and RhCp derivatives A computational mechanistic study. 2006 , 691, 4434-4445	60
1503	Oxidative addition to main group versus transition metals: Insights from the Activation Strain model. 2006 , 691, 4341-4349	39
1502	Synthesis and ligand properties towards gold and silver of the ferrocenylamidobenzimidazole ligand. 2006 , 691, 4181-4188	8
1501	A density functional investigation of charge transfer and structural distortions of cuprous(I) bis-phenanthroline under photo-induced excitation. 2006 , 179, 149-155	13
1500	DFT calculations of magnetic parameters for molybdenum complexes and hydroxymethyl intermediates trapped on silica surface. 2006 , 63, 788-94	5
1499	A DFT overview of high-valent iron, cobalt and nickel tetraamidomacrocyclic ligand (TAML) complexes: the end of innocence?. 2006 , 100, 620-6	12
1498	When being straight bends rules: a rationale for the linear FeNO unit in the low-spin square-pyramidal {FeNO} ₇ tetracyanonitrosylferrate(2-) anion. 2006 , 100, 2069-73	10
1497	The role of density functional theory in chemistry: Some historical landmarks and applications to zeolites. 2006 , 762, 1-7	20
1496	Geometry, solvent, and polar effects on the relationship between calculated core-electron binding energy shifts (Δ E _{BE}) and Hammett substituent (ρ) constants. 2006 , 758, 61-69	28

1495	HFI and DFT study of the bonding in complexes of halogen and interhalogen diatomics with Lewis base. 2006 , 760, 175-182	27
1494	Complexes in insulators: Role of the electric field from the host lattice. 2006 , 759, 195-199	13
1493	Trans effect and inverse trans effect in MLX ₅ complexes (M=Mo, U; L=O, S; X=Cl, Br): A rationalization within density functional theory study. 2006 , 762, 109-121	15
1492	SO ₃ complexes with nitrogen containing ligands as the object of nuclear quadrupole interactions and density functional theory calculations. 2006 , 761, 195-201	3
1491	Actinide(III) and lanthanide(III) complexes with nitrogen ligands: Counterions and ligand substituent effects on the metal-ligand bond. 2006 , 771, 105-110	42
1490	Density functional study of closed-shell attractions of (X=N, O, P, S, As, Se) systems. 2006 , 773, 15-20	5
1489	What is the best theoretical method to study molybdenum dithiolene complexes?. 2006 , 773, 59-70	20
1488	A relativistic DFT study of cyclopentadienyl actinide complexes with no transition-metal analogues. 2006 , 777, 61-73	14
1487	A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. 2006 , 125, 194101	3551
1486	Direct nitric oxide detection in aqueous solution by copper(II) fluorescein complexes. 2006 , 128, 14364-73	237
1485	The Effect of Steric Hindrance on the Association of Telluradiazoles through Te-N Secondary Bonding Interactions. 2006 , 6, 181-186	95
1484	Potential Application of K ⁺ Ligands in Actinide Separations. 2006 , 201-218	1
1483	Comparative theoretical study of N-heterocyclic carbenes and other ligands bound to Au(I). 2006 , 1, 623-8	33
1482	Titanium and zirconium complexes with non-salicylaldimine-type imine-phenoxy chelate ligands: syntheses, structures, and ethylene-polymerization behavior. 2006 , 1, 878-87	28
1481	Modeling proline ligation in the heme-dependent CO sensor, CooA, using small-molecule analogs. 2006 , 11, 642-50	7
1480	Structure, redox, pK _a , spin. A golden tetrad for understanding metalloenzyme energetics and reaction pathways. 2006 , 11, 674-94	80
1479	Structure and bonding of methyl alkali metal molecules. 2006 , 12, 563-8	8
1478	Density functional study of closed-shell attraction on X(ML) ₃ + (X = O, S, Se; M = Au, Ag, Cu) systems. 2007 , 13, 255-65	7

1477	The Silicon Carbonyls Revisited: On the Existence of a Planar Si(CO) ₄ . 2006 , 115, 448-459	10
1476	EPR properties of Au atoms adsorbed on various sites of the MgO(1 0 0) surface from relativistic DFT calculations. 2006 , 600, 2434-2442	21
1475	Adsorption of cyclohexadiene, cyclohexene and cyclohexane on Pt(111). 2006 , 600, 3121-3134	33
1474	Trigonal bipyramidal iron(III) and manganese(III) oxo, sulfido, and selenido complexes. An electronic-structural overview. 2006 , 100, 707-15	10
1473	Seven clues to the origin and structure of class-I ribonucleotide reductase intermediate X. 2006 , 100, 771-9	28
1472	A challenge to chemical intuition: donor-acceptor interactions in H ₃ B-L and H ₂ B ⁺ -L (L=CO; EC ₅ H ₅ , E=N-Bi). 2006 , 12, 4620-9	22
1471	The versatility of pentalene coordination to transition metals: a density functional theory investigation. 2006 , 12, 2048-65	53
1470	An investigation of lanthanum coordination compounds by using solid-state ¹³⁹ La NMR spectroscopy and relativistic density functional theory. 2005 , 12, 159-68	34
1469	Atropisomeric discrimination in new Ru(II) complexes containing the C(2)-symmetric didentate chiral phenyl-1,2-bisoxazolinic ligand. 2006 , 12, 2798-807	30
1468	Computational study of solvent effects and the vibrational spectra of Anderson polyoxometalates. 2006 , 12, 2094-102	13
1467	Hydrogen-hydrogen bonding in planar biphenyl, predicted by atoms-in-molecules theory, does not exist. 2006 , 12, 2889-95	280
1466	Bond orders between molecular fragments. 2006 , 12, 2252-62	10
1465	The challenge of the so-called electron configurations of the transition metals. 2006 , 12, 4101-14	27
1464	Supramolecular switches based on the guanine-cytosine (GC) Watson-Crick pair: effect of neutral and ionic substituents. 2006 , 12, 3032-42	45
1463	Direct estimate of the strength of conjugation and hyperconjugation by the energy decomposition analysis method. 2006 , 12, 3617-29	109
1462	Toward the complete prediction of the ¹ H and ¹³ C NMR spectra of complex organic molecules by DFT methods: application to natural substances. 2006 , 12, 5514-25	167
1461	A model of the chemical bond must be rooted in quantum mechanics, provide insight, and possess predictive power. 2006 , 12, 2902-5	191
1460	Structure and bonding in first-row transition-metal dicarbides: are they related to the stability of met-cars?. 2006 , 12, 6963-75	44

1459	Computational modeling of polyoxotungstates by relativistic DFT calculations of (^{183}W) NMR chemical shifts. 2006 , 12, 8460-71		47
1458	Orbital overlap and chemical bonding. 2006 , 12, 9196-216		254
1457	Terminally coordinated AsS and PS ligands. 2006 , 12, 8603-8		18
1456	Alpha-stabilization of carbanions: fluorine is more effective than the heavier halogens. 2006 , 45, 823-6		39
1455	"Naked" Ga^+ and In^+ as pure acceptor ligands: structure and bonding of $[\text{GaPt}(\text{GaCp}^*)_4][\text{BArF}]$. 2006 , 45, 5207-10		56
1454	Diamagnetic-paramagnetic conversion of tris(2-pyridylthio)methylcopper(III) through a structural change from trigonal bipyramidal to octahedral. 2006 , 45, 7611-4		52
1453	Dancing on a fullerene surface: isomerization of $\text{Y}(3)\text{N}@\text{(N-ethylpyrrolidino-C}(80))$ from the 6,6 to the 5,6 regioisomer. 2006 , 45, 8176-80		76
1452	Relationship Between the Nearest-Neighbor Exchange Coupling Constants and the Number of Exchange Interactions in the Cyano-Bridged $\text{MnMo}_6(\text{CN})_{18}$ Cluster: Density Functional Theory Calculations. 2006 , 2006, 2292-2298		5
1451	New Polynuclear MoBe Complexes with Ferrocenylamidobenzimidazole Ligands. 2006 , 2006, 4096-4103		8
1450	How Do the Different Defect Structures and Element Substitutions Affect the Nonlinear Optical Properties of Lacunary Keggin Polyoxometalates? A DFT Study. 2006 , 2006, 4179-4183		30
1449	A DFT Study on the Electronic and Redox Properties of $[\text{PW}_{11}\text{O}_{39}(\text{ReN})]_n$ ($n = 3, 4, 5$) and $[\text{PW}_{11}\text{O}_{39}(\text{OsN})]_2$. 2006 , 2006, 5126-5129		21
1448	Prediction of spectroscopic constants for diatomic molecules in the ground and excited states using time-dependent density functional theory. <i>Journal of Computational Chemistry</i> , 2006 , 27, 163-73	3.5	13
1447	Starting SCF calculations by superposition of atomic densities. <i>Journal of Computational Chemistry</i> , 2006 , 27, 926-32	3.5	42
1446	DFT calculations of ^{57}Fe Mössbauer isomer shifts and quadrupole splittings for iron complexes in polar dielectric media: applications to methane monooxygenase and ribonucleotide reductase. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1292-306	3.5	52
1445	DFT models for copper(II) bispidine complexes: structures, stabilities, isomerism, spin distribution, and spectroscopy. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1263-77	3.5	67
1444	Proton affinities of main-group-element hydrides and noble gases: trends across the periodic table, structural effects, and DFT validation. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1486-93	3.5	38
1443	A QM/MM study on the aqueous solvation of the tetrahydroxouranyl $[\text{UO}_2(\text{OH})_4]^{2-}$ complex ion. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1156-62	3.5	12
1442	On the accuracy of density functional theory for iron-sulfur clusters. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1385-97	3.5	88

1441	Performance of DFT in modeling electronic and structural properties of cobalamins. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1429-37	3.5	98
1440	Assessment of the performance of density-functional methods for calculations on iron porphyrins and related compounds. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1577-92	3.5	72
1439	A theoretical study of the structure and bonding of UOX4 (X = F, Cl, Br, I) molecules: the importance of inverse trans influence. 2006 , 7, 455-62		27
1438	An alternative approach to the g-matrix: theory and applications. 2006 , 7, 1575-89		129
1437	Nanoswitches based on DNA base pairs: why adenine-thymine is less suitable than guanine-cytosine. 2006 , 7, 1971-9		18
1436	Stabilisierung von Carbanionen: Fluor betrifft die schwereren Halogene. 2006 , 118, 838-841		15
1435	Nacktes Ga ⁺ und In ⁺ als reine Acceptorliganden: Struktur und Bindungsverhältnisse von [GaPt(GaCp*) ₄][BARF]. 2006 , 118, 5331-5334		32
1434	Diamagnetic/Paramagnetic Conversion of Tris(2-pyridylthio)methylcopper(III) through a Structural Change from Trigonal Bipyramidal to Octahedral. 2006 , 118, 7773-7776		10
1433	Dancing on a Fullerene Surface: Isomerization of Y3N@(N-Ethylpyrrolidino-C80) from the 6,6 to the 5,6 Regioisomer. 2006 , 118, 8356-8360		18
1432	Time-dependent density functional study of the electronic potential energy curves and excitation spectrum of the oxygen molecule. 2006 , 125, 44314		21
1431	On the degeneracy of atomic states within exact-exchange (spin-) density functional theory. 2006 , 125, 084105		11
1430	Calculation of nuclear magnetic resonance shieldings using frozen-density embedding. 2006 , 125, 194104		60
1429	Third-order interactions in symmetry-adapted perturbation theory. 2006 , 125, 154107		86
1428	Towards the engineering of enantioselective properties of supported platinum catalysts. 2006 , 32, 1241-1247	6	
1427	Watson/Crick hydrogen bonds: nature and role in DNA replication. 2006 , 79-97		2
1426	Group Transfer Polymerizations of Acrylates Catalyzed by Mononuclear Early d-Block and f-Block Metallocenes: A DFT Study. 2006 , 25, 3619-3630		27
1425	Sensitivity of photoelectron circular dichroism to structure and electron dynamics in the photoionization of carvone and related chiral monocyclic terpenone enantiomers. 2006 , 125, 234306		36
1424	Insertion reaction of carbon dioxide into Sn-OR bond. Synthesis, structure and DFT calculations of di- and tetranuclear isopropylcarbonato tin(IV) complexes. 2006 , 5167-75		49

1423	Calculation of excitation energies of open-shell molecules with spatially degenerate ground states. II. Transformed reference via intermediate configuration Kohn-Sham time dependent density functional theory oscillator strengths and magnetic circular dichroism C terms. 2006 , 124, 144105	26
1422	Origin of fine structure in si photoelectron spectra at silicon surfaces and interfaces. 2006 , 96, 157601	50
1421	Performance of the Vignale-Kohn functional in the linear response of metals. 2006 , 74,	19
1420	Assessment of a simple correction for the long-range charge-transfer problem in time-dependent density-functional theory. 2006 , 124, 214102	118
1419	High-field/ high-frequency EPR study on stable free radicals formed in sucrose by gamma-irradiation. 2006 , 40, 553-63	21
1418	Optimized effective potential method in current-spin-density-functional theory. 2006 , 74,	23
1417	Water solvent effect on the first hyperpolarizability of p-nitrophenol and p-nitrophenylphosphate: a time-dependent density functional study. 2006 , 124, 174502	9
1416	First-principles calculation of the EPR g tensor in extended periodic systems. 2006 , 73,	16
1415	Off-center instability in SrCl ₂ :Fe ⁺ : Role of unoccupied 4p orbitals. 2006 , 73,	16
1414	A DFT STUDY ON THE ELECTRONIC CHARACTER OF P700+. 2006 , 05, 733-741	2
1413	Charge transport along phenylenevinylene molecular wires. 2006 , 32, 695-705	13
1412	Formation of unprecedented actinide triple bond carbon in uranium methyldyne molecules. 2007 , 104, 18919-24	74
1411	Orbital currents in the Colle-Salvetti correlation energy functional and the degeneracy problem. 2007 , 127, 124103	9
1410	Interface between platinum(111) and liquid isopropanol (2-propanol): a model for molecular dynamics studies. 2007 , 126, 074702	23
1409	Time-dependent picture of the charge-transfer contributions to surface enhanced Raman spectroscopy. 2007 , 126, 244709	101
1408	Theoretical investigation of electronic structures and excitation energies of doubly N-confused porphyrin and its group 11 transition metal (III) complexes. 2007 , 126, 245106	10
1407	Electronic structures of two kinds of oligoborane radical anions: mixed-valence description of a reduced p-phenylenediborane and spin density distributions in distorted octahedral clusters [B ₆ Hal ₆] ⁻ Hal ₃ ≡Cl, Br, I. 2007 , 5, 267-276	10
1406	Electronic spectrum of UO ₂ (2+) and [UO ₂ Cl ₄] ²⁻ calculated with time-dependent density functional theory. 2007 , 126, 194311	61

1405	Exact functional derivative of the nonadditive kinetic-energy bifunctional in the long-distance limit. 2007 , 126, 234116	61
1404	Development of Constraint Algorithm for the Number of Electrons in Molecular Orbitals Consisting Mainly 4f Atomic Orbitals of Rare-Earth Elements and Its Introduction to Tight-Binding Quantum Chemical Molecular Dynamics Method. 2007 , 46, 2505-2509	8
1403	3d impurities in normal and inverted perovskites: Differences are not explained by ligand field theory. 2007 , 75,	23
1402	Analysis of the Vignale-Kohn current functional in the calculation of the optical spectra of semiconductors. 2007 , 75,	25
1401	Anomalous superhyperfine tensor observed in BaFCl doped with the 5d1 ion La2+: Role of 5d π hybridization. 2007 , 75,	4
1400	Alternative perspective on density-functional perturbation theory. 2007 , 76,	5
1399	Resonance vibrational Raman optical activity: a time-dependent density functional theory approach. 2007 , 127, 134101	68
1398	On the Reaction of Hexachlorocyclotriphosphazene with Heptamethyldisilazane. Crystal Structure of P ₃ N ₃ Cl ₅ {N(CH ₃)[Si(CH ₃) ₃]}. 2007 , 72, 1407-1419	3
1397	Chapter 2 DFT modeling and spectroscopic investigations into molecular aspects of DeNOx catalysis. 2007 , 27-65	8
1396	Nucleophilic substitution at silicon (S _N 2@Si) via a central reaction barrier. 2007 , 72, 2201-7	142
1395	Computational Design of High Hydrogen Adsorption Efficiency in Molecular Bulflower π 2007 , 111, 4487-4490	40
1394	Direct estimate of conjugation and aromaticity in cyclic compounds with the EDA method. 2007 , 135, 403-21; discussion 489-506	114
1393	Electronic Properties of N-Heterocyclic Carbene (NHC) Ligands: Synthetic, Structural, and Spectroscopic Studies of (NHC)Platinum(II) Complexes. 2007 , 26, 5880-5889	168
1392	Complexation of Cu ⁺ in Hydrothermal NaCl Brines: Ab initio molecular dynamics and energetics. 2007 , 71, 714-722	63
1391	pH modulates the quinone position in the photosynthetic reaction center from Rhodospirillum rubrum sphaeroides in the neutral and charge separated states. 2007 , 371, 396-409	126
1390	Covalency in the f-element-halogen bond: Computational studies of [M(N(E)PH ₂) ₂] ₃ (M = La, U, Pu; E = O, S, Se, Te). 2007 , 444-445, 369-375	41
1389	Chemical insights in the concept of hybrid drugs: the antitumor effect of nitric oxide-donating aspirin involves a quinone methide but not nitric oxide nor aspirin. 2007 , 50, 2424-31	126
1388	Probing lead(II) bonding environments in 4-substituted pyridine adducts of (2,6-Me ₂ C ₆ H ₃ S) ₂ Pb: an X-ray structural and solid-state ²⁰⁷ Pb NMR study. 2007 , 46, 8625-37	43

1387	A combined experimental and theoretical study of uranium polyhydrides with new evidence for the large complex UH ₄ (H ₂) ₆ . 2007 , 111, 6383-7	34
1386	Interaction of metal porphyrins with fullerene C ₆₀ : a new insight. 2007 , 111, 4374-82	25
1385	Local-density-functional calculations of the vacancy-oxygen center in Ge. 2007 , 75,	9
1384	Prediction of the ¹ H and ¹³ C NMR spectra of alpha-D-glucose in water by DFT methods and MD simulations. 2007 , 72, 7373-81	93
1383	Transition metal-carbon complexes. A theoretical study. 2007 , 129, 7596-610	101
1382	Spin-orbit relativistic time-dependent density functional calculations of the metal and ligand pre-edge XAS intensities of organotitanium complexes: TiCl ₄ , Ti(eta ⁵ -C ₅ H ₅)Cl ₃ , and Ti(eta ⁵ -C ₅ H ₅) ₂ Cl ₂ . 2007 , 111, 5270-9	49
1381	QM/MM Methods for Biological Systems. 2006 , 173-290	325
1380	Syntheses, structures and redox properties of some complexes containing the Os(dppe)Cp* fragment, including [{Os(dppe)Cp*} ₂ (mu-C triple bond CC triple bond C)]. 2007 , 5387-99	49
1379	Tuning second-order NLO responses through halogen bonding. 2007 , 2590-2	103
1378	Organobismuth(III) Dihalides with T-Shaped Geometry Stabilized by Intramolecular N->Bi Interactions and Related Diorganobismuth(III) Halides. 2007 , 26, 1196-1203	62
1377	Hydrogen storage in molecular clathrates. 2007 , 107, 4133-51	332
1376	DFT modeling of sandwich complexes involving cationic palladium chains and polyenic or polycyclic aromatic hydrocarbons. 2007 , 46, 5283-91	11
1375	Energy decomposition analysis of metal-metal bonding in [M ₂ X ₈] ₂ - (X=Cl, Br) complexes of 5f (U, Np, Pu), 5d (W, Re, Os), and 4d (Mo, Tc, Ru) elements. 2007 , 46, 3557-65	34
1374	Donor-Acceptor Properties of Ligands from the Natural Orbitals for Chemical Valence. 2007 , 26, 6576-6580	270
1373	Ester versus polyketone formation in the palladium-diphosphine catalyzed carbonylation of ethene. 2007 , 129, 3989-4000	55
1372	Host-guest adaptability within oxothiomolybdenum wheels: structures, studies in solution and DFT calculations. 2007 , 3043-54	36
1371	Hydrogen generation from weak acids: electrochemical and computational studies of a diiron hydrogenase mimic. 2007 , 129, 12521-30	308
1370	The role of substituents on functionalized 1,10-phenanthroline in controlling the emission properties of cationic iridium(III) complexes of interest for electroluminescent devices. 2007 , 46, 8533-47	160

- 1369 Heterolytic activation of H-X (X = H, Si, B, and C) bonds: an experimental and theoretical investigation. **2007**, 129, 5587-96 45
- 1368 Sulfur K-edge XAS and DFT studies on NiII complexes with oxidized thiolate ligands: implications for the roles of oxidized thiolates in the active sites of Fe and Co nitrile hydratase. **2007**, 46, 4989-96 32
- 1367 Three-dimensional local structure refinement using a full-potential XANES analysis. **2007**, 75, 49
- 1366 Calculation of the Term of Magnetic Circular Dichroism. A Time-Dependent Density Functional Theory Approach. **2007**, 3, 434-47 41
- 1365 Cyclometallated iridium(III) complexes with substituted 1,10-phenanthrolines: a new class of highly active organometallic second order NLO-phores with excellent transparency with respect to second harmonic emission. **2007**, 4116-8 79
- 1364 Ligand field photofragmentation spectroscopy of [Ag(L)N]₂⁺ complexes in the gas phase: experiment and theory. **2007**, 127, 064311 13
- 1363 First-principles theoretical investigation of the electronic couplings in single crystals of phenanthroline-based organic semiconductors. **2007**, 126, 164704 45
- 1362 Applications of Quantum Chemical Methods in Zeolite Science. **2007**, 701-XXI 15
- 1361 New members of a class of iron-thiolate-nitrosyl compounds: trinuclear iron-thiolate-nitrosyl complexes containing Fe(3)S(6) core. **2007**, 129, 1151-9 21
- 1360 Fe L-edge X-ray absorption spectroscopy of low-spin heme relative to non-heme Fe complexes: delocalization of Fe d-electrons into the porphyrin ligand. **2007**, 129, 113-25 121
- 1359 Au₃₄: A Fluxional Core-Shell Cluster. **2007**, 111, 8228-8232 98
- 1358 Role of rotational entropy in benzyl isocyanide isomerization. **2007**, 105, 2919-2926 1
- 1357 Evaluating High Performance Computing Systems at the Naval Research Laboratory. **2007**, 56
- 1356 Large fullerenes stabilized by encapsulation of metallic clusters. **2007**, 4161-3 56
- 1355 Theoretical investigation of the energies and geometries of photoexcited uranyl(VI) ion: a comparison between wave-function theory and density functional theory. **2007**, 127, 214302 63
- 1354 Electron-sponge behavior and electronic structures in cobalt-centered pentagonal prismatic Co₁₁Te₇(CO)₁₀ and Co₁₁Te₅(CO)₁₅ cluster anions. **2007**, 46, 501-9 18
- 1353 Studies on photocatalytically active materials containing structure elements of a pyridinium alkaloid from Punica granatum. **2007**, 17, 2793 9
- 1352 Hyperconjugative stabilization in alkyl carbocations: direct estimate of the beta-effect of group-14 elements. **2007**, 111, 8028-35 33

1351	NaAlH ₄ Clusters with Two Titanium Atoms Added. 2007 , 111, 8206-8213	20
1350	Redox-Active Complexes Containing Group 8 Metal Centers Linked by C ₂ Bridges. 2007 , 26, 3735-3745	60
1349	Relating the Radical Stabilization Energy and Steric Bulk of a Hydrocarbyl Group to the Strength of its Bonds with Metals and Hydrogen. A Theoretical Study. 2007 , 26, 1627-1634	21
1348	Geometric structure of X(AuPH ₃) ₄ ⁺ (X = N, P, As, Sb): T _d or C _{4v} ?. 2007 , 111, 1562-6	12
1347	A solid-state ⁵⁵ Mn NMR spectroscopy and DFT investigation of manganese pentacarbonyl compounds. 2007 , 9, 1226-38	18
1346	Highly polar bonds and the meaning of covalency and ionicity--structure and bonding of alkali metal hydride oligomers. 2007 , 135, 451-68; discussion 489-506	16
1345	An ytterbium(II) complex with dimethyl ester of oxydiacetic acid. 2007 , 2779-83	2
1344	A DFT based investigation into the electronic structure and properties of hydride rich rhodium clusters. 2007 , 1781-92	15
1343	Rationalizing the different products in the reaction of N ₂ with three-coordinate MoL ₃ complexes. 2007 , 1939-47	15
1342	Decomposition of CH ₂ O by lanthanum: a theoretical study. 2007 , 111, 11894-903	3
1341	The dithiolene ligand--'innocent' or 'non-innocent'? A theoretical and experimental study of some cobalt-dithiolene complexes. 2007 , 135, 469-88; discussion 489-506	31
1340	Probing key coordination interactions: configurationally restricted metal activated CXCR ₄ antagonists. 2007 , 5008-18	32
1339	Finding a needle in a haystack: direct determination of vibrational signatures in complex systems. 2007 , 31, 818	57
1338	Structure and electronic spectra of DNA mini-hairpins with G(n):C(n) stems. 2007 , 111, 13101-6	15
1337	Cyanides and isocyanides of first-row transition metals: molecular structure, bonding, and isomerization barriers. 2007 , 111, 6334-44	48
1336	Density Functional Theory and Kinetic Studies of Methanation on Iron Surface. 2007 , 111, 11012-11025	46
1335	Gas-phase chemistry of actinides ions: new insights into the reaction of UO ⁺ and UO ₂ ⁺ with water. 2007 , 129, 4229-39	67
1334	Cyclotrimerization Reactions Catalyzed by Rhodium(I) Half-Sandwich Complexes: A Mechanistic Density Functional Study. 2007 , 26, 3816-3830	68

1333	Geometry Optimization of a Ru(IV) Allyl Dicationic Complex: A DFT Failure?. 2007 , 3, 665-70	15
1332	Toward a Separate Reproduction of the Contributions to the Hartree-Fock and DFT Intermolecular Interaction Energies by Polarizable Molecular Mechanics with the SIBFA Potential. 2007 , 3, 824-37	93
1331	Metallaborane reactivity. A stoichiometric mechanism for the insertion of two alkynes into an iridaborane framework via a disposable molybdenum chaperone. 2007 , 129, 3392-401	16
1330	On the bonding of first-row transition metal cations to guanine and adenine nucleobases. 2007 , 111, 9823-9	33
1329	Stabilization of acepentalene by coordination to transition metals: a DFT investigation. 2007 , 46, 3295-300	7
1328	Continuous-wave and pulse EPR study of the copper(II) complex of N-confused tetraphenylporphyrin: direct observation of a sigma metal-carbon bond. 2007 , 46, 1847-55	17
1327	Solid-state NMR spectroscopic study of coordination compounds of XeF(2) with metal cations and the crystal structure of [Ba(XeF(2))(5)][AsF(6)](2). 2007 , 46, 6069-77	20
1326	Singlet diradical complexes of chromium, molybdenum, and tungsten with azo anion radical ligands from M(CO) ₆ precursors. 2007 , 46, 8584-93	41
1325	The formulation and implementation of analytic energy gradients for periodic density functional calculations with STO/NAO Bloch basis set. 2007 , 105, 2583-2596	16
1324	Testing if the interstitial atom, X, of the nitrogenase molybdenum-iron cofactor is N or C: ENDOR, ESEEM, and DFT studies of the S = 3/2 resting state in multiple environments. 2007 , 46, 11437-49	77
1323	Mechanistically Designed Dual-Site Catalysts for the Alternating ROMP of Norbornene and Cyclooctene. 2007 , 26, 3585-3596	85
1322	Signature of the conformational preferences of small peptides: a theoretical investigation. 2007 , 111, 8650-8	20
1321	"Open rather than closed" malonate methano-fullerene derivatives. The formation of methanofulleroid adducts of Y ₃ N@C ₈₀ . 2007 , 129, 10423-30	112
1320	Theoretical Modeling of Ethylene Insertion by Nickel Iminophosphonamide and Amidinate Complexes. 2007 , 26, 6612-6623	24
1319	The Nature of the Ru≡NO Bond in Ruthenium Tetraammine Nitrosyl Complexes. 2007 , 26, 5815-5825	53
1318	Ligand-field dependence of the excited state dynamics of Hangman bisporphyrin dyad complexes. 2007 , 111, 8258-68	14
1317	A density functional study of the various forms of UN ₄ O ₁₂ containing uranyl nitrate. 2007 , 111, 10789-803	7
1316	Alkynyl ruthenium colorimetric sensors: optimizing the selectivity toward fluoride anion. 2007 , 46, 5922-32	39

- 1315 Metal-metal bonding in tetracyanometalates (M=PtII, PdII, NiII) of monovalent thallium. Crystallographic and spectroscopic characterization of the new compounds $Tl_2Ni(CN)_4$ and $Tl_2Pd(CN)_4$. **2007**, 46, 4642-53 22
- 1314 VTVH-MCD and DFT studies of thiolate bonding to $[FeNO]_7/[FeO_2]_8$ complexes of isopenicillin N synthase: substrate determination of oxidase versus oxygenase activity in nonheme Fe enzymes. **2007**, 129, 7427-38 98
- 1313 Photoelectron spectroscopy and electronic structure calculations of d1 vanadocene compounds with chelated dithiolate ligands: implications for pyranopterin Mo/W enzymes. **2007**, 46, 10639-46 30
- 1312 Synthesis of Low Density Poly(ethylene) Using Nickel Iminophosphonamide Complexes. **2007**, 40, 2993-3004 35
- 1311 Cerium(III) and Cerium(IV) Bis(β -pentalene) Sandwich Complexes: Synthetic, Structural, Spectroscopic, and Theoretical Studies. **2007**, 26, 3111-3119 52
- 1310 Spectroelectrochemistry and DFT analysis of a new $\{RuNO\}_n$ redox system with multifrequency EPR suggesting conformational isomerism in the $\{RuNO\}_7$ state. **2007**, 46, 9254-61 21
- 1309 Spin coupling in the supramolecular structure of a new tetra(quinoline-TEMPO)yttrium(III) complex. **2007**, 46, 660-9 4
- 1308 Which Configuration is More Stable for $La_2@C_{80}D_{3d}$ or D_{2h} ? Recomputation with ZORA Methods within ADF. **2007**, 111, 7862-7867 33
- 1307 Parametrization of an empirical correction term to density functional theory for an accurate description of pi-stacking interactions in nucleic acids. **2007**, 111, 13124-34 39
- 1306 Multimetalloenes. A Theoretical Study. **2007**, 26, 4731-4736 102
- 1305 Ab initio molecular dynamics of heme in cytochrome c. **2007**, 111, 1157-64 7
- 1304 C₃-symmetric trinuclear molybdenum cluster sulfides: configurational stability, supramolecular stereocontrol, and absolute configuration assignment. **2007**, 46, 10717-23 20
- 1303 Theoretical study on the mechanism of the [2+1] thermal cycloaddition between alkenes and stable singlet (phosphino)(silyl)carbenes. **2007**, 72, 357-66 29
- 1302 Sulfur K-edge XAS as a probe of sulfur-centered radical intermediates. **2007**, 129, 3034-5 29
- 1301 Solvent and intermolecular effects on first hyperpolarizabilities of organometallic tungsten-carbonyl complexes, a TDDFT study. **2007**, 111, 7925-32 17
- 1300 Probing variable axial ligation in nickel superoxide dismutase utilizing metalloprotein-based models: insight into the superoxide disproportionation mechanism. **2007**, 129, 14605-18 58
- 1299 Enhanced diradical nature in oxyallyl derivatives leads to near infra red absorption: a comparative study of the squaraine and croconate dyes using computational techniques. **2007**, 111, 3378-86 67
- 1298 Synthesis, structure, and unexpected magnetic properties of $La_3Re_2O_{10}$. **2007**, 46, 8739-45 9

1297	Size-Dependence of the Enhanced Raman Scattering of Pyridine Adsorbed on Agn (n = 28, 20) Clusters. 2007 , 111, 4756-4764	166
1296	Table salt and other alkali metal chloride oligomers: structure, stability, and bonding. 2007 , 46, 5411-8	17
1295	Bonding in Low-Coordinate Environments: Electronic Structure of Pseudotetrahedral Iron-Imido Complexes. 2007 , 3, 448-57	35
1294	Reactions of nitrogen monoxide on cobalt cluster ions: reaction enhancement by introduction of hydrogen. 2007 , 111, 422-8	22
1293	Cooperative CH \cdots N Interactions in the Crystal Structure of 2,5-Di(3-biphenyl)-1,1-dimethyl-3,4-diphenyl-silole and Its Effect on Its Electronic Properties. 2007 , 111, 9543-9547	21
1292	EDA study of pi-conjugation in tunable Bis(gem-diethynylethene) fluorophores. 2007 , 72, 7367-72	24
1291	Electronic structure and FeNO conformation of nonheme iron-thiolate-NO complexes: an experimental and DFT study. 2007 , 129, 10446-56	66
1290	Opto-Electronic Properties of Fluorene-Based Derivatives as Precursors for Light-Emitting Diodes. 2007 , 111, 5812-5820	20
1289	Coordination and Reactivity Diversity of N-Piperidineethyl-Functionalized Indenyl Ligands: Synthesis, Structure, Theoretical Calculation, and Catalytic Activity of Organolanthanide Complexes with the Ligands. 2007 , 26, 1512-1522	36
1288	Ethylenebis(triphenylphosphine)platinum as a probe for niobium-mediated diphosphorus chemistry. 2007 , 46, 7387-93	35
1287	A new look at the ylidic bond in phosphorus ylides and related compounds: energy decomposition analysis combined with a domain-averaged fermi hole analysis. 2007 , 111, 2859-69	25
1286	Iron-molybdenum charge-transfer hybrids containing organometallic and inorganic fragments bridged by aryldiazenido ligands in a mu-eta(6):eta(1) coordination mode: syntheses, characterization, X-ray structures, electrochemistry, and theoretical investigation. 2007 , 46, 1123-34	6
1285	Evaluation of the SCF Combination of KS-DFT and 3D-RISM-KH; Solvation Effect on Conformational Equilibria, Tautomerization Energies, and Activation Barriers. 2007 , 3, 458-76	55
1284	Density Functional Theory Investigation into the Stereocontrol of the Syndiospecific Polymerization of Propylene Catalyzed by Cs-Symmetric Zirconocenes. 2007 , 26, 2024-2036	28
1283	Optimized geometry of the cluster Gd ₂ O ₃ and proposed antiferromagnetic alignment of f-electron magnetic moment. 2007 , 111, 10162-5	15
1282	Cyclopropanation of Cyclohexenone by Diazomethane Catalyzed by Palladium Diacetate: Evidence for the Formation of Palladium(0) Nanoparticles. 2007 , 26, 3306-3314	34
1281	Infrared and DFT investigations of the XC[triple bond]ReX ₃ and HC[triple bond]ReX ₃ complexes: Jahn-Teller distortion and the methylidyne C-X(H) stretching absorptions. 2007 , 46, 8728-38	20
1280	Relativistic two-component formulation of time-dependent current-density functional theory: application to the linear response of solids. 2007 , 127, 174111	20

1279	Reaction Mechanisms for C-D Bond Coupling from Pt ₄ CH ₂ ⁺ and O ₂ : A Relativistic Density Functional Study. 2007 , 26, 6076-6081	5
1278	Influence of Different Ligands X (X = F, Cl, Br, I, NO ₂ , CN) on the Rate and Mechanism for Methane Activation by PtCl ₂ X ₂ in Aqueous Solution. A Density Functional Theory Study. 2007 , 26, 2277-2284	15
1277	Electronic structure of some substituted iron(II) porphyrins. Are they intermediate or high spin?. 2007 , 111, 5927-35	40
1276	Evidence for tetraphenylporphyrin monoacids. 2007 , 46, 5979-88	50
1275	Hyperelectronic Metal-Carborane Analogues of Cymantrene (MnCp(CO) ₃) Anions: Electronic and Structural Noninnocence of the Tricarbadiaboranyl Ligand. 2007 , 26, 4471-4482	20
1274	Termination and Transfer Reactions in the Group Transfer Polymerizations of Acrylates Catalyzed by Mononuclear Early d-Block and f-Block Metallocenes: A DFT Study. 2007 , 26, 2157-2166	12
1273	Bonding analyses, formation energies, and vibrational properties of M-R ₂ dtc complexes (M=Ag(I), Ni(II), Cu(II), or Zn(II)). 2007 , 111, 13075-87	25
1272	Molecular Orbital Model for Pyridine/Pyridyl Adsorption on Metal Surfaces. 2007 , 111, 5493-5496	11
1271	Conformational behavior of basic monomeric building units of glycosaminoglycans: isolated systems and solvent effect. 2007 , 111, 2313-21	12
1270	Oxidative properties of FeO ₂ ⁺ : electronic structure and solvation effects. 2007 , 9, 156-66	57
1269	Linked and Fused Tungstaborane Clusters: Synthesis, Characterization, and Electronic Structures of bis-(η -C ₅ Me ₅ W) ₂ B ₅ H ₈) ₂ and (η -C ₅ Me ₅ W) ₂ {Fe(CO) ₃ } _n B ₆ -nH ₁₀ -n, n = 0, 1. 2007 , 26, 5377-5385	54
1268	Proton assisted oxygen-oxygen bond splitting in cytochrome p450. 2007 , 129, 6204-9	41
1267	Bimetallic Complexes of Metallacyclopentynes: cis versus trans and Planarity versus Nonplanarity. 2007 , 26, 2149-2156	11
1266	Charge Transfer through Isomeric Unsaturated Hydrocarbons. Redox Switchable Optical Properties and Electronic Structure of Substituted Indenes with a Pendant Ferrocenyl. 2007 , 26, 5867-5879	30
1265	Metal-mediated J coupling in DNA base pairs: relativistic DFT predictions. 2007 , 129, 11360-1	46
1264	Electronic Structure of Trigonal-Planar Transition-Metal-Imido Complexes: Spin-State Energetics, Spin-Density Profiles, and the Remarkable Performance of the OLYP Functional. 2007 , 3, 689-702	101
1263	Introduction. 2007 , 15, 307	2
1262	Hafnium Bis(phenoxyimino) Dibenzyl Complexes and Their Activation toward Olefin Polymerization. 2007 , 26, 1444-1460	30

1261	Solid-state (⁶³ Cu and ⁶⁵ Cu) NMR spectroscopy of inorganic and organometallic copper(I) complexes. 2007 , 129, 13049-65	57
1260	Spectroscopic and quantum chemical studies on low-spin FeIV=O complexes: Fe-O bonding and its contributions to reactivity. 2007 , 129, 15983-96	190
1259	Silicate chain formation in the nanostructure of cement-based materials. 2007 , 127, 164710	52
1258	Effects of benzoannulation and alpha-octabutoxy substitution on the photophysical behavior of nickel phthalocyanines: a combined experimental and DFT/TDDFT study. 2007 , 46, 2080-93	40
1257	Catalytic Carbon-Halogen Bond Activation: Trends in Reactivity, Selectivity, and Solvation. 2007 , 3, 514-29	99
1256	Coordination mode of nitrate in uranyl(VI) complexes: a first-principles molecular dynamics study. 2007 , 46, 5196-206	32
1255	Analyzing and Interpreting NMR Spin-Spin Coupling Constants Using Molecular Orbital Calculations. 2007 , 84, 156	61
1254	Tetranuclear complexes of [Fe(CO) ₂ (C ₅ H ₅) ₂] ⁺ with TCNX ligands (TCNX=TCNE, TCNQ, TCNB): intramolecular electron transfer alternatives in compounds (μ ₄ -TCNX)[ML _n] ₄ . 2007 , 46, 7312-20	15
1253	Relativistic Effects on the Topology of the Electron Density. 2007 , 3, 2182-97	57
1252	Experimental and theoretical examination of C-CN and C-H bond activations of acetonitrile using zerovalent nickel. 2007 , 129, 7562-9	124
1251	Couplings between electronic transitions in a subsystem formulation of time-dependent density functional theory. 2007 , 126, 134116	177
1250	Substituent effects in formally quintuple-bonded ArCrCrAr compounds (Ar = terphenyl) and related species. 2007 , 46, 11277-90	135
1249	Structurally homologous beta- and meso-alkynyl amidinium porphyrins. 2007 , 46, 8668-75	23
1248	Controlling phosphorescence color and quantum yields in cationic iridium complexes: a combined experimental and theoretical study. 2007 , 46, 5989-6001	226
1247	Theoretical study of metal-ligand interaction in Sm(III), Eu(III), and Tb(III) complexes of coumarin-3-carboxylic acid in the gas phase and solution. 2007 , 46, 10926-36	26
1246	Valence-to-Core X-Ray Emission Spectroscopy as a Tool for Investigation of Organometallic Systems. 2007 ,	
1245	Downfolding and N-ization of Basis Sets of Slater Type Orbitals. 2007 ,	1
1244	Tuning the electronic communication in heterobimetallic mixed-valence ions of (1-ferrocenyl)- and (2-ferrocenyl)indenyl rhodium isomers. 2007 , 13, 1955-68	38

1243	A comparative relativistic DFT and ab initio study on the structure and thermodynamics of the oxofluorides of uranium(IV), (V) and (VI). 2007 , 13, 4932-47	127
1242	Progress in the understanding of drug-receptor interactions, part 2: experimental and theoretical electrostatic moments and interaction energies of an angiotensin II receptor antagonist (C30H30N6(O)3S). 2007 , 13, 6942-56	18
1241	Breaking chemistry's strongest bond: can three-coordinate [M{N(R)Ar}3] complexes cleave carbon monoxide?. 2007 , 13, 4264-72	23
1240	Aromaticity in metallabenzenes. 2007 , 13, 5873-84	132
1239	Cyanation: providing a three-in-one advantage for the design of n-type organic field-effect transistors. 2007 , 13, 4750-8	176
1238	Bridge over troubled water: resolving the competing photosystem II crystal structures. 2007 , 13, 5082-9	44
1237	Diboryl and diboranyl porphyrin complexes: synthesis, structural motifs, and redox chemistry: diborenyl porphyrin or diboranyl isophlorin?. 2007 , 13, 5982-93	88
1236	Aromaticity: molecular-orbital picture of an intuitive concept. 2007 , 13, 6321-8	70
1235	Towards new organometallic wires: tetraruthenium complexes bridged by phenylenevinylene and vinylpyridine ligands. 2007 , 13, 10257-72	44
1234	Is this a chemical bond? A theoretical study of Ng2@C60 (Ng=He, Ne, Ar, Kr, Xe). 2007 , 13, 8256-70	154
1233	The nature of the AgI...AgI interaction in different Ag(NH3)2 dimers embedded in supramolecular solids. 2007 , 13, 8583-90	28
1232	Stable pentacoordinate carbocations: structure and bonding. 2007 , 13, 8620-6	24
1231	The electronic structure of the tris(ethylene) complexes [M(C2H4)3] (M=Ni, Pd, and Pt): a combined experimental and theoretical study. 2007 , 13, 10078-87	45
1230	Selective binding and easy separation of C70 by nanoscale self-assembled capsules. 2007 , 46, 202-5	117
1229	Synthesis and electronic structure of a ferroborene. 2007 , 46, 5215-8	61
1228	Bismuth and lead hanging-carboxylate porphyrins: an unexpected homobimetallic lead(II) complex. 2007 , 46, 5120-4	38
1227	C(NHC)2: divalent carbon(0) compounds with N-heterocyclic carbene ligands-theoretical evidence for a class of molecules with promising chemical properties. 2007 , 46, 8695-8	319
1226	Chirality, agostic interactions, and pyramidity in actinide methylidene complexes. 2007 , 46, 9045-9	37

1225	Molecular photochromic systems: a theoretical and experimental investigation on zinc(II) dithizonate. 2007 , 21, 246-254		2
1224	Selective Binding and Easy Separation of C70 by Nanoscale Self-Assembled Capsules. 2007 , 119, 206-209		41
1223	Synthese und Elektronenstruktur eines Ferroborirens. 2007 , 119, 5307-5310		28
1222	Bismuth and Lead Hanging-Carboxylate Porphyrins: An Unexpected Homobimetallic Lead(II) Complex. 2007 , 119, 5212-5216		13
1221	C(NHC) ₂ : zweibindige Kohlenstoff(0)-Verbindungen mit N-heterocyclischen Carbenliganden □ theoretische Belege für eine Molekülklasse mit vielversprechenden Eigenschaften. 2007 , 119, 8850-8853		167
1220	Chirality, Agostic Interactions, and Pyramidity in Actinide Methylidene Complexes. 2007 , 119, 9203-9207		9
1219	Addition Energies and Vibrational Fine Structure Measured in Electromigrated Single-Molecule Junctions Based on an Oligophenylenevinylene Derivative. 2007 , 19, 281-285		115
1218	Electronic structure of CO--an exercise in modern chemical bonding theory. <i>Journal of Computational Chemistry</i> , 2007 , 28, 117-26	3.5	89
1217	Unicorns in the world of chemical bonding models. <i>Journal of Computational Chemistry</i> , 2007 , 28, 15-24	3.5	174
1216	Covalent versus ionic bonding in alkalimetal fluoride oligomers. <i>Journal of Computational Chemistry</i> , 2007 , 28, 238-50	3.5	14
1215	Energy landscapes of nucleophilic substitution reactions: a comparison of density functional theory and coupled cluster methods. <i>Journal of Computational Chemistry</i> , 2007 , 28, 1551-1560	3.5	87
1214	Geometry optimization using generalized, chemically meaningful constraints. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2226-36	3.5	75
1213	Model transition states for methane diazonium ion methylation of guanine runs in oligomeric DNA. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2352-65	3.5	9
1212	A Theoretical Study of the Nearest Cu ^{II} -Cu Antiferromagnetic Exchange Coupling Interactions in [LaCu ₆] and [YCu ₆]. 2007 , 2007, 1261-1267		3
1211	An Unusual Carbonyl Chemical Shift in a Carbonylhexairidium Cluster: A Combined Solid-State NMR and DFT Approach. 2007 , 2007, 3477-3483		11
1210	Electronic Structure of Linearly Coordinated EQ Complexes of the Type [(N ₃ N)W(EQ)] [N ₃ N = N(CH ₂ CH ₂ NSiMe ₃) ₃ ; E = P, As, Sb, Bi; Q = O, S, Se, Te]: A DFT Study. 2007 , 2007, 2443-2453		3
1209	Red-to-Yellow Pressure-Induced Phase Transition in Pt(bpy)Cl ₂ : Spectroscopic Study Supported by DFT Calculations. 2007 , 2007, 5735-5742		10
1208	Electronic Structures and Spectroscopic Properties of [Pt(CNMe) ₂ (CN) ₂] _n (n = 1-4): A Theoretical Exploration of Promising Phosphorescent Materials. 2007 , 2007, 2181-2188		13

1207	Proton Affinities in Water of Maingroup-Element Hydrides [Effects of Hydration and Methyl Substitution. 2007 , 2007, 3646-3654	82
1206	Cleavage of CO by Mo[N(R)Ar] ₃ Complexes. 2007 , 2007, 3736-3741	15
1205	Olefin Complexes of Low-Valent Rhenium. 2007 , 2007, 5246-5261	18
1204	Coordination Alternatives in Dinuclear Bis(pyridin-2-ylalkyl)benzylaminecopper(II) Complexes with OH ⁻ RO ⁻ F ⁻ or Cl ⁻ Bridges: Experimental Structures and DFT Preferences. 2007 , 2007, 5500-5510	17
1203	Decomposition Cascades of Dicoordinate Copper(I) Chalcogenides. 2007 , 2007, 5294-5299	6
1202	Double Group Transfer Reactions as Indicators of Aromatic Stabilization. 2007 , 2007, 5410-5415	17
1201	Transition-state energy and position along the reaction coordinate in an extended activation strain model. 2007 , 8, 1170-81	158
1200	Nucleophilic substitution at phosphorus centers (S _N 2@p). 2007 , 8, 2452-63	55
1199	¹ H, ¹³ C and ¹⁵ N NMR coordination shifts in gold(III), cobalt(III), rhodium(III) chloride complexes with pyridine, 2,2'-bipyridine and 1,10-phenanthroline. 2007 , 45, 24-36	56
1198	Investigation of the dissociative adsorption for cyclopropane on the copper surface by density functional theory and quantum chemical molecular dynamics method. 2007 , 601, 679-685	3
1197	The nature of metal-metal bond of the dimetallocene complexes [M ₂ (η -C ₅ R ₅) ₂] (M=Zn, Cd, Hg; R=H, Me): An energy decomposition analysis. 2007 , 805, 127-132	31
1196	Structure and bonding differences in C ₃ N ₄ and Si ₃ N ₄ isomers [A comparative study of [Si ₃ N ₄] and [C ₃ N ₄] potential energy surfaces using DFT and MP2 methodologies. 2007 , 807, 73-85	2
1195	Bonding and aromaticity of cyclic phosphazenes viewed as interaction of D _{nh} fragments. 2007 , 820, 148-158	17
1194	Photocatalytic decolorization of Remazol Black 5 (RB5) and Procion Red MX-5B [therm of adsorption, kinetic of decolorization and mineralization. 2007 , 77, 100-109	97
1193	A TDDFT study on the excitation of P700. 2007 , 434, 111-115	4
1192	Theoretical investigation on intramolecular electron transfer in polypeptides. 2007 , 440, 302-307	7
1191	Theoretical description of metal-gand bonding within f-element complexes: A successful and necessary interplay between theory and experiment. 2007 , 10, 888-896	26
1190	Computational spectroscopy and DFT investigations into nitrogen and oxygen bond breaking and bond making processes in model deNO _x and deN ₂ O reactions. 2007 , 119, 219-227	42

1189	Electronic transitions and bonding properties in a series of five-coordinate d ⁶ -electron complexes [Mn(CO) ₃ (L ₂)] ⁺ (L ₂ =chelating redox-active σ-donor ligand). 2007 , 251, 557-576	60
1188	Metal–ligand bonding in metallocenes: Differentiation between spin state, electrostatic and covalent bonding. 2007 , 360, 179-189	167
1187	Copper(II) complexes with unsymmetrical pentadentate ed _{3a} -type diamino-tricarboxylate ligands. Crystal structures, configurational analysis and DFT study of complexes. 2007 , 360, 2420-2431	25
1186	Dicoordinate copper(I) chalcogenides [Structure and bonding. 2007 , 360, 3511-3517	10
1185	On the ground state T _g ? _g (T _g =2T _{2g} , 3T _{1g}) Jahn–Teller-coupling in hexacyano complexes of 3d-transition metals. 2007 , 838, 157-163	11
1184	Periodic trends in metal–metal bonding in edge-shared [M ₂ Cl ₁₀] ⁴⁻ systems. 2007 , 26, 2942-2948	8
1183	Theoretical studies on the electronic structure and spectral properties of versatile diarylethene-containing 1,10-phenanthroline ligands and their rhenium(I) complexes. 2007 , 692, 5368-5374	24
1182	Theoretical investigation of the bonding properties of N-heterocyclic carbenes coordinated to electron-rich d ⁸ metal centers. 2007 , 692, 5709-5716	38
1181	Sulfur K-edge XAS of WVO vs. MoVO bis(dithiolene) complexes: contributions of relativistic effects to electronic structure and reactivity of tungsten enzymes. 2007 , 101, 1594-600	20
1180	Comment on On the calculation of the electrostatic potential, electric field and electric field gradient from the aspherical pseudoatom model by Volkov, King, Coppens & Farrugia (2006). 2007 , 63, 198-200; author reply 201-3	10
1179	(Ph ₄ P) ₂ [Be ₂ F ₆] ²⁻ ·CH ₃ CN: Synthese, Schwingungsspektrum, Kristallstruktur und quantenchemische Rechnungen. 2007 , 633, 1183-1188	10
1178	Core Electron Binding Energy (CEBE) as Descriptors in Quantitative Structure–Activity Relationship (QSAR) Analysis of Cytotoxicities of a Series of Simple Phenols. 2007 , 26, 378-384	4
1177	Nuclear Fukui functions from nonintegral electron number calculations. 2007 , 107, 807-815	11
1176	Bonding analysis of N-heterocyclic carbene tautomers and phosphine ligands in transition-metal complexes: a theoretical study. 2007 , 2, 1555-67	216
1175	Structural, spectral, electric-field-induced second harmonic, and theoretical study of Ni(II), Cu(II), Zn(II), and VO(II) complexes with [N ₂ O ₂] unsymmetrical schiff bases of S-methylisothiosemicarbazide derivatives. 2007 , 46, 884-95	106
1174	Interaction of plasmon and molecular resonances for rhodamine 6G adsorbed on silver nanoparticles. 2007 , 129, 7647-56	258
1173	Charge Transport along Coiled Conjugated Polymer Chains. 2007 , 111, 11104-11112	37
1172	Tetrakis(thiadiazole)porphyrazines. 5. Electrochemical and DFT/TDDFT studies of the free-base macrocycle and its Mg(II), Zn(II), and Cu(I) complexes. 2007 , 46, 4145-57	47

1171	Structural characterization of molybdenum(V) species in aqueous HCl solutions. 2007 , 46, 4430-45	16
1170	High-field EPR, ENDOR and ELDOR on bacterial photosynthetic reaction centers. 2007 , 31, 59-98	41
1169	Magnetic field dependence of ^{13}C photo-CIDNP MAS NMR in plant photosystems I and II. 2007 , 31, 193-204	11
1168	On convergence of the normalized elimination of the small component (NESC) method. 2007 , 117, 333-338	50
1167	Computational NMR spectroscopy: reversing the information flow. 2007 , 117, 603-619	95
1166	Theory of oxides surfaces, interfaces and supported nano-clusters. 2007 , 117, 827-845	26
1165	An integrated computational tool for the study of the optical properties of nanoscale devices: application to solar cells and molecular wires. 2007 , 117, 1093-1104	34
1164	Transition metal impurities in wide gap materials: are the electronic properties well described through the ligand field theory?. 2007 , 118, 665-671	8
1163	Hypervalence and the delocalizing versus localizing propensities of $\text{H}\beta$, $\text{Li}\beta$, $\text{CH}\beta$ and $\text{SiH}\beta$. 2007 , 18, 813-819	23
1162	Hypothetical Hypercloso Octahedral M_4N_2 Clusters: A New Mode of Dinitrogen Coordination?. 2007 , 18, 729-740	7
1161	On the Electronic Structure of Distorted Cubic Rhodium Cluster Complexes Containing Bridging Germanium or Phosphorus Ligands. 2007 , 18, 720-728	1
1160	Synthesis and DFT Defined $\text{trans}(\text{O}_5\text{O}_6)$ Molecular Structure of $\text{Cs}[\text{Fe}(\text{1,3-pddadp})] \cdot 2\text{H}_2\text{O}$. Strain Analysis and Spectral Assignment of the Complex. 2007 , 138, 823-832	3
1159	Altered spin state equilibrium in the T309V mutant of cytochrome P450 2D6: a spectroscopic and computational study. 2007 , 12, 645-54	9
1158	Natural orbitals for chemical valence as descriptors of chemical bonding in transition metal complexes. 2007 , 13, 347-55	385
1157	Localization of ligand binding site in proteins identified in silico. 2007 , 13, 665-75	18
1156	Pi-pi stacking tackled with density functional theory. 2007 , 13, 1245-57	111
1155	On the structure and relative stability of uranyl(VI) sulfate complexes in solution. 2007 , 10, 905-915	25
1154	Theoretical and experimental study of methane steam reforming reactions over nickel catalyst. 2007 , 253, 4427-4437	47

1153	Cd-metallothionein: Analysis of local atomic structure. 2007 , 575, 162-164	7
1152	Theoretical study of the hydrogen adsorption on AlB nanowire. 2008 , 184, 60-76	9
1151	Quantum chemical molecular dynamical investigation of alkyl nitrite photo-dissociated on copper surfaces. 2008 , 254, 6991-6999	1
1150	In situ infrared spectroscopic characterization of a bismuth-ethanol interface. 2008 , 53, 8166-8171	7
1149	Energy-level alignment in the adsorption of phosphonyl reagents on γ -Al ₂ O ₃ . 2008 , 602, 1938-1947	16
1148	Understanding the π -facial diastereoselectivity in the addition of chiral diaminophosphino(silyl)carbenes to activated olefins. 2008 , 19, 2353-2358	5
1147	From Electron Density Flow Towards Activation: Benzene Interacting with Cu(I) and Ag(I) Sites in ZSM-5. DFT Modeling. 2008 , 126, 241-246	13
1146	The Electronic Structure and Bonding of the First p-Block Paddlewheel Complex, Bi ₂ (trifluoroacetate) ₄ , and Comparison to d-Block Transition Metal Paddlewheel Complexes: A Photoelectron and Density Functional Theory Study. 2008 , 19, 275-294	5
1145	Quadrupole coupling constants and isomeric Mössbauer shifts for halogen-containing gold, platinum, niobium, tantalum and antimony compounds. 2008 , 181, 27-36	4
1144	A vibrational circular dichroism implementation within a Slater-type-orbital based density functional framework and its application to hexa- and hepta-helicenes. 2008 , 119, 245-263	75
1143	The strength of the σ and π bonds in Re ₂ Cl ₂ . 2008 , 120, 313-320	22
1142	The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. 2008 , 120, 215-241	19079
1141	Role of hydration in determining the structure and vibrational spectra of L-alanine and N-acetyl-L-alanine N ² -methylamide in aqueous solution: a combined theoretical and experimental approach. 2008 , 119, 191-210	109
1140	Competition between Bailar and Ray-Dutt paths in conformational interconversion of tris-chelated complexes: a DFT study. 2008 , 120, 447-457	6
1139	Analysis of the metal-ligand bonds in [Mo(X)(NH ₂) ₃] (X = P, N, PO, and NO), [Mo(CO) ₅ (NO)] ⁺ , and [Mo(CO) ₅ (PO)] ⁺ . 2008 , 120, 351-361	12
1138	Charge density analysis of two proton transfer complexes: Understanding hydrogen bonding and determination of in-crystal dipole moments. 2008 , 120, 613-620	14
1137	Coordination and binding geometry of methyl-coenzyme M in the red _{1m} state of methyl-coenzyme M reductase. 2008 , 13, 1275-89	7
1136	Applications of natural orbitals for chemical valence in a description of bonding in conjugated molecules. 2008 , 14, 681-7	176

1135	DFT-based molecular modeling and vibrational study of the La(III) complex of 3,3'-(benzylidene)bis(4-hydroxycoumarin). 2008 , 14, 353-66	30
1134	Theoretical study of the novel sandwich compound [Au3Cl3Tr 2]2+. 2008 , 14, 417-25	17
1133	On the Application of the Bond Transferability Postulate to Transition-Metal Complexes: Study of FeF6 3- and FeOF5 4- Centers in KMgF3. 2008 , 34, 149-156	5
1132	H2O2 activation by heteropolyacids with defect structures: the case of [(XO4)W10O32]n- [X = Si, Ge, n = 8; X = P, n = 7]. 2008 , 21, 596-602	17
1131	Inductive and resonance effects based on core-electron binding energy shift. 2008 , 108, 2326-2333	5
1130	Copper binding sites in the C-terminal domain of mouse prion protein: A hybrid (QM/MM) molecular dynamics study. 2008 , 70, 1084-98	20
1129	Dimerization of the 2-(Methylselenomethyl)benzimidazole-silver(I) Cation Involving a AgI...AgI Interaction. 2008 , 634, 2343-2346	8
1128	Intramolecular alkyl phosphine dehydrogenation in cationic rhodium complexes of tris(cyclopentylphosphine). 2008 , 14, 1004-22	41
1127	Fused tricyclic phosphiranes--analysis of phosphorus chemical shieldings. 2008 , 14, 1499-507	11
1126	Molecular and electronic structures of one-electron oxidized Ni(II)-(dithiosalicylidenediamine) complexes: Ni(III)-thiolate versus Ni(II)-thiyl radical states. 2008 , 14, 2564-76	45
1125	Hypervalent silicon versus carbon: ball-in-a-box model. 2008 , 14, 819-28	82
1124	Understanding lead chemistry from topological insights: the transition between holo- and hemidirected structures within the [Pb(CO)n]2+ model series. 2008 , 14, 2730-43	36
1123	Divalent carbon(0) chemistry, part 1: Parent compounds. 2008 , 14, 3260-72	331
1122	Divalent carbon(0) chemistry, part 2: Protonation and complexes with main group and transition metal Lewis acids. 2008 , 14, 3273-89	261
1121	Structural, magnetic coupling and oxidation state trends in models of the CaMn4 cluster in photosystem II. 2008 , 14, 5482-94	29
1120	Hypervalent versus nonhypervalent carbon in noble-gas complexes. 2008 , 14, 6901-11	36
1119	Effects of geometric isomerism and anions on the kinetics and mechanism of the stepwise formation of long-range DNA interstrand cross-links by dinuclear platinum antitumor complexes. 2008 , 14, 6391-405	15
1118	Microsolvation effects on the optical properties of crystal violet. 2008 , 14, 7351-7	22

1117	Models of the ox1 state of methylcoenzyme M reductase: where are the electrons?. 2008 , 14, 9981-9		3
1116	pi-Bonding in complexes of benzannulated biscarbenes, -germylenes, and -stannylenes: an experimental and theoretical study. 2008 , 14, 10716-21		48
1115	Computational NMR spectroscopy of organoarsenicals and the natural polyarsenic compound arsenicin A. 2008 , 14, 10445-52		24
1114	On the origin of circular dichroism in trigonal dihedral d6 complexes of bidentate ligands containing only sigma-orbitals. A qualitative model based on a density functional theory study of Lambda-[Co(en)3]3+. 2008 , 20, 938-50		17
1113	Infrared spectroscopy of dioxouranium(V) complexes with solvent molecules: effect of reduction. 2008 , 9, 1278-85		36
1112	Hangman salen platforms containing dibenzofuran scaffolds. 2008 , 1, 941-9		14
1111	PyFrag--Streamlining your reaction path analysis. <i>Journal of Computational Chemistry</i> , 2008 , 29, 312-5	3.5	41
1110	cclib: a library for package-independent computational chemistry algorithms. <i>Journal of Computational Chemistry</i> , 2008 , 29, 839-45	3.5	3652
1109	QUILD: QUAntum-regions interconnected by local descriptions. <i>Journal of Computational Chemistry</i> , 2008 , 29, 724-34	3.5	114
1108	A flexible implementation of frozen-density embedding for use in multilevel simulations. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1011-8	3.5	121
1107	Reaction mechanisms of dissociative chemisorption of HI, I2, and CH3I on a magic cluster Al13-. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1626-31	3.5	11
1106	The trans effect in square-planar platinum(II) complexes--a density functional study. <i>Journal of Computational Chemistry</i> , 2008 , 29, 2370-81	3.5	62
1105	QM/MM vibrational mode tracking. <i>Journal of Computational Chemistry</i> , 2008 , 29, 2460-70	3.5	20
1104	Influence of the Copper Coordination Geometry on the DNA Cleavage Activity of Clip-Phen Complexes Studied by DFT. 2008 , 2008, 612-619		21
1103	Electron-Sponge Behavior, Reactivity and Electronic Structures of Cobalt-Centered Cubic Co9Te6(CO)8 Clusters. 2008 , 2008, 1959-1968		14
1102	Synthesis, Radiolabelling and Confocal Fluorescence Microscopy of Styrene-Derivatised Bis(thiosemicarbazonato)zinc and -copper Complexes. 2008 , 2008, 1985-1993		26
1101	Cationic Triple-Decker Complexes with a Bridging 4-Borataborepine Ligand: Synthesis, Structure, and Bonding. 2008 , 2008, 3320-3329		6
1100	Density Functional Theory Studies of the Magnetostructural Correlations in the Cyano-Bridged Mo2Ni and Mo2Ni3 Systems. 2008 , 2008, 2199-2206		4

1099	Complexes of Yb ³⁺ with EDTA and CDTA [Molecular and Electronic Structure. 2008 , 2008, 3075-3082	21
1098	Nucleophilic Substitution at C, Si and P: How Solvation Affects the Shape of Reaction Profiles. 2008 , 2008, 649-654	57
1097	Methylgallium as a terminal ligand in [(Cp*Ga)4Rh(GaCH3)] ⁺ . 2008 , 47, 3438-41	43
1096	The low basicity of phosphabenzene: first examples of protonation, alkylation, and silylation reactions. 2008 , 47, 3801-4	32
1095	Metal-metal distances at the limit: a coordination compound with an ultrashort chromium-chromium bond. 2008 , 47, 7246-9	150
1094	Dramatic remote substituent effects on the electronic spin state of bis(scorpionate) iron(II) complexes. 2008 , 47, 8687-91	23
1093	Modeling Electron and Hole Transport in Fluoroarene-Oligothiophene Semiconductors: Investigation of Geometric and Electronic Structure Properties. 2008 , 18, 332-340	104
1092	Methylgallium als terminaler Ligand in [(Cp*Ga)4Rh(GaCH3)] ⁺ . 2008 , 120, 3487-3490	19
1091	The Low Basicity of Phosphabenzene: First Examples of Protonation, Alkylation, and Silylation Reactions. 2008 , 120, 3861-3864	8
1090	Metall-Metall-Abstände am Limit: ein Komplex mit ultrakurzer Cr-Cr-Bindung. 2008 , 120, 7356-7359	59
1089	Dramatic Remote Substituent Effects on the Electronic Spin State of Bis(scorpionate) Iron(II) Complexes. 2008 , 120, 8815-8819	2
1088	Crystal structures, theoretical calculations, spectroscopic and electrochemical properties of Cr(III) complexes with dipicolinic acid and 1,10-phenanthroline. 2008 , 27, 502-512	44
1087	Density functional theory calculations of novel Rh(I) diphosphinite catalysts. 2008 , 27, 2529-2538	3
1086	A europium(II) complex with bis-pyridino-18-crown-6. 2008 , 27, 2688-2692	12
1085	An attempt towards coordination supramolecularity from Mn(II), Ni(II) and Cd(II) with a new hexadentate [N4O2] symmetrical Schiff base ligand: Syntheses, crystal structures, electrical conductivity and optical properties. 2008 , 27, 3359-3370	18
1084	Unusual hydrothermal synthesis of a heteroaromatic macrocyclic complex. 2008 , 27, 3700-3702	6
1083	Computational studies of CO and CO ⁺ : Density functional theory and time-dependent density functional theory. 2008 , 109, 2546-2560	7
1082	An investigation of the formation of 1,3,5-heterosubstituted benzene rings by cyclo-condensation of acetyl-substituted organometallic complexes. 2008 , 693, 1957-1967	9

- 1081 Tunable electronic coupling in iron-chromium mixed-valence ions of methylated Cp-indene ligands. **2008**, 693, 3797-3809 8
- 1080 Both Met(109) and Met(112) are utilized for Cu(II) coordination by the amyloidogenic fragment of the human prion protein at physiological pH. **2008**, 102, 2103-13 27
- 1079 The electronic properties and electron affinity of the hydrogenated nanodiamonds with surface reconstructions. **2008**, 255, 2623-2626 6
- 1078 One-electron quantum capping potential for hybrid QM/MM studies of silicate molecules and solids. **2008**, 454, 65-69 14
- 1077 The luminescent $[Mo_6X_8(NCS)_6]_2$ (X=Cl, Br, I) clusters?: A computational study based on time-dependent density functional theory including spin-orbit and solvent-polarity effects. **2008**, 455, 38-41 24
- 1076 Electronic structure and molecular properties of the $[Mo_6X_8L_6]_2$ (X = Cl, Br, I; L = F, Cl, Br, I) clusters. **2008**, 460, 438-441 52
- 1075 Analysis of electron density distributions from subsystem density functional theory applied to coordination bonds. **2008**, 461, 353-359 62
- 1074 Spin-orbit effects on the aromaticity of the Re_3Cl_9 and Re_3Br_9 clusters. **2008**, 467, 94-96 33
- 1073 Hydrogen and dihydrogen bonding of transition metal hydrides. **2008**, 345, 95-102 28
- 1072 Synthesis and conformational studies of chiral meso-(β -unsaturated)-porphyrins. **2008**, 64, 10874-10881 7
- 1071 Tricarbonylchromium complexes of [5]- and [6]metacyclophane: an experimental and theoretical study. **2008**, 64, 11641-11646 10
- 1070 Halogen-halogen interactions in $[Mo_3X_7Y_7]_3$ clusters (X=S, Se, Te; Y=Cl, Br, I). **2008**, 849, 112-115 3
- 1069 Explaining the HOMO and LUMO distribution on individual ligands in mer-Alq₃ and its CH₃N substituted derivatives. **2008**, 850, 79-83 16
- 1068 Accurate calculation of N1s and C1s core electron binding energies of substituted pyridines. Correlation with basicity and with Hammett substituent constants. **2008**, 863, 33-38 15
- 1067 The nature of the metal-nitric oxide bond in the $[M(CN)_5(NO)]_q$ (M = Cr, Mn, Fe, Ru, Os, and Co) and trans- $[Ru(NH_3)_4L(NO)]_q$ (L = pyrazine, pyridine, N₂, H₂O, Cl⁻, CN⁻, NO₂⁻) complexes: A bond-energy decomposition analysis. **2008**, 865, 28-35 13
- 1066 A TD-DFT study on dissociative loss of the axial and equatorial carbonyl for HCo(CO)₄. **2008**, 865, 88-93 2
- 1065 A DFT study of H adsorption on Pt(111) and PtRu(111) surfaces. **2008**, 254, 5827-5830 7
- 1064 Synthesis and properties of new trinuclear Mo(II) complexes containing imidazole and benzimidazole ferrocene units. **2008**, 361, 1584-1596 21

1063	Structural Model Studies for the High-Valent Intermediate Q of Methane Monooxygenase from Broken-Symmetry Density Functional Calculations. 2008 , 361, 973-986	55
1062	Assignment of Pre-edge Features in the Ru K-edge X-ray Absorption Spectra of Organometallic Ruthenium Complexes. 2008 , 361, 1059	38
1061	Development of palladium L-edge X-ray absorption spectroscopy and its application for chloropalladium complexes. 2008 , 361, 1047-1058	18
1060	Metal-Sulfur dπ-backbonding of the oxidations of metal-thiolate complexes: Photoelectron spectroscopy of (η ⁵ -C ₅ H ₅)Fe(CO) ₂ SR (SR=SCH ₃ , StBu) and (η ⁵ -C ₅ H ₅)Re(NO)(PR ₃)SCH ₃ (PR ₃ =PiPr ₃ , PPh ₃). 2008 , 361, 1122-1133	9
1059	Toward an expanded oxygen atom transfer reactivity scale: Computational investigation of the energetics of oxo transfer reaction couples. 2008 , 361, 1166-1176	27
1058	The role of 5-R-1,10-phenanthroline (R=CH ₃ , NO ₂) on the emission properties and second-order NLO response of cationic Ir(III) organometallic chromophores. 2008 , 361, 4070-4076	39
1057	Some considerations on the proper use of computational tools in transition metal chemistry. 2008 , 361, 3820-3831	69
1056	Photoelectron spectroscopy of dithiolatodiiironhexacarbonyl models for the active site of [FeFe] hydrogenases: Insight into the reorganization energy of the rotated structure in the enzyme. 2008 , 890, 281-288	30
1055	THEORETICAL STUDIES OF THE TETRACHLOROCUPRATE(II) ANION: ADF GEOMETRY OPTIMIZATION, AND CALCULATION OF THE PES, EPR PARAMETERS, AND VIBRATIONAL FREQUENCIES. 2008 , 07, 53-65	1
1054	A Dichromium(II) Bis(β-pentalene) Double-Sandwich Complex with a Spin Equilibrium: Synthetic, Structural, Magnetic, and Theoretical Studies. 2008 , 27, 2013-2020	31
1053	Structure and bonding of the MCN molecules, M=Cu,Ag,Au,Rg. 2008 , 128, 224303	27
1052	Direct metal-metal interaction contributions to quadratic hyperpolarizability: a study on dirhenium complexes. 2008 , 112, 4965-72	20
1051	Photophysical properties of natural light-harvesting complexes studied by subsystem density functional theory. 2008 , 112, 2207-17	82
1050	Frontside versus Backside S(N) ₂ substitution at group 14 atoms: origin of reaction barriers and reasons for their absence. 2008 , 3, 1783-92	52
1049	Sterically congested uranyl complexes with seven-coordination of the UO ₂ unit: the peculiar ligation mode of nitrate in [UO ₂ (NO ₃) ₂ (Rbtp)] complexes. 2008 , 47, 6850-62	59
1048	Physicochemical properties of zwitterionic L- and DL-alanine crystals from their experimental and theoretical charge densities. 2008 , 112, 5163-74	53
1047	Watson-crick base pairs with thiocarbonyl groups: How sulfur changes the hydrogen bonds in DNA. 2008 , 6, 15-21	6
1046	Quantum-chemical investigation of the effect of grain-boundary segregation on wear resistance of steel. 2008 , 29, 99-107	4

1045	Halide ligand-more than just sigma-donors? A structural and spectroscopic study of homologous organonickel complexes. 2008 , 47, 11324-33	35
1044	Pseudopolymorphism in Nickel(II) Complexes with 6-Methylpicolinate. Synthesis, Structural, Spectroscopic, Thermal, and Density Functional Theory Studies. 2008 , 8, 3465-3473	23
1043	DFT at its best: metal- versus ligand-centered reduction in nickel hydroporphyrins. 2008 , 112, 15158-73	13
1042	Nucleophilicity and leaving-group ability in frontside and backside S(N)2 reactions. 2008 , 73, 7290-9	170
1041	Reaction Coordinates and the Transition-Vector Approximation to the IRC. 2008 , 4, 920-8	34
1040	Linkage Isomerism of Nitriles in Rhodium Half-Sandwich Metallacycles. 2008 , 27, 4028-4030	18
1039	An electrochemical study of antineoplastic gallium, iron and ruthenium complexes with redox noninnocent alpha-N-heterocyclic chalcogensemicarbazones. 2008 , 47, 11032-47	51
1038	E2 and SN2 Reactions of X(-) + CH3CH2X (X = F, Cl); an ab Initio and DFT Benchmark Study. 2008 , 4, 929-40	76
1037	[Re(eta(5)-C5H5)(CO)3]+ family of 17-electron compounds: monomer/dimer equilibria and other reactions. 2008 , 130, 2692-703	66
1036	Theoretical study on a novel series of fullerene-containing organometallics Fe(eta5-C55X5)2 (X = CH, N, B) and their large third-order nonlinear optical properties. 2008 , 112, 8086-92	21
1035	Redox properties of ruthenium nitrosyl porphyrin complexes with different axial ligation: structural, spectroelectrochemical (IR, UV-visible, and EPR), and theoretical studies. 2008 , 47, 7106-13	45
1034	Aromaticity and antiaromaticity in 4-, 6-, 8-, and 10-membered conjugated hydrocarbon rings. 2008 , 112, 12816-22	35
1033	Theoretical Modeling of Zeolite Nanoparticle Surface Acidity for Heavy Oil Upgrading. 2008 , 112, 6794-6810	45
1032	Computational and experimental tools in solving some mechanistic problems in the chemistry of Fischer carbene complexes. 2008 , 4671-82	50
1031	A DFT perspective on the structures and electronic spectra of the orange and blue isomers of photochromic dithizonatophenylmercury(II). 2008 , 112, 2211-8	21
1030	Enhanced Hydrogen Uptake and the Electronic Structure of Lithium-Doped MetalOrganic Frameworks. 2008 , 112, 9278-9284	69
1029	On the origin of alternating bond distortions and the emergence of chirality in polyoxometalate anions. 2008 , 130, 8223-33	98
1028	A computational study on some viable targets for gas-phase synthesis of metal complexes of the cyclic (B6C)-2 and their bonding pattern. 2008 , 112, 10365-77	12

1027	Time-dependent DFT studies of metal core-electron excitations in Mn complexes. 2008 , 112, 11223-34	17
1026	Binding between endohedral Na atoms in Si clathrate I; a first principles study. 2008 , 20, 385209	3
1025	From SiO molecules to silicates in circumstellar space: atomic structures, growth patterns, and optical signatures of Si _n O _m clusters. 2008 , 2, 1729-37	38
1024	Three-dimensional local structure of photoexcited Cu diimine complex refined by quantitative XANES analysis. 2008 , 112, 5363-7	47
1023	Local symmetry change in BaF ₂ :Mn ²⁺ at approximately 50 K: microscopic insight. 2008 , 128, 124513	12
1022	Redox transitions of chromium, manganese, iron, cobalt and nickel protoporphyrins in aqueous solution. 2008 , 10, 1023-31	49
1021	Empirical corrections to density functional theory highlight the importance of nonbonded intramolecular interactions in alkanes. 2008 , 112, 11495-500	46
1020	Nature of the Fe ₄₂ center in KTaO ₃ : A density functional theory study. 2008 , 78,	6
1019	Influence of internal electric fields on bonding and properties of impurities in insulators: Mn ²⁺ in LiBaF ₃ and normal perovskites. 2008 , 78,	21
1018	Uranium and Lanthanide Complexes with the 2-Mercapto Benzothiazolate Ligand: Evidence for a Specific Covalent Binding Site in the Differentiation of Isostructural Lanthanide(III) and Actinide(III) Compounds. 2008 , 27, 33-42	37
1017	On the origin of paramagnetism in planar nickel(II) complexes. 2008 , 1989-92	16
1016	PARTICULAR MECHANISMS ON INSERTION OF ETHYLENE INTO Zr-H BOND OF Cp ₂ ZrH ₂ : A DFT STUDY. 2008 , 07, 933-941	1
1015	Stable Geometric and Electronic Structures of Gold-Coated Nanoparticles ₁₂ (M = 5d Transition Metals, from Hf to Hg): lh or Oh?. 2008 , 112, 12646-12652	23
1014	Symmetry breaking effect in the ferrocene electronic structure by hydrocarbon-monosubstitution: an experimental and theoretical study. 2008 , 128, 154315	17
1013	Ground state of octahedral platinum hexafluoride. 2008 , 77,	33
1012	Half-metallic finite zigzag single-walled carbon nanotubes from first principles. 2008 , 78,	42
1011	Models, Mysteries and Magic of Molecules. 2008 ,	8
1010	The chemical bond between Au(I) and the noble gases. Comparative study of NgAuF and NgAu ⁺ (Ng = Ar, Kr, Xe) by density functional and coupled cluster methods. 2008 , 130, 1048-60	222

1009	All-Electron Scalar Relativistic Basis Sets for Third-Row Transition Metal Atoms. 2008 , 4, 908-19	832
1008	Cholesky Decomposition-Based Multiconfiguration Second-Order Perturbation Theory (CD-CASPT2): Application to the Spin-State Energetics of Co(III)(diiminato)(NPh). 2008 , 4, 694-702	300
1007	Accurate Spin-State Energies for Iron Complexes. 2008 , 4, 2057-66	289
1006	Detecting delocalization. 2008 , 32, 1359	14
1005	Computational Strategies for Identification of Bimetallic Ethylene Epoxidation Catalysts. 2008 , 265-281	1
1004	Theoretical mechanism study of UF ₆ hydrolysis in the gas phase. 2008 , 112, 8877-83	17
1003	Influence of polyoxometalate ligands on the nature of high-valent transition metal nitrido species. A theoretical analysis of experimentally known and unprecedented compounds. 2008 , 5166-72	36
1002	LiSc(BH ₄) ₄ : a novel salt of Li ⁺ and discrete Sc(BH ₄) ₄ ⁻ complex anions. 2008 , 112, 7551-5	146
1001	Infrared spectroscopy of discrete uranyl anion complexes. 2008 , 112, 508-21	47
1000	Alkane hydroxylation by peroxy acids: a comparison with the cytochrome P450 hydroxylation. 2008 , 112, 12855-61	6
999	Theoretical study of the oxygen exchange in uranyl hydroxide. An old riddle solved?. 2008 , 130, 13735-44	58
998	The contrasting chemistry and cancer cell cytotoxicity of bipyridine and bipyridinediol ruthenium(II) arene complexes. 2008 , 47, 11470-86	86
997	Bonding of Imidazol-2-ylidene Ligands in Nickel Complexes. 2008 , 27, 3410-3414	51
996	Understanding and predicting distorted T- versus Y-geometries for neutral chromous complexes supported by a sterically encumbering beta-diketiminate ligand. 2008 , 130, 17351-61	30
995	Pentadienyl Complexes of Alkali Metals: Structure and Bonding□ 2008 , 27, 827-833	25
994	Crystal engineering for pi-pi stacking via interaction between electron-rich and electron-deficient heteroaromatics. 2008 , 73, 4608-14	61
993	A New Approach to the Photochemically Controlled Crown Ethers: (Tetramethylcyclobutadiene)cobalt Complexes with Benzo-15-Crown-5 and Dibenzo-18-Crown-6□ 2008 , 27, 3654-3658	17
992	Heterometallic cuboidal clusters M(3)M'Q(4) (M = Mo, W; M' = Sn, Pb, As, Sb; Q = S, Se): from coordination compounds to supramolecular adducts. 2008 , 47, 306-14	21

991	On the sensitivity of f electrons to their chemical environment. 2008 , 130, 2180-3	44
990	Investigation of the redox behavior of ferroquine, a new antimalarial. 2008 , 5, 710-6	92
989	Synthesis, characterization, and DFT/TD-DFT calculations of highly phosphorescent blue light-emitting anionic iridium complexes. 2008 , 47, 980-9	212
988	Direct space decomposition of ELI-D: interplay of charge density and pair-volume function for different bonding situations. 2008 , 112, 9814-28	66
987	Vibrational excitations in weakly coupled single-molecule junctions: a computational analysis. 2008 , 2, 1445-51	52
986	From Discrete Electronic States to Plasmons: TDDFT Optical Absorption Properties of Ag _n (n = 10, 20, 35, 56, 84, 120) Tetrahedral Clusters. 2008 , 112, 11272-11279	223
985	Band Gap Tunable, Donor-Acceptor-Donor Charge-Transfer Heteroquinoid-Based Chromophores: Near Infrared Photoluminescence and Electroluminescence. 2008 , 20, 6208-6216	301
984	2D-3D transition of gold cluster anions resolved. 2008 , 77,	243
983	Simulating charge transport in tris(8-hydroxyquinoline) aluminium (Alq(3)). 2008 , 10, 1852-8	155
982	Importance of the basis set for the spin-state energetics of iron complexes. 2008 , 112, 6384-91	115
981	Theory of 1,3-dipolar cycloadditions: distortion/interaction and frontier molecular orbital models. 2008 , 130, 10187-98	627
980	Thermodynamic, kinetic, and computational study of heavier chalcogen (S, Se, and Te) terminal multiple bonds to molybdenum, carbon, and phosphorus. 2008 , 47, 2133-41	37
979	Surface complexation of U(VI) on goethite (FeOOH). 2008 , 72, 298-310	168
978	Mechanism of charge transport in self-organizing organic materials. 2008 , 27, 87-138	183
977	Carbon complexes as electronically and sterically tunable analogues of carbon monoxide in coordination chemistry. 2008 , 130, 16646-58	37
976	Electronic structure, absorption spectra, and hyperpolarisabilities of some novel push-pull zinc porphyrins. A DFT/TDDFT study. 2008 , 106, 147-160	11
975	Mapping the d-d excited-state manifolds of transition metal beta-diiminato-imido complexes. Comparison of density functional theory and CASPT2 energetics. 2008 , 112, 12792-8	18
974	Implementation of a density functional theory-based method for the calculation of the hyperfine A-tensor in periodic systems with the use of numerical and Slater type atomic orbitals: application to paramagnetic defects. 2008 , 112, 4521-6	9

- 973 Hydration of hydrogentungstate anions at different pH conditions: a car-parrinello molecular dynamics study. **2008**, 47, 7745-50 27
- 972 A re-evaluation of the two-step spin crossover in the trinuclear cation $[\text{Co}_3(\text{dipyridylamido})_4\text{Cl}_2]^+$. **2008**, 608-14 21
- 971 What can quantum chemistry tell us about Pa(V) hydration and hydrolysis?. **2008**, 32, 2080 16
- 970 Engineering delocalizing π electronic $[\text{CuI}_3(\beta\text{-OH})(\text{Epz})_3]^{2+}$ species into organometallic frameworks by Ag- π coordination. **2008**, 10, 1467 18
- 969 The donor ability of the chelated carbonate ligand: protonation and metallation of $[(\text{L})\text{Co}(\text{O}_2\text{CO})]^+$ complexes in aqueous solution. **2008**, 4984-92 10
- 968 State-resolved UV photofragmentation spectrum of the metal dication complex $[\text{Zn}(\text{pyridine})_4]^{2+}$. **2008**, 4153-5 13
- 967 Photoinduced bond cleavage in CH_3ReO_3 : excited state dynamics. **2008**, 32, 1904 6
- 966 Mercury-fluorine interactions: a matrix isolation investigation of $\text{Hg}\dots\text{F}_2$, HgF_2 and HgF_4 in argon matrices. **2008**, 10, 4594-605 14
- 965 6-Coordinate tungsten(VI) tris-*n*-isopropylanilide complexes: products of terminal oxo and nitrido transformations effected by main group electrophiles. **2008**, 4458-63 13
- 964 Protein-induced geometric constraints and charge transfer in bacteriochlorophyll-histidine complexes in LH2. **2008**, 10, 6971-8 18
- 963 Solvent dependence of the *g*-anisotropy in the ESR of cyanide-bridged mixed-valence complexes. **2008**, 6257-64 5
- 962 Tuning the thermodynamic stability of oxothiomolybdenum wheels: crystal structures, studies in solution and DFT calculations. **2008**, 4565-74 22
- 961 A computational study of the electronic structure, bonding, and spectral properties of tripodal tetraamine Co(III) carbonate complexes. **2008**, 2433-41 11
- 960 Electronic structure of the mononuclear Ag(II) complex $[\text{Ag}([\text{18}]\text{aneS}(4)\text{O}(2))]^{2+}$ ($[\text{18}]\text{aneS}(4)\text{O}(2) = 1,10\text{-dioxo-4,7,13,16-tetrathiacyclooctadecane}$). **2008**, 1305-7 13
- 959 $\text{Pi}^*\text{-pi}^*$ bonding interactions generated by halogen oxidation of zirconium(IV) redox-active ligand complexes. **2008**, 130, 4364-74 82
- 958 A tungsten(VI) nitride having a $\text{W}_2(\mu\text{-N})_2$ core. **2008**, 47, 1560-7 15
- 957 Cluster carbonyls of the $[\text{Re}(6)(\mu_3\text{-Se})(8)]^{2+}$ core: synthesis, structural characterization, and computational analysis. **2008**, 4247-53 16
- 956 The gas-phase structure of 1-selena-closo-dodecaborane(11), $1\text{-SeB}_{11}\text{H}_{11}$, determined by the concerted use of electron diffraction and computational methods. **2008**, 96-100 11

955	Investigating CN- cleavage by three-coordinate M[N(R)Ar] ₃ complexes. 2008 , 338-44	15
954	Isolation of the first Li/halogen phosphinidenoid transition-metal complex. 2008 , 2674-6	32
953	DFT survey of monoboron and diboron corroles: regio- and stereochemical preferences for a constrained, low-symmetry macrocycle. 2008 , 4464-73	22
952	A tetranuclear organorhenium(i) complex of the 2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-p-quinodimethane radical anion, TCNQF ⁻ (-). 2008 , 5749-53	14
951	Structural analysis of the Mn(IV)/Fe(III) cofactor of Chlamydia trachomatis ribonucleotide reductase by extended X-ray absorption fine structure spectroscopy and density functional theory calculations. 2008 , 130, 15022-7	51
950	A charge-dipole model for the static polarizability of nanostructures including aliphatic, olefinic, and aromatic systems. 2008 , 112, 1277-85	33
949	An Investigation of the Accuracy of Different DFT Functionals on the Water Exchange Reaction in Hydrated Uranyl(VI) in the Ground State and the First Excited State. 2008 , 4, 569-77	61
948	Oxidation of methanol by FeO ₂ ⁺ in water: DFT calculations in the gas phase and ab initio MD simulations in water solution. 2008 , 112, 1000-12	38
947	Sterically Demanding, Sulfonated, Triarylphosphines: Application to Palladium-Catalyzed Cross-Coupling, Steric and Electronic Properties, and Coordination Chemistry. 2008 , 27, 576-593	76
946	P ₂ addition to terminal phosphide M[triple bond]P triple bonds: a rational synthesis of cyclo-P ₃ complexes. 2008 , 130, 9524-35	58
945	Probing variable amine/amide ligation in Ni(II)N ₂ S ₂ complexes using sulfur K-edge and nickel L-edge X-ray absorption spectroscopies: implications for the active site of nickel superoxide dismutase. 2008 , 47, 2649-60	41
944	Role of s-p orbital mixing in the bonding and properties of second-period diatomic molecules. 2008 , 112, 2437-46	22
943	Bonding in Low-Coordinate Environments: Electronic Structure of Distorted Square-Planar Iron-Imido Complexes With Pincer-Type Ligands. 2008 , 4, 1576-84	3
942	Electrostatic and covalent contributions in the coordination bonds of transition metal complexes. 2008 , 112, 2469-76	4
941	ZEOBUILDER: A GUI toolkit for the construction of complex molecular structures on the nanoscale with building blocks. 2008 , 48, 1530-41	46
940	On the origin of circular dichroism in trigonal dihedral cobalt (III) complexes of unsaturated bidentate ligands. 2008 , 47, 4762-73	19
939	Tetra-2,3-pyrazinoporphyrazines with externally appended pyridine rings. 5. Synthesis, physicochemical and theoretical studies of a novel pentanuclear palladium(II) complex and related mononuclear species. 2008 , 47, 3903-19	36
938	Trinuclear Mo ₃ S ₇ clusters coordinated to dithiolate or diselenolate ligands and their use in the preparation of magnetic single component molecular conductors. 2008 , 47, 9400-9	46

- 937 Computational study of iron bis(dithiolene) complexes: redox non-innocent ligands and antiferromagnetic coupling. **2008**, 47, 10037-45 16
- 936 Modeling the vibronic spectra of transition metal complexes: the ligand-field spectrum of $[\text{PtCl}_4]^{2-}$. **2008**, 47, 4817-25 9
- 935 Phosphaalkenes as long-lived phosphorus cluster surface functional groups: intramolecular P=C addition to a niobium-supported P7 cage. **2008**, 47, 9363-71 22
- 934 A New Class of Efficient Electrocatalysts for the Reduction of Protons into Hydrogen Based on the $[\text{Mo}_2\text{O}_2\text{S}_2]^{2+}$ Building Block. **2008**, 112, 1109-1114 40
- 933 The role of H bonding and dipole-dipole interactions on the electrical polarizations and charge mobilities in linear arrays of urea, thiourea, and their derivatives. **2008**, 129, 204301 13
- 932 DFT analysis of g and ^{13}C hyperfine coupling tensors for model $\text{Ni}(\text{I})(\text{CO})(n)\text{L}(m)$ ($n = 1-4$, $\text{L} = \text{H}_2\text{O}$, OH^-) complexes epitomizing surface nickel(I) carbonyls. **2008**, 112, 12208-19 17
- 931 Electronic structure and metal-metal interactions in trinuclear face-shared $[\text{M}_3\text{X}_{12}]^{3-}$ ($\text{M} = \text{Mo}, \text{W}$; $\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$) systems. **2008**, 47, 3072-83 9
- 930 Vanadium(V) compounds with the bis-(hydroxylamino)-1,3,5-triazine ligand, H₂bihyat: synthetic, structural, and physical studies of $[\text{V}_2(\text{V})\text{O}_3(\text{bihyat})_2]$ and of the enhanced hydrolytic stability species $\text{cis-}[\text{V}(\text{V})\text{O}_2(\text{bihyat})]^-$. **2008**, 47, 11698-710 26
- 929 Effect of charge and composition on the structural fluxionality and stability of nine atom tin-bismuth Zintl analogues. **2008**, 47, 10953-8 21
- 928 Correlation between Density Functional Studies and Experimental Data of Three New 19-Electron Metal Sandwich Complexes Containing Amido, Ester, and Thioester Cyclopentadienyl Substituents. **2008**, 27, 3693-3700 4
- 927 Improved description of nuclear magnetic resonance chemical shielding constants using the M06-L meta-generalized-gradient-approximation density functional. **2008**, 112, 6794-9 80
- 926 Why does cyanide pretend to be a weak field ligand in $[\text{Cr}(\text{CN})_5]^{3-}$? **2008**, 47, 4413-20 13
- 925 Theoretical comparison of ketene dimerization in the gas and liquid phase. **2008**, 112, 3192-200 12
- 924 Structural, spectroscopic, and theoretical elucidation of a redox-active pincer-type ancillary applied in catalysis. **2008**, 130, 3676-82 134
- 923 Evaluation of the carbene hydride mechanism in the carbon-carbon bond formation process of alkane metathesis through a DFT study. **2008**, 130, 7984-7 31
- 922 Dendritic molecular switch: chiral folding and helicity inversion. **2008**, 130, 16812-22 52
- 921 Diastereoselective Synthesis of New Rhodium-Based Amphiphilic Polyol-Cp Systems. **2008**, 27, 945-954
- 920 Stabilization of an all-metal antiaromatic molecule (Al_4Li_4) using BH and C as caps. **2008**, 47, 2098-102 7

919	Structural and spectroscopic characterization of a charge-separated uranium benzophenone ketyl radical complex. 2008 , 130, 6567-76	94
918	Coordinating Tectons: Bipyridyl Terminated Allenylidene Complexes. 2008 , 27, 1716-1726	28
917	Mechanism of thioredoxin-catalyzed disulfide reduction. Activation of the buried thiol and role of the variable active-site residues. 2008 , 112, 2511-23	34
916	Quantifying the Donor/Acceptor Properties of Carbon Monoxide and Its Carbo-mer Using ELF Analysis. 2008 , 27, 5263-5272	10
915	Topological analysis of electron densities from Kohn-Sham and subsystem density functional theory. 2008 , 128, 044114	48
914	Understanding the stabilization of metal carbide endohedral fullerenes M ₂ C ₂ @C ₈₂ and related systems. 2008 , 112, 4550-5	82
913	The ketene intermediate in the photochemistry of ortho-nitrobenzaldehyde. 2008 , 10, 3872-82	44
912	Crystallographic, electrochemical, and electronic structure studies of the mononuclear complexes of Au(I)/(II)/(III) with [9]aneS ₂ O ([9]aneS ₂ O = 1-oxa-4,7-dithiacyclononane). 2008 , 47, 9919-29	29
911	Solution behavior and structural properties of Cu(I) complexes featuring m-terphenyl isocyanides. 2008 , 47, 9010-20	64
910	Carbon dioxide activation with sterically pressured mid- and high-valent uranium complexes. 2008 , 130, 12536-46	211
909	Probing the Mechanism of Carbon-Hydrogen Bond Activation by Photochemically Generated Hydridotris(pyrazolyl)borato Carbonyl Rhodium Complexes: New Experimental and Theoretical Investigations. 2008 , 27, 189-201	25
908	NMR solvent shifts of acetonitrile from frozen density embedding calculations. 2008 , 112, 2640-7	37
907	Further shortening of the C-C single bond in substituted tetrahedranyl tetrahedrane systems: an energy decomposition analysis. 2008 , 112, 12919-24	8
906	Effects of complex formation on vibrational circular dichroism spectra. 2008 , 112, 6978-91	71
905	Reversible redox-switchable second-order optical nonlinearity in polyoxometalate: a quantum chemical study of [PW ₁₁ O ₃₉ (ReN)] ⁿ⁻ (n = 3-7). 2008 , 47, 5245-52	43
904	Structural model studies for the peroxo intermediate P and the reaction pathway from P→Q of methane monooxygenase using broken-symmetry density functional calculations. 2008 , 47, 2975-86	52
903	Breathing orbital valence bond method in diffusion Monte Carlo: C-H bond dissociation of acetylene. 2008 , 112, 8964-9	10
902	Chemical reactivity of D _{3h} C ₇₈ (metallo)fullerene: regioselectivity changes induced by Sc ₃ N encapsulation. 2008 , 130, 6206-14	70

8901	Experimental and theoretical investigations of the thermodynamic stability of Ba-c(60) and K-C(60) compound clusters. 2008 , 2, 1000-14	11
900	Infrared spectra and electronic structures of agostic uranium methyldiene molecules. 2008 , 47, 1435-42	49
899	ENDOR characterization of a synthetic diiron hydrazido complex as a model for nitrogenase intermediates. 2008 , 130, 546-55	25
898	Toward a chemical mechanism of proton pumping by the B-type cytochrome c oxidases: application of density functional theory to cytochrome ba3 of <i>Thermus thermophilus</i> . 2008 , 130, 15002-21	60
897	The role of peripheral alkyl substituents: a theoretical study of substituted and unsubstituted uranyl isoamethyryn complexes. 2008 , 47, 805-11	20
896	Synthetic and Computational Studies of Thiocarbonyl/Organyl Coupling Reactions (1). 2008 , 27, 5548-5558	19
895	Why Do C1-Symmetric ansa-Zirconocene Catalysts Produce Lower Molecular Weight Polymers for Ethylene/Propylene Copolymerization than for Ethylene/Propylene Homopolymerization?. 2008 , 27, 2861-2867	19
894	Ligand-bound S = 1/2 FeMo-cofactor of nitrogenase: hyperfine interaction analysis and implication for the central ligand X identity. 2008 , 47, 6162-72	51
893	Circular dichroism of trigonal dihedral chromium(III) complexes: a theoretical study based on open-shell time-dependent density functional theory. 2008 , 47, 11656-68	25
892	Highly Efficient Pyridylpyrazole Ligands for the Heck Reaction. A Combined Experimental and Computational Study. 2008 , 27, 1084-1091	54
891	Photophysical behavior of open-shell first-row transition-metal octabutoxynaphthalocyanines: CoNc(OBu)8 and CuNc(OBu)8 as case studies. 2008 , 47, 4275-89	15
890	Valence electronic structure of benzo-2,1,3-chalcogenadiazoles studied by photoelectron spectroscopy and density functional theory. 2008 , 47, 6220-6	29
889	Mechanistic aspects of the reaction of Th ⁺ and Th ²⁺ with water in the gas phase. 2008 , 47, 2083-8	30
888	Synthesis and molecular and electronic structures of a series of Mo ₃ CoSe ₄ cluster complexes with three different metal electron populations. 2008 , 47, 3661-8	9
887	Synthesis and Characterization of Titanium Complexes Bearing Two β -Enaminoketonato Ligands with Electron-Withdrawing Groups and Their Behavior in Ethylene Polymerization. 2008 , 27, 3642-3653	33
886	Theoretical study on the considerable second-order nonlinear optical properties of naphthylimido-substituted hexamolybdates. 2008 , 112, 9919-23	43
885	Density Functional Theory Study of the TiH ₂ Interaction with a NaAlH ₄ Cluster. 2008 , 112, 15759-15764	20
884	Corrole as a binucleating ligand: preparation, molecular structure and density functional theory study of diboron corroles. 2008 , 130, 2888-9	38

883	Electrochemical oxidation of double-stranded polybisnorbornenes containing linearly aligned ferrocene linkers. 2008 , 4484-6	22
882	Electronic excitations and spectra in single-stranded DNA. 2008 , 130, 7607-12	68
881	Bond multiplicity in transition-metal complexes: applications of two-electron valence indices. 2008 , 112, 7256-63	192
880	Theoretical Investigations of the Effects of J-Aggregation on the Linear and Nonlinear Optical Properties of E-4-(4-Dimethylaminostyryl)-1-methylpyridinium [DAMS ⁺]. 2008 , 112, 1213-1226	20
879	Experimental and theoretical comparison of actinide and lanthanide bonding in M[N(EPR(2))(2)](3) complexes (M = U, Pu, La, Ce; E = S, Se, Te; R = Ph, iPr, H). 2008 , 47, 29-41	161
878	Anionic Roussin's red esters (RREs) syn-/anti-[Fe(μ -SEt)(NO) ₂] ₂ (-): the critical role of thiolate ligands in regulating the transformation of RREs into dinitrosyl iron complexes and the anionic RREs. 2008 , 47, 6040-50	68
877	Weak π -Olefin Bonding in Palladium and Platinum Allyl Cationic Complexes Containing Chiral Monodentate Ligands with η -Phenyl Methyl Amine Side Chains. 2008 , 27, 2949-2958	13
876	Synthesis and structural characterisation of an yttrium-alkyl-alkylidene. 2008 , 1747-9	85
875	Adsorption and reaction of 1-epoxy-3-butene on Pt(111): implications for heterogeneous catalysis of unsaturated oxygenates. 2008 , 130, 5507-14	22
874	A nickel hydride complex in the active site of methyl-coenzyme m reductase: implications for the catalytic cycle. 2008 , 130, 10907-20	64
873	A biomimetic approach to oxidized sites in the xanthine oxidoreductase family: synthesis and stereochemistry of tungsten(VI) analogue complexes. 2008 , 130, 12794-807	35
872	Hyperfine energy levels of alkali-metal dimers: Ground-state polar molecules in electric and magnetic fields. 2008 , 78,	85
871	A Solid-State NMR, X-ray Diffraction, and Ab Initio Investigation into the Structures of Novel Tantalum Oxyfluoride Clusters. 2008 , 20, 2205-2217	25
870	Influence of Cis and Trans Ligands in Platinum(II) Complexes on the Ability of the Platinum Center to Activate C-H Bonds. A Density Functional Theory Study. 2008 , 27, 1743-1749	30
869	Oxidative Addition of S-H Bonds to Dimethylplatinum(II) Complexes: Evidence for a Binuclear Mechanism. 2008 , 27, 6521-6530	47
868	Zero Field NMR of BiFeO ₃ . 2008 , 368, 131-136	
867	Effect of structural dynamics on charge transfer in DNA hairpins. 2008 , 130, 5157-66	140
866	STRUCTURE AND PROPERTIES OF PERFLUOROALKYLATED PHTHALOCYANINES: A THEORETICAL STUDY. 2008 , 07, 541-563	8

865	ASSESSMENT OF SOME RECENTLY DEVELOPED DENSITY FUNCTIONALS FOR CALCULATIONS ON IRON PORPHYRINS. 2008 , 07, 615-628	2
864	Cu ⁺ , Ag ⁺ and Na ⁺ Cationic Sites in ZSM-5 Interacting with Benzene: DFT Modeling. 2008 , 174, 709-712	5
863	Intercalation of daunomycin into stacked DNA base pairs. DFT study of an anticancer drug. 2008 , 26, 115-30	41
862	Theoretical characterization of titanyl phthalocyanine as a p-type organic semiconductor: short intermolecular pi-pi interactions yield large electronic couplings and hole transport bandwidths. 2008 , 128, 034701	88
861	Pressure effects on CrCl ₆ (3-) embedded in cubic Cs ₂ NaMCl ₆ (M=Sc,Y) lattices: study through periodic and cluster calculations. 2008 , 128, 144708	21
860	A subsystem density-functional theory approach for the quantum chemical treatment of proteins. 2008 , 128, 155102	79
859	Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism. II. Calculation of A terms. 2008 , 128, 234102	41
858	Simulation of vibrational energy transfer in two-dimensional infrared spectroscopy of amide I and amide II modes in solution. 2008 , 129, 055101	54
857	Orbital-free effective embedding potential at nuclear cusps. 2008 , 129, 074107	44
856	A revised electronic Hessian for approximate time-dependent density functional theory. 2008 , 129, 184114	62
855	Multifunctional metal-doped carbon nanocapsules. 2008 , 129, 234702	5
854	Efficient evaluation of the Fourier transform over products of Slater-type orbitals on different centers. 2008 , 41, 485205	6
853	Aromaticity in Heterocyclic and Inorganic Benzene Analogues. 2008 , 61, 209	25
852	Transition State Energy Decomposition Study of Acetate-Assisted and Internal Electrophilic Substitution C _{Br} Bond Activation by (acac-O,O) ₂ Ir(X) Complexes (X = CH ₃ COO, OH). 2008 , 27, 6440-6445	58
851	An electrostatic interaction model for frequency-dependent polarizability: methodology and applications to hydrocarbons and fullerenes. 2008 , 19, 025203	18
850	Electron-nucleus cusp correction and forces in quantum Monte Carlo. 2008 , 128, 114106	24
849	A theoretical study of the excited states of AmO ₂ n ⁺ , n=1,2,3. 2008 , 128, 164315	16
848	First-principles study of the mode-1 fracture of Fe-TiX interfaces (X=C,N). 2008 , 78,	3

847	Calculation of local excitations in large systems by embedding wave-function theory in density-functional theory. 2008 , 10, 5353-62	123
846	A relativistic density functional study of gaseous uranium tetrahalides. 2008 , 106, 1907-1912	5
845	Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism. III. Temperature-dependent magnetic circular dichroism induced by spin-orbit coupling. 2008 , 129, 104105	29
844	Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism: calculation of B terms. 2008 , 128, 144105	40
843	Pseudo-Jahn-Teller origin of the low barrier hydrogen bond in N(2)H(7) (+). 2008 , 129, 124313	15
842	Microscopic origin of the different colors displayed by MgAl ₂ O ₄ :Cr ³⁺ and emerald. 2008 , 78,	15
841	Electron Transfer from Hydrogen Molecule to Au(111) During Dissociative Adsorption: A First-Principles Study. 2008 , 77, 054705	7
840	Atomistic and electronic structure of bimetallic cobalt/rhenium clusters from density functional theory calculations. 2008 , 128, 084712	8
839	X-Ray Absorption Spectroscopic Study on Polymerization of Aqueous Aluminate by DV-X α Molecular-Orbital Method. 2008 , 54, 193-207	1
838	Quantum Molecular Biological Methods Using Density Functional Theory. 2009 ,	1
837	. 2009 ,	6
836	Electronic structure of the azide group in 3 cent-azido-3 cent-deoxythymidine (AZT) compared to small azide compounds. 2009 , 14, 2656-68	33
835	Cyanide complexes of Ti(IV): a computational study. 2009 , 131, 094507	3
834	On the calculation of general response properties in subsystem density functional theory. 2009 , 131, 084104	41
833	On the Kohn-Sham density response in a localized basis set. 2009 , 131, 044103	12
832	Density functional estimations of Heisenberg exchange constants in oligonuclear magnetic compounds: Assessment of density functional theory versus ab initio. 2009 , 131, 224316	12
831	Color shift in Al ₂ O ₃ ?xCr ₂ O ₃ solid solutions and the electroneutrality principle. 2009 , 79,	7
830	Bis(cyclopentadienyl)dihydrido Mo and W complexes as Lewis bases [A computational study about their adducts with BX ₃ (X = F, Cl) and Al(CH ₃) ₃ . 2009 , 87, 1406-1414	8

829	Combining relativistic quantum-chemistry theories and electron-momentum spectroscopy to study valence-electron structures of molecules. 2009 , 80,	15
828	Nonmetallic electronegativity equalization and point-dipole interaction model including exchange interactions for molecular dipole moments and polarizabilities. 2009 , 131, 044101	24
827	A new all-round density functional based on spin states and S(N)2 barriers. 2009 , 131, 094103	104
826	Intramolecular interactions of L-phenylalanine revealed by inner shell chemical shift. 2009 , 131, 044321	24
825	Computational Methods: Transition Metal Clusters. 2009 ,	
824	Potential antitumor gold drugs:DFT and XANES studies of local atomic and electronic structure. 2009 , 190, 012210	3
823	A charge-dipole interaction model for the frequency-dependent polarizability of silver clusters. 2009 , 20, 195204	16
822	Analysis of one-bond Se-Se nuclear couplings in diselenides and 1,2-diselenoles on the basis of molecular orbital theory: torsional angular dependence, electron density influence, and origin in $j(\text{Se}, \text{Se})$. 2009 , 381925	3
821	Solvent-resistant structures of base-free lithium and potassium allyl complexes, $\text{M}[(\text{SiMe}_3)_n\text{C}_3\text{H}_5-n]$ ($\text{M} = \text{Li}, n= 3$; $\text{M} = \text{K}, n= 2$). 2009 , 8, 225-235	14
820	The electronic structure of the primary electron donor of reaction centers of purple bacteria at atomic resolution as observed by photo-CIDNP ^{13}C NMR. 2009 , 106, 22281-6	68
819	Electronic structure and TDDFT optical absorption spectra of silver nanorods. 2009 , 113, 4445-50	89
818	How silylene defects at (100) Si surfaces can account for the anomalous features observed via x-ray photoelectron spectroscopy. 2009 , 130, 184702	6
817	Observation of Zr^{2+} , Cd^{2+} , Hf^{2+} , W^{2+} , and Pt^{2+} in the gas phase. 2009 , 130, 144312	13
816	Virial theorem in the Kohn-Sham density-functional theory formalism: accurate calculation of the atomic quantum theory of atoms in molecules energies. 2009 , 131, 021101	37
815	All-electron CI calculations of 3d transition-metal L(2,3) XANES using zeroth-order regular approximation for relativistic effects. 2009 , 21, 104209	4
814	Counterintuitive assignment of the lines observed by x-ray photoelectron spectroscopy at the hydrogen-terminated (1 0 0) surface of silicon. 2009 , 42, 225301	1
813	Surface-enhanced vibrational raman optical activity: a time-dependent density functional theory approach. 2009 , 113, 4437-44	31
812	Divalent carbon(0) compounds. 2009 , 81, 597-614	183

811	The irreducible bundle: further structure in the kinetic energy distribution. 2009 , 130, 204108	21
810	Relativistic hybrid density functional calculations of indirect nuclear spin-spin coupling tensors ρ Comparison with experiment for diatomic alkali metal halides., 2009 , 87, 927-941	23
809	Atoms in boxes: From confined atoms to electron-atom scattering. 2009 , 131, 104108	22
808	Fluctuations at the base pair level effecting charge transfer in DNA. 2009 , 113, 3955-62	19
807	Activation of ethane C-H and C-C bonds by gas phase Th ⁺ and U ⁺ : a theoretical study. 2009 , 113, 14699-705	22
806	Magnetic anisotropy and molecular assembling in d complex cation-complex anion type coordination compounds. 2009 , 11, 760-765	8
805	Creating a GUI for Zori, a Quantum Monte Carlo Program. 2009 , 11, 41-47	4
804	Spin Relaxation in Ru-Chromophore-Linked Azine/Diquat Radical Pairs. 205-220	
803	References. 2009 , 615-656	
802	Customized Electronic Coupling in Self-Assembled Donor-Acceptor Nanostructures. 2009 , 19, 3567-3573	50
801	Phosphinidene Addition to Conjugated Allenes. 2009 , 351, 1132-1138	4
800	Trimetallic Nitride Endohedral Fullerenes: Experimental and Theoretical Evidence for the M ₃ N ₆ @C _{2n} model. 2009 , 121, 1453-1456	7
799	A Ditopic Ion-Pair Receptor Based on Stacked Nucleobase Quartets. 2009 , 121, 3335-3337	23
798	Lithium-Ammoniak-Lösungen: eine molekulare Betrachtung. 2009 , 121, 8344-8381	8
797	Absolute configuration of eremophilane sesquiterpenes from <i>Petasites hybridus</i> : comparison of experimental and calculated circular dichroism spectra. 2010 , 22, 308-19	21
796	New applications and challenges for computational ROA spectroscopy. 2009 , 21 Suppl 1, E98-104	36
795	A VCD robust mode analysis of induced chirality: the case of pulegone in chloroform. 2009 , 21 Suppl 1, E287-97	59
794	Divergent electronic structures of isoelectronic metaloclusters: tungsten(II) halides and rhenium(III) chalcogenide halides. 2009 , 15, 2581-93	32

- 793 A comparison of N₂ cleavage in Schrock's Mo[N₃N] and Laplaza-Cummins' Mo[N(R)Ar]₃ systems. **2009**, 15, 646-55 15
- 792 Influence of endohedral confinement on the electronic interaction between He atoms: a He₂@C₂₀H₂₀ case study. **2009**, 15, 1985-90 96
- 791 Rare tautomers of 1-methyluracil and 1-methylthymine: tuning relative stabilities through coordination to PtII complexes. **2009**, 15, 209-18 29
- 790 Metal nitride cluster fullerene M₃N@C₈₀ (M=Y, Sc) based dyads: synthesis, and electrochemical, theoretical and photophysical studies. **2009**, 15, 864-77 92
- 789 Dihydrogen bonding: donor-acceptor bonding (AH...HX) versus the H₂ molecule (A-H₂-X). **2009**, 15, 5814-22 31
- 788 The steric nature of the bite angle. **2009**, 15, 6112-5 54
- 787 Dinitrogen activation by Fryzuk's [Nb(P(2)N(2))] complex and comparison with the Laplaza-Cummins [Mo{N(R)Ar}(3)] and Schrock [Mo(N(3)N)] systems. **2009**, 15, 11373-83 9
- 786 Electronic structure and redox properties of metal nitride endohedral fullerenes M(3)N@C(2n) (M=Sc, Y, La, and Gd; 2n=80, 84, 88, 92, 96). **2009**, 15, 10997-1009 75
- 785 Transition-metal complexes [(PMe(3))(2)Cl(2)M(E)] and [(PMe(3))(2)(CO)(2)M(E)] with naked group 14 atoms (E=C-Sn) as ligands; part 1: parent compounds. **2009**, 15, 8807-16 21
- 784 Transition-metal complexes [(PMe(3))(2)Cl(2)M(E)] and [(PMe(3))(2)(CO)(2)M(E)] with naked group 14 atoms (E=C-Sn) as ligands; part 2: complexation with W(CO)(5). **2009**, 15, 8817-24 15
- 783 Ligand strain and the nature of spin crossover in binuclear complexes: two-step spin crossover in a 4,4'-bipyridine-bridged iron(II) complex [{Fe(dpia)(NCS)(2)}₂(4,4'-bpy)] (dpia = di(2-picoly)amine; 4,4'-bpy = 4,4'-bipyridine). **2009**, 15, 10070-82 48
- 782 Reactivity and regioselectivity of noble gas endohedral fullerenes Ng@C(60) and Ng(2)@C(60) (Ng=He-Xe). **2009**, 15, 13111-23 42
- 781 The stereospecific ligand exchange at a pseudo-benzylic T-4 iridium centre in planar-chiral cycloiridium (eta(6)-arene)tricarbonylchromium complexes. **2009**, 15, 10830-42 14
- 780 Resolving conformation dichotomy for Y- and T-shaped three-coordinate Ni(I) carbonyl complexes with relativistic DFT analysis of EPR fingerprints. **2009**, 15, 11802-7 11
- 779 Double group transfer reactions: role of activation strain and aromaticity in reaction barriers. **2009**, 15, 13022-32 72
- 778 Synthesis, structure and reactivity of stable homoleptic gold(I) alkene cations. **2009**, 15, 12196-200 42
- 777 Understanding chemical shielding tensors using group theory, MO analysis, and modern density-functional theory. **2009**, 34A, 91-123 89
- 776 Magnetic anisotropy in a family of experimentally synthesized and theoretically modeled M'6M8(CN₂₄) systems. **2009**, 10, 2496-502 1

- 775 Homolytic versus heterolytic dissociation of alkalimetal halides: the effect of microsolvation. **2009**, 10, 2955-65 13
- 774 Subsystem-based theoretical spectroscopy of biomolecules and biomolecular assemblies. **2009**, 10, 3148-73 82
- 773 Carbon-Silicon Bond Activation by [Pd(ItBu)₂] The Molecular Structures of [Pd(Me₃Si)(ItBu)(H)]₂ and [Pd(CH₂ItBu)₂]. **2009**, 2009, 1844-1850 15
- 772 The Nature of the Metal-Carbene Bond in Normal and Abnormal Pyridylidene, Quinolyliidene and Isoquinolyliidene Complexes. **2009**, 2009, 1892-1904 31
- 771 A Quantum Chemical Study of the Structure, Bonding Characteristics and Nonlinear Optical Properties of Aryloxido and Salicylaldehyde Derivatives of [XW₅O₁₈]₃ (X = Zr or Ti). **2009**, 2009, 2529-2535 23
- 770 Experimental and Theoretical Evidence of H₂ Interactions in Supramolecular Assemblies Based on TTF-CH=CH-Py Ligands Tethered to Mo₆Cl₈ Octahedral Molybdenum Halide Cluster Cores. **2009**, 2009, 2153-2161 39
- 769 How To Tune Acid-Induced Ring Enlargement Reactions The Strange Case of 2H-Azaphosphirene Complexes and Its Surprising Dichotomy. **2009**, 2009, 2062-2065 12
- 768 PECD study of a single-conformer molecule: a critical comparison of experiment and theory.. **2022**, 0
- 767 Decomposition Mechanism of Isoprenoid Hydrocarbon -Menthane in the Presence of Pt@FGS Nanoparticles: A ReaxFF-MD Study.. **2022**,
- 766 12-Membered Ring Carbides with Stabilization of Actinide Atoms.. **2022**,
- 765 Chiral Emissive Lanthanide Complexes from Enantiopure [6]Helicene-bis(pyrazolyl)-pyridine Ligands. 0
- 764 Hole Tetrel Bonds Lewis Acid Properties of Metallylenes. **2022**, 12, 112 1
- 763 Experimental and Simulation Studies on Nonwoven Polypropylene-Nitrile Rubber Blend: Recycling of Medical Face Masks to an Engineering Product.. **2022**, 7, 4791-4803 1
- 762 Stereoelectronic interactions: A booster for J transmission.. **2022**,
- 761 Corrosion inhibition studies of ferrocenyl Schiff bases in a mild acidic medium through experimental methods and DFT calculations. 0
- 760 Insight into the Adsorption Structure of TIPS-Pentacene on Noble Metal Surfaces. **2022**, 126, 2689-2698
- 759 Square tetravalent chalcogen bonds in dimeric aggregates: a joint crystallographic survey and theoretical study. **2022**, 24, 975-986 1
- 758 Development and application of ReaxFF methodology for understanding the chemical dynamics of metal carbonates in aqueous solutions.. **2022**, 2

757	Carbene-Metal Complexes As Molecular Scaffolds for Construction of through-Space Thermally Activated Delayed Fluorescence Emitters.. 2022 ,	3
756	Borophene as a rising star in materials chemistry: Synthesis, properties and applications in analytical science and energy devices.	2
755	Reactivity of the superhalogen/superalkali ion encapsulating C fullerenes. 2021 ,	1
754	Estimations of Fe-N interaction energies of iron(0)-dicarbene and its reduced analogue by EDA-NOCV analyses: crucial steps in dinitrogen activation under mild conditions.. 2022 , 12, 3465-3475	0
753	Cu(II), Mn(II) and Zn(II) complexes of hydrazones with a quaternary ammonium moiety: synthesis, experimental and theoretical characterization and cytotoxic activity. 2021 ,	3
752	Ferrocene functionalized enantiomerically pure Schiff bases and their Zn(ii) and Pd(ii) complexes: a spectroscopic, crystallographic, electrochemical and computational investigation.	0
751	Efficient Fluorescent Detection of Mercuric Ions Based on 2-Thienylbenzimidazole/Cucurbit[7]uril Complexes. 2022 , 02,	
750	Theoretical Insights on Improving Amidoxime Selectivity for Potential Uranium Extraction from Seawater.. 2022 ,	0
749	New rhodium(II)-ED3AP-complex: Crystal structure, characterization and computational chemistry. 2022 , 3-3	
748	New Hypercoordinating Organostannanes for the Modular Functionalization of Mono- and Polystannanes: Synthetic and Computational Studies**.	
747	The Magnetic Behaviour of CoTPP Supported on Coinage Metal Surfaces in the Presence of Small Molecules: A Molecular Cluster Study of the Surface -Effect.. 2022 , 12,	0
746	Bonding and stability of dinitrogen-bonded donor base-stabilized Si(0)/Ge(0) species [(cAAC-Si/Ge)(N)] ₃ : EDA-NOCV analysis.. 2022 , 12, 4081-4093	
745	Long-chain mercury carboxylates relevant to saponification in oil and tempera paintings: XRPD and ssNMR complementary study of their crystal structures.. 2022 ,	0
744	Computational Investigation of the Metal and Ligand Substitution Effects on the Structure and Electronic States of the Phosphoramidate Tetramer Complexes of Cu(I), Ni(I), Co(I), and Fe(I).. 2022 , 61, 1471-1485	0
743	Exceptional Manganese(II) Stability and Manganese(II) / Zinc(II) Selectivity with Rigid Polydentate Ligands.. 2022 ,	3
742	B-DNA Structure and Stability: The Role of Nucleotide Composition and Order.. 2022 , e202100231	
741	Nature of hydride and halide encapsulation in Ag cages: insights from the structure and interaction energy of [Ag(X){SP(OPr)}] (X = H, F, Cl, Br, I) from relativistic DFT calculations.. 2021 , 24, 452-458	
740	Near-infrared emitting copper(I) complexes with a pyrazolylpyrimidine ligand: exploring relaxation pathways.. 2022 ,	1

739	The effects of polar solvents on structural, electronic, and optical properties of organic dyes.	
738	The Second Excited Triplet-State Facilitates TADF and Triplet-Triplet Annihilation Photon Upconversion via a Thermally Activated Reverse Internal Conversion. 2102275	2
737	Stabilisation of Li(0)-Li(0) bond by normal and mesoionic carbenes and electride characteristics of the complexes.	1
736	Photoelectron Circular Dichroism as a Probe of Chiral Hydrocarbons. 2022, 4, 31-41	1
735	Modelling the physical properties of environmentally friendly optical magnetic switches: DFT and TD-DFT. 2022, 355-384	2
734	Spin Orbit Coupling in Orthogonal Charge Transfer States: (TD-)DFT of Pyrene-Dimethylaniline.. 2022, 27,	2
733	Bifunctional Iminophosphorane-Catalyzed Enantioselective Sulfa-Michael Addition to Unactivated α -Unsaturated Amides.. 2022,	3
732	Path-dependency of energy decomposition analysis & the elusive nature of bonding.. 2022,	4
731	Near-infrared circular dichroism of the ytterbium DOTMA complex: an investigation.. 2022,	0
730	Covalency between the uranyl ion and dithiophosphate by sulfur K-edge X-ray absorption spectroscopy and density functional theory.. 2022, 29, 11-20	0
729	What Singles out Alumanyl Anions? A Comparative Computational Study of the Carbon Dioxide Insertion Reaction in Gold-Alumanyl, -Gallyl, and -Indyl Complexes.. 2022,	3
728	C(sp ⁿ)-X (n = 1-3) Bond Activation by Palladium.. 2021,	0
727	Evolution of plasmon-like excited states in silver nanowires and nanorods.. 2022, 156, 074301	2
726	Dinitrogen Binding Relevant to FeMoco of Nitrogenase: Clear Visualization of σ -Donation and π -Backdonation from Deformation Electron Densities around Carbon/Silicon-Iron Site.	0
725	Formation of twelve-fold iodine coordination at high pressure.. 2022, 13, 412	4
724	How Polytetrafluoroethylene Lubricates Iron: An Atomistic View by Reactive Molecular Dynamics.. 2022,	1
723	Photophysical Properties of Benzophenone-Based TADF Emitters in Relation to Their Molecular Structure.. 2022,	2
722	Highly efficient wideband solar energy conversion employing singlet-triplet transitions.	0

- 721 Theoretical Study of the Geometry of Dibenzoazepine Analogues.. **2022**, 27,
- 720 Methods for Interpreting the Partitioning and Fate of Petroleum Hydrocarbons in a Sea Ice Environment.. **2022**, ○
- 719 Metalloligand-based coordination polymer embedding the nitrosyl ruthenium complex for photoactive materials with bound nitric oxide.. **2022**,
- 718 Highly stable actinide(III) complexes supported by doubly aromatic ligands.. **2022**, ○
- 717 Insight Into the Stability and Electronic and Optical Properties of N-Heterocyclic Carbene Analogues of Halogen/Phosphine-Protected Au Superatomic Clusters.. **2022**, ○
- 716 Probing the Lewis Acidity of Boronic Acids through Interactions with Arene Substituents.. **2021**, ○
- 715 Infrared spectroscopic signature of the structural diversity of the water heptamer. **2022**, 3, 100748 3
- 714 Deciphering the Role of Noncovalent Interactions in the Conformations of Dibenzo-1,5-dichalcogenocines.. **2022**, e202100518 ○
- 713 Do nitrate ions preferentially bind to Ln/An ion in nuclear waste treatment? [Answers from DFT calculations. **2022**, 215, 115691 2
- 712 Near-Infrared fluorescent unsymmetrical aza-BODIPYs: Synthesis, photophysics and TD-DFT calculations.. **2022**, 271, 120898 ○
- 711 Tetranuclear Cu(II) complex with [2+4] Cu₄O₄ cubane based core framework derived from 2-[[2-(1-hydroxy-ethyl)-phenylimino]-methyl]-6-methoxy-phenol: Quantifying conventional and unconventional interactions and QTAIM analysis. **2022**, 1254, 132396 3
- 710 Atomic-scale probing of defect-assisted Ga intercalation through graphene using ReaxFF molecular dynamics simulations. **2022**, 190, 276-290 3
- 709 Investigation of bond orientational order of new Schiff base and theoretical study on Covid-19 activity: A molecular dynamics based on DFT and molecular docking analysis. **2022**, 792, 139390 ○
- 708 A bowl-shaped phenoxido-bridged binuclear zinc complex: Experimental and theoretical studies. **2022**, 534, 120807 ○
- 707 Influence of fluorosubstitution on physical properties of the smectogenic chiral ester. **2022**, 150, 111756 1
- 706 -Block metal complexes with bis(pyrazol-1-yl)acetato ligands.. **2022**, ○
- 705 Insights into the Factors Controlling the H_β Bond Cleavage Reactions by Five-Membered G13/P (G13 = Group 13 Element) and B/G15 (G15 = Group 15 Element) Frustrated Lewis Pairs. ○
- 704 Imidazo[1,5-a]pyridine-based derivatives as highly fluorescent dyes. **2022**, 120849 1

703	Stabilization of Interstellar CSi Species by Donor Base Ligands: L-CSi-L; L = cAAC, NHC, and PMe.. 2022,			1
702	Mössbauer Property Calculations on Fe ₃₃ H ₂₀ Cu ₂ + Dinuclear Center Models of the Resting Oxidized as-Isolated Cytochrome c Oxidase.. 2022,			
701	Rational design of iron catalysts for C-X bond activation.. <i>Journal of Computational Chemistry</i> , 2022,	3.5		0
700	A terminal neptunium(V)-mono(oxo) complex.. 2022,			2
699	Formation and infrared spectroscopic characterization of carbon suboxide complexes TM- η -C O and the inserted ketylidene complexes OCTMCCO (TM=Cu, Ag, Au) in solid neon.. <i>Journal of Computational Chemistry</i> , 2022,	3.5		0
698	A strategy toward therapeutic improvement of electric field-sensitive gemcitabine prodrugs in 2D metal-organic frameworks in view of their structure and interactions. 2022, 109281			
697	Ultrafast Solution-Phase Photophysical and Photochemical Dynamics of Hexaiodobismuthate(III), the Heart of Bismuth Halide Perovskite Solar Cells.. 2022,			0
696	Hydrogen Bonds with Fluorine in Ligand-Protein Complexes-the PDB Analysis and Energy Calculations.. 2022, 27,			3
695	All-Electron BSE@ Method for -Edge Core Electron Excitation Energies.. 2022,			1
694	EDA-NOCV Analysis of Donor-Base-Stabilized Elusive Monomeric Aluminum Phosphides [(L)P-Al(L'); L, L' = cAAC, NHC, PMe].. 2022, 7, 5730-5738			0
693	Photoionization Observables from Multi-Reference Dyson Orbitals Coupled to B-Spline DFT and TD-DFT Continuum.. 2022, 27,			1
692	Study on crystallization process of SiO ₂ based SiO ₂ -Li ₂ O nano-wire glass ceramic: A molecular dynamics simulation based on SCC-DFTB calculations.			
691	Synthesis and Computational Characterization of Organic UV-Dyes for Cosensitization of Transparent Dye-Sensitized Solar Cells. 2021, 26,			1
690	How Solvation Influences the S ₂ versus E ₂ Competition.. 2021,			3
689	NMR Response of the Tetrel Bond Donor. 2022, 126, 851-865			2
688	Investigation on micro-mechanism of palm oil as natural ester insulating oil for overheating thermal fault analysis of transformers.			4
687	Quasi-aromatic MBius chelates of Cadmium(II) nitrite and/or nitrate..			
686	Density Functional Theory for Transition Metal Catalysis. 2022,			

685	Preorganization of N,O-hybrid phosphine oxide chelators for effective extraction of trivalent Am/Eu ions: a computational study. 2022 , 46, 5761-5770	1
684	Multi-electron excitation contributions towards primary and satellite states in the photoelectron spectrum.. 2022 ,	2
683	Transition Structures, Reaction Paths, and Kinetics: Methods and Applications in Catalysis. 2022 ,	
682	Energy decomposition analysis of cationic carbene analogues with group 13 and 16 elements as a central atom: a comparative study.. 2022 ,	1
681	Looking at platinum carbonyl nanoclusters as .. 2022 ,	1
680	Vibrationally resolved photoelectron angular distributions of ammonia.. 2022 ,	1
679	Superatomic Salts with Controlled Ionicity.	
678	Unraveling differences in aluminyl and carbene coordination chemistry: bonding in gold complexes and reactivity with carbon dioxide.	2
677	Can a Wanzlick-like equilibrium exist between dicoordinate borylenes and diborenes?.	1
676	The effect of different energy portions on the 2D/3D stability swapping for 13-atom metal clusters.. 2022 ,	0
675	Parameter free evaluation of S ₂ reaction rates for halide substitution in halomethane.. 2022 ,	
674	Catalytic properties of the ferryl ion in the solid state: a computational review.	
673	Environment Effects on X-Ray Absorption Spectra With Quantum Embedded Real-Time Time-Dependent Density Functional Theory Approaches.. 2022 , 10, 823246	0
672	Strength and Nature of Host-Guest Interactions in Metal-Organic Frameworks from a Quantum-Chemical Perspective.. 2022 ,	0
671	Influence of Hydrogen Bonds and π Interactions on the Fluorescence of Crystalline (N-Alkylpyridyl)enamino-pyrrolo[2,3-b]quinoxalin-2-one Derivatives. 2022 , 22, 1571-1582	1
670	An ETS-NOCV-based computational strategies for the characterization of concerted transition states involving CO.. <i>Journal of Computational Chemistry</i> , 2022 ,	3-5 1
669	Analysis of Weak Interactions in Crystals of Fenamic Acids π thacridine Complexes. 2022 , 22, 1554-1570	
668	First principles study of layered silicon carbide as anode in lithium ion battery.	0

667	Elucidating Sulfide Activation Mode in Metal-Catalyzed Sulfoxidation Reactivity.. 2022 ,		0
666	Polycyclic Aromatic Hydrocarbons (PAHs) in Interstellar Ices: A Computational Study into How the Ice Matrix Influences the Ionic State of PAH Photoproducts.. 2022 , 6, 766-774		0
665	The BCL Method for DSSC: Basis and Applications. 2022 , 12, 2358		
664	Benchmark Study on the Calculation of Sn NMR Chemical Shifts.. 2022 , 61, 3903-3917		1
663	Understanding the catalysis by bis-selenonium cations as bidentate chalcogen bond donors. 2022 , 1, 100008		1
662	Bonding situation in isolable silver(I) carbonyl complexes of the Scorpionates.. <i>Journal of Computational Chemistry</i> , 2022 ,	3.5	1
661	Systematic QM Region Construction in QM/MM Calculations Based on Uncertainty Quantification.. 2022 ,		2
660	Effects of π -conjugation on the charge-transport properties of hole-transporting materials featuring diphenylamine- π -quinacridone for perovskite solar cells: A theoretical study.		
659	Scattering effects from neighboring atoms in core-level WSe ₂ photoemission. 2022 , 105,		
658	Evolution of Vibrational Spectra in the Manganese-Silicon Clusters MnSi _n , n = 10, 12, and 13, and Cationic [MnSi _n] ⁺ .. 2022 ,		1
657	Unoccupied electronic structure of actinide dioxides. 2022 , 105,		3
656	Carbonate complexation enhances hydrothermal transport of rare earth elements in alkaline fluids.. 2022 , 13, 1456		3
655	Inverse Design of Nanoclusters for Light-Controlled CO-HCOOH Interconversion.. 2022 , 2523-2532		0
654	CSiGaAl and CGeGaAl having planar tetracoordinate carbon atoms in their global minimum energy structures.. <i>Journal of Computational Chemistry</i> , 2022 ,	3.5	4
653	Free and open source software for computational chemistry education.		1
652	Phosphorescence and Photophysical Parameters of Porphycene in Cryogenic Matrices. 2022 , 2, 217-224		
651	Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins. 2022 , 5,		0
650	The Unusual Structural Behavior of Heteroleptic Aryl Copper(I) Thiolato Molecules: Cis vs Trans Structures and London Dispersion Effects. 2022 , 41, 794-801		0

649	Influence of conventional hydrogen bonds in the intercalation of phenanthroline derivatives with DNA: The important role of the sugar and phosphate backbone.. <i>Journal of Computational Chemistry</i> , 2022 ,	3.5	1
648	Discrimination of Excited States of Acetylacetone through Theoretical Molecular-Frame Photoelectron Angular Distributions.. 2022 , 27,		
647	Terminal end-on coordination of dinitrogen versus isoelectronic CO: A comparison using the charge displacement analysis.. <i>Journal of Computational Chemistry</i> , 2022 ,	3.5	0
646	Periodic DFTB for Supported Clusters: Implementation and Application on Benzene Dimers Deposited on Graphene. 2022 , 10, 39		1
645	Bonding analysis of the C2 precursor Me3E(C2I(Ph)FBF3 (E = C, Si, Ge). 2022 ,		
644	Doped TiO2 slabs for water splitting: a DFT study. 2022 ,		
643	Double pentavalent pnictogen-bonding interactions in the homodimers of pnictogenoxide species: CSD search and theoretical study. 2022 , 1209, 113636		2
642	Quantitative assessment of ligand substituent effects on σ and π contributions to Fe-N bonds in spin crossover FeII complexes.. 2022 ,		
641	Halogen Bonds Exist between Noncovalent Ligands and Natural Nucleic Acids.. 2022 ,		1
640	Synthesis and Characterization of Ternary Clusters Containing the [As] Anion, [MM'As] (M = Nb or Ta; M' = Cu or Ag).. 2022 ,		2
639	Design of Active Defects in Semiconductors: 3D Electron Diffraction Revealed Novel Organometallic Lead Bromide Phases Containing Ferrocene as Redox Switches. 2201126		1
638	Vibronic Coupling in Spherically Encapsulated, Diatomic Molecules: Prediction of a Renner-Teller-like Effect for Endofullerenes.. 2022 ,		1
637	The Role of Hydrogen Bonds in Interactions between [PdCl] Dianions in Crystal.. 2022 , 27,		2
636	Probing the Potential of Hitherto Unexplored Base-Stabilized Borylenes in Dinitrogen Binding.. 2022 ,		0
635	Dinaphthotetrathienoacenes: Synthesis, Characterization, and Applications in Organic Field-Effect Transistors.. 2022 , e2105674		3
634	How the Chalcogen Atom Size Dictates the Hydrogen-Bond Donor Capability of Carboxamides, Thioamides, and Selenoamides.. 2022 ,		0
633	Relativistic Spin-Orbit Electronegativity and the Chemical Bond between a Heavy Atom and a Light Atom.. 2022 ,		1
632	Enhancement of the Water Affinity of Histidine by Zinc and Copper Ions.. 2022 , 23,		1

- 631 Suitability of Carbazoyl Hauser and Turbo-Hauser Bases as Magnesium-Based Electrolytes. 0
- 630 Physicochemical Properties and Atomic-Scale Interactions in Polyaniline (Emeraldine Base)/Starch Bio-Based Composites: Experimental and Computational Investigations.. **2022**, 14, 0
- 629 Indenyl and Allyl Palladate Complexes Bearing N-Heterocyclic Carbene Ligands: an Easily Accessible Class of New Anticancer Drug Candidates. 0
- 628 Quantum chemical studies of the electronic structures of anti-tumor agents: AuIII+ (LEPorphine, tetraphenylporphyrin). **2022**, 1211, 113685
- 627 Cluster approach to scattering in MoS2 photoemission. **2022**, 557, 111476
- 626 DFT, MD simulations and experimental analysis of adsorptive complexation and isotope separation of gadolinium ion with macrocyclic crown ether embedded polymeric resin. **2022**, 289, 120709 0
- 625 Theoretical study on the extraction behaviors of MoO22+ with organophosphorous extractants. **2022**, 355, 118969 1
- 624 Structure-sensitive marker bands of metallocorroles: A resonance Raman study of manganese and gold corrole derivatives.. **2022**, 231, 111783 1
- 623 Pyridyl anchored indolium dyes for the p-type dye sensitized solar cell. **2022**, 202, 110244 1
- 622 Donation and back-donation in cis- and trans-[(η -C5H5)Fe(η -CO)(ECO)]2 tautomers: Which relative is more generous? An ETS-NOCV bond analysis. **2022**, 536, 120897
- 621 Electronic structure of platinum(II)-phosphine-tin(II)trihalide complexes. **2022**, 1260, 132743
- 620 A DFT study of silver decorated bismuthene for gas sensing properties and effect of humidity. **2022**, 145, 106635 1
- 619 Investigating electronic properties and electron transport in molecular junctions of new model CoNiO2 doped with Li and Na via extended tight-binding based on DFT computational method. **2022**, 318, 132179
- 618 Investigation of green solvents for the extraction of phenol and natural alkaloids: Solvent and extractant selection. **2022**, 442, 136054 1
- 617 First Principal Simulation of Palladium Nanocatalysts Surfaces. **2021**, 15, 1270-1277
- 616 Combined ReaxFF and Ab Initio MD Simulations of Brown Coal Oxidation and Coal-Water Interactions.. **2021**, 24, 0
- 615 CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. **2021**, 7
- 614 Quantum-chemical approaches in the study of fullerene and its derivatives by the example of the most typical cycloaddition reactions: A review. **2022**, 122, 1

613	Unsaturated Sulfur Crown Ethers Can Extract Mercury(II) and Show Promise for Future Copernicium(II) Studies: A Combined Experimental and Computational Study.. 2021 ,	0
612	Pyrene Core-based Dopant-free Hole Transporting Materials for Perovskite Solar Cells: A Theoretical Design and Experimental Verification. 2022 , 126, 160-168	2
611	Iridium(VII) Corrole Terminal Carbides Should Exist as Stable Compounds. 2022 , 2, 159-163	0
610	Study of the Electronic Structure of M ₂ (CH ₂ CMe ₃) ₆ (M = Mo, W) by Photoelectron Spectroscopy and Density Functional Theory. 2022 , 41, 29-40	1
609	Improving the Silicon Interactions of GFN-xTB. 2021 ,	1
608	CO Cleavage Reaction Driven by Alkylidyne Complexes of Group 6 Metals and Uranium: A Density Functional Theory Study on Energetics, Reaction Mechanism, and Structural/Bonding Properties. 2021 ,	
607	Synthesis and n-Type Semiconducting Properties of Bis(dioxaborin) Compounds Containing a Extended 2,2'-Bithiophene Structure. 2021 ,	3
606	Estimations of Fe-N Intrinsic Interaction Energies of Iron-Sulfur/Nitrogen-Carbon Sites: A Deeper Bonding Insight by EDA-NOCV Analysis of a Model Complex of the Nitrogenase Cofactor.. 2021 , 6, 33932-33942	0
605	Experimental and Computational Study of a Tetraazamacrocyclic Bis(aryloxy) Uranyl Complex and of the Analogues {E?U?NR} (E = O and NR).. 2021 ,	0
604	Ligation of Boratabenzene and 9-Borataphenanthrene to Coinage Metals. 2021 ,	0
603	Nature of C-H...Halogen Bonding and its Role in Organocatalysis. 2021 , 2021, 6102-6110	1
602	Data-Centric Architecture for Self-Driving Laboratories with Autonomous Discovery of New Nanomaterials.. 2021 , 12,	1
601	Plasmonic Circular Dichroism in Chiral Gold Nanowire Dimers.. 2021 , 27,	2
600	A promising strategy for increasing phosphorescent quantum yield: The ligand 10-cyclic chelate of the tetradentate Pt(II) complex. 2022 , 36,	1
599	Designing a Solution-Stable Distannene: The Decisive Role of London Dispersion Effects in the Structure and Properties of {Sn(CH-2,4,6-Cy)} (Cy = Cyclohexyl).. 2021 , 143, 21478-21483	2
598	Electron Density Geometry and the Quantum Theory of Atoms in Molecules.. 2021 , 125, 10622-10631	1
597	Performance of GFN1-xTB for periodic optimization of metal organic frameworks.. 2022 ,	0
596	UV-selective organic absorbers for the cosensitization of greenhouse-integrated dye-sensitized solar cells: synthesis and computational study.. 2022 , 12, 11420-11435	3

595	Core-electron contributions to the molecular magnetic response.. 2022,	4
594	A new design of SiO ₂ /Na ₂ O/Al ₂ O ₃ glass/ceramic and determination of elastic modulus and density of states via molecular dynamics simulations based on density functional tight-binding calculations. 1	
593	How Ionization Catalyzes Diels-Alder Reactions.. 2022,	0
592	Theoretical Insights into the Selective Separation of Am(III)/Eu(III) Using Hydrophilic Triazolyl-Based Ligands.. 2022,	0
591	First Principles Study of Layered CrGeTe ₃ as Lithium Intercalation Compound.	
590	A 2D perchlorinated sp ² -carbon framework. 2022, 100858	1
589	Three-body CsD ₂ calculation in Pd ₁₂ cage and E2 transition in ultra-low energy nuclear reaction. 2022, 6, 045003	
588	Electrochemical Oxidation and Speciation of Lanthanides in Potassium Carbonate Solution.	
587	Possible catalytic activity of N,N-coordinated mono-cationic copper bound Pyrazol-1-yl(1H-pyrrol-2-yl)methanone complex: a computational study. 1	
586	Revealing the nature of optical activity in carbon dots produced from different chiral precursor molecules.. 2022, 11, 92	3
585	Time-dependent density functional theory study of the optical properties of tetrahedral aluminum nanoparticles.. <i>Journal of Computational Chemistry</i> , 2022,	3-5 0
584	The stability and chemical bonding of a series tridentate ligand-actinyl complexes: [AnO ₂ (L) ₂] ²⁺ (An: U and Am). 2022, 119118	1
583	Basic Functions. 2022, 17-46	0
582	Adsorption and Activation of CO ₂ on a Au ₁₉ Pt Subnanometer Cluster in Aqueous Environment. 2022, 113701	
581	Greener Strategy for Lupanine Purification from Lupin Bean Wastewaters Using a Molecularly Imprinted Polymer.. 2022,	0
580	Ligand Shell Isomerization Induces Different Fluorescence Origins of Two Au Nanoclusters.. 2022, 3718-3725	0
579	Functional, Aromatic, and Fluorinated Monothiosemicarbazones: Investigations into Their Structures and Activity toward the Gallium-68 Incorporation by Microwave Irradiation.. 2022, 7, 13750-13777	
578	Presentation_1.pptx. 2018,	

577 Table_1.docx. 2018,

576 Image_1.TIF. 2018,

575 Image_10.TIF. 2018,

574 Image_2.TIF. 2018,

573 Image_3.TIF. 2018,

572 Image_4.TIF. 2018,

571 Image_5.TIF. 2018,

570 Image_6.TIF. 2018,

569 Image_7.TIF. 2018,

568 Image_8.TIF. 2018,

567 Image_9.TIF. 2018,

566 Table_1.pdf. 2018,

565 Video_1.AVI. 2018,

564 Table_1.DOCX. 2018,

563 Data_Sheet_1.PDF. 2020,

562 High-temperature thermal decomposition of iso-octane based on reactive molecular dynamics simulations.. 2022, 28, 124

1

561 Probing Noncovalent Interactions in [3,3]Metaparacyclophanes.. 2022,

560 Missing Link in the Growth of Lead-Based Zintl Clusters: Isolation of the Dimeric Plumbaspherene [CuPb].. 2022,

559	Dual Metalation in a Two-Dimensional Covalent Organic Framework for Photocatalytic C-N Cross-Coupling Reactions.. 2022 ,	10
558	Binding methane to a metal centre.. 2022 ,	2
557	Band-filling effects in single-crystalline oligomer models for doped PEDOT: 3,4-ethylenedioxythiophene (EDOT) dimer salt with hydrogen-bonded infinite sulfate anion chains.	
556	Anion-anion interaction within Ch(CH)X (Ch = S, Se, Te; X = Cl, Br, I) dimers stabilized by chalcogen bonds.. 2022 ,	2
555	New phosphotetradecavanadate hybrids: crystal structure, DFT analysis, stability and binding interactions with bio-macromolecules.. 2022 ,	0
554	Molecule-like and Lattice Vibrations in Metal Clusters.	0
553	Composition-driven Archetype Dynamics in Polyoxovanadates□	2
552	On surface chemical reactions of free-base and titanyl porphyrins with r-TiO(110): a unified picture.. 2022 ,	1
551	Magnetic coupling induced by the interaction between endohedral metal borofullerenes.. 2022 , 12, 13401-13405	
550	Neighborhoods and functionality in metals.. 2022 ,	
549	Relativistic DFT Calculations of Changes in NMR Chemical Shifts in Aqueous Solutions of Heavy-Metal Nitrates. 2022 , 8, n/a	
548	Basic studies toward ultrafast soft x-ray photoelectron diffraction; its application to probing local structure in iodobenzene molecules.. 2022 , 9, 024303	0
547	Direct Electron Transfer between Aromatic Molecules inside and outside the ZSM-5 Zeolite Channels: An Identification of the EPR Spectra of 1,3,5-Trimethylbenzene Radical Cations. 2022 , 126, 7421-7430	
546	Chemical Mechanism of AlF3 Etching during AlMe3 Exposure: A Thermodynamic and DFT Study. 2022 , 126, 7410-7420	2
545	First steps towards achieving both ultranonlocality and a reliable description of electronic binding in a meta-generalized gradient approximation. 2022 , 4,	0
544	Hydrogen Activation and Spillover on Anatase TiO2-Supported Ag Single-Atom Catalysts. 2022 , 126, 7482-7491	2
543	Bypassing the statistical limit of singlet generation in sensitized upconversion using fluorinated conjugated systems.. 2022 , 1	1
542	Gold-Aluminylyl and Gold-Diarylboryl Complexes: Bonding and Reactivity with Carbon Dioxide.. 2022 , 61, 7327-7337	1

- 541 LFDFT A Practical Tool for Coordination Chemistry. **2022**, 10, 70 1
- 540 The New Ag-S Cluster [AgS(SBu)][CFCOO] with a Unique hcp Ag Kernel and Ag Keplerian-Shell-Based Structural Architecture and Its Photoresponsivity.. **2022**, 2
- 539 Bulky and Stable Copper(I)-Phenanthroline Complex: Impact of Steric Strain and Symmetry on the Excited-State Properties.. **2022**, 61, 7296-7307 2
- 538 Vanadium(IV) coordination complexes with excellent biological activities: a synthetic, characterization, and density functional theory approach. 1-18 0
- 537 Cage-size effects on the encapsulation of P by fullerenes.. *Journal of Computational Chemistry*, **2022**, 3-5 1
- 536 Theoretical Studies of Furan and Thiophene Nanothreads: Structures, Cycloaddition Barriers, and Activation Volumes.. **2022**, 0
- 535 Ultrafast Vibrational Response of Activated C-D Bonds in a Chloroform-Platinum(II) Complex.. **2022**, 4447-4454
- 534 Density functional theoretical analysis of micro-adsorption of isotopes of hydrogen molecule and atom by uranium. **2022**, 0
- 533 A 300-fold conductivity increase in microbial cytochrome nanowires due to temperature-induced restructuring of hydrogen bonding networks.. **2022**, 8, eabm7193 4
- 532 Nitrogen reduction to ammonia triggered by heterobimetallic uranium-group 10 metal complexes of phosphinoaryl oxides: A relativistic DFT study. **2022**, 525, 112345 0
- 531 Slippery coating without loss of lubricant. **2022**, 444, 136606 0
- 530 A stack-guiding unit constructed 2D COF with improved charge carrier transport and versatile photocatalytic functions. **2022**, 445, 136713 1
- 529 Hydrogen adsorption and storage behaviors of Li-decorated PdS₂ monolayer: An extended tight-binding study based on DFT. **2022**, 0
- 528 Predicting the Thermodynamics of Ionic Liquids: What to Expect from PC-SAFT and COSMO-RS?. **2022**, 0
- 527 Prediction of SEI Formation in All-Solid-State Batteries: Computational Insights from PCL-based Polymer Electrolyte Decomposition on Li-Metal. 1
- 526 Synthesis and characterisation of the ternary intermetalloid clusters {M@[As8(ZnMes)₄]}₃ (M = Nb, Ta) from binary [M@[As8]3] precursors. 1
- 525 Theoretical Insights on Molecular Designing of Hot-Exciton based Thermally Activated Delayed Fluorescence Molecules. 2
- 524 Infrared spectroscopy of Be(CO) in the gas phase: electron transfer and C-C coupling of CO.. **2022**,

- 523 Insight into the Complexation of Heptavalent Technetium with Tri-n-Butyl Phosphate: A Computational Study. **2022**, 139705
- 522 Relationship between Halogen-Halogen Interaction and Electric Conductivity in Thiazolo[2,3-a]isoquinolin-7-ium Triiodides. **2022**, 133306
- 521 The hunter falls prey: photoinduced oxidation of C60 in inclusion complex with perfluorocycloparaphenylene.. **2022**, 0
- 520 The influence of trans-ligand to NO on the thermal stability of photoinduced side-bond coordinated linkage isomer. 0
- 519 Corrosion protection performance of silicon-based coatings on carbon steel in NaCl solution: a theoretical and experimental assessment of the effect of plasma-enhanced chemical vapor deposition pretreatment. **2022**, 12, 15601-15612 0
- 518 Construction of the Largest Metal-Centered Double-Ring Tubular Boron Clusters Based on Actinide Metal Doping. 1
- 517 Development, structural, spectroscopic and investigation of new complexes relevant as anti-toxoplasma metallopharmacs. **2022**, 133380 0
- 516 Clarifying notes on the bonding analysis adopted by the energy decomposition analysis. 4
- 515 Chemical Bonding in Actinyl (V/VI) Dipyrimethyrin Complexes for the Actinide Series from Americium to Californium: A Computational Investigation. 0
- 514 In Silico Optimization of Charge Separating Dyes for Solar Energy Conversion. 0
- 513 Modelling the Radical Chemistry on Ice Surfaces: An Integrated Quantum Chemical and Experimental Approach. **2022**, 9, 0
- 512 Experimental and Theoretical Evidence of a Pb-Pb Ditetrel Bond Without a σ -Hole. 0
- 511 Vapor-Liquid Equilibrium Study of the Monochlorobenzene π ,6-Dichloropyrimidine Binary System. **2022**, 7, 17670-17678
- 510 Silver(I) and gold(I) complexes with bitriazole-based N-heterocyclic carbene ligand: solid state features and behavior in solution.
- 509 Donor-Acceptor-Donor Hot Exciton Triads for High Reverse Intersystem Crossing in OLEDs. 2200509 0
- 508 Mesoionic Carbene Complexes of Uranium(IV) and Thorium(IV).
- 507 Cucurbit[7]uril as Nanoreactor for the Fixation of CO₂ with Oxirane: A Density Functional Theory Investigation. **2022**, 7, 0
- 506 Reactive Molecular Dynamics Study of Hygrothermal Degradation of Crosslinked Epoxy Polymers. 1

- 505 Model Compounds for Intermediates and Transition States in Sonogashira and Negishi Coupling: d8d10 Bonds in Large Heterobimetallic Complexes Are Weaker than Computational Chemistry Predicts. 0
- 504 Cluster of Hexamolybdenum [Mo₆Cl₁₄]₂ for Sensing Nitroaromatic Compounds. 0
- 503 Optimization of the r2SCAN-3c Composite Electronic-Structure Method for Use with Slater-Type Orbital Basis Sets. 0
- 502 A Theoretical Study of Unsupported Uranium-Ruthenium Bonds Based on Tripodal Ligands.
- 501 Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings.
- 500 Multiple Surface Site Three-Dimensional Structure Determination of a Supported Molecular Catalyst. 3
- 499 Reaction Entropies in Solution from Analytical Three-Dimensional Reference Interaction Site Model Derivatives with Application to Redox and Spin-Crossover Processes. 1
- 498 Electronic Structure and Spectroscopy of f-Element Tris(cyclopentadienyl) Complexes. 285-327
- 497 Electric Fields in Enzyme Catalysis. **2022**,
- 496 Effect of unwanted guest molecules on the stacking configuration of covalent organic frameworks: a periodic energy decomposition analysis. 1
- 495 How do structural factors determine the linear and non-linear optical properties of fluorene-containing quadrupolar fluorophores? A theoretical answer. 1
- 494 How to capture C₂O₂: Structures and bonding of neutral and charged complexes [(NHC)-C₂O₂-(NHC)]_q (NHC = N-heterocyclic carbene; q = 0, 1+, 2+).
- 493 Pure blue phosphorescent platinum(ii) emitters supported by NHC-based pincer type ligands with unitary emission quantum yields. 1
- 492 An ultrastable thiolate/diglyme ligated cluster: Au₂₀(PET)₁₅(DG)₂. 1
- 491 Characterization of Pt-doping effects on nanoparticle emission: A theoretical look at Au₂₄Pt(SH)₁₈ and Au₂₄Pt(C₃H₇)₁₈.
- 490 Computational descriptor analysis on excited state behaviours of a series of TADF and non-TADF compounds.
- 489 Ligand-Core Interaction in Ligand-Protected Ag₂₅(XR)₁₈ (X= S, Se, Te) Superatoms. Evaluation of Anchor Atom Role via Relativistic DFT Calculations.
- 488 Prediction of anharmonic, condensed-phase IR spectra using a composite approach: Discrete encapsulated chloride hydrates. **2022**, 387, 111660

- 487 Thermal Conductivity of Two-Dimensional Benzobisoxazole-Linked Covalent Organic Frameworks with Nanopores: Implications for Thermal Management Applications. 2
- 486 Electronic structure of two-dimensional-layered PbTiO₃ perovskite crystal: an extended tight-binding study based on DFT. **2022**, 45, 0
- 485 Theoretical studies on excited-state properties and luminescence mechanism of a Carbene-Metal-Amide Au(I) complex with thermally activated delayed fluorescence.
- 484 The effect of molecular decoration on formation of curved and twisted graphene. **2022**, 113795
- 483 Palladium-Catalyzed Activation of Carbon-Halogen Bonds: Electrostatics-Controlled Reactivity. 1
- 482 Actinium coordination chemistry: A density functional theory study with monodentate and bidentate ligands. *Journal of Computational Chemistry*, 3.5
- 481 Au-Au Chemical Bonding in Nitronyl Nitroxide Gold(I) Derivatives. 0
- 480 Pressure Effects on 3d n ($n=4, 9$) Insulating Compounds: Long Axis Switch in Na₃MnF₆ not Due to the Jahn-Teller Effect. 0
- 479 Role of Cl...I halogen bonds in tuning the crystals of Uranyl-Dichlorothiophene carboxylate based hybrid cluster materials through N-donor counter ions. **2022**, 133524
- 478 Molecular Arrangement Control of [1]Benzothieno[3,2-b][1]benzothiophene (BTBT) via Charge-Assisted Hydrogen Bond. 1
- 477 Benzenetriimide-Based Molecular Conductor with Antiferro- to Ferromagnetic Switching Induced by Structural Change of π -Stacked Array.
- 476 Automated Rational Design of Metal-Organic Polyhedra. 0
- 475 Compression Produces a Square-Planar Iron Tetracarbonyl. **2022**, 61, 9055-9062
- 474 Calculation of absolute Raman scattering cross-sections using vibrational self-consistent field/vibrational configuration interaction wave functions. *Journal of Computational Chemistry*, 3.5 1
- 473 The Nature of the Polar Covalent Bond. 3
- 472 Electrochemical Study of Vicinal Dibromide Dehalogenation Catalyzed by Cobaloximes. **2022**, 169, 063518
- 471 C-H and Si-H Activation Reactions at Ru/Ga Complexes: A Combined Experimental and Theoretical Case Study on the Ru-Ga Bond.
- 470 Theoretical Studies on the Structure and Intramolecular Interactions of Fagopyrins-Natural Photosensitizers of Fagopyrum. **2022**, 27, 3689 1

- 469 Elucidation of Metal Local Environments in Single-Atom Catalysts Based on Carbon Nitrides. 2202080 2
- 468 Direct assembly between closed-shell coinage metal superatoms. 1
- 467 Breaking the scaling relations for efficient N₂-to-NH₃ conversion by a bowl active site design: Insight from LaRuSi and isostructural electrides. **2022**, 43, 2183-2192
- 466 Electron transfer assessment between stannol ring of triple-decker complexes and M(CO)₅ (M = Cr, Mo, W), MnCp(CO)₂ and CoCp(CO) metallic fragments: Bonding and energy decomposition analysis. **2022**, 223, 115960 0
- 465 Theoretical Studies on the Interaction of Uranyl with Carboxylic Acids and Oxime Ligands. **2022**, 80, 708
- 464 Push-pull organic dyes and dye-catalyst assembly featuring a benzothiadiazole unit for photoelectrochemical hydrogen production.
- 463 Theoretical insights into selective extraction of uranium from seawater with tetradentate N,O-mixed donor ligands.
- 462 Cooperative pentavalent pnictogen bonding versus dominant hydrogen bonding in POCl₃-diethylether dimer characterized using matrix isolation infrared spectroscopy and ab initio computations. **2022**, 387, 111672 0
- 461 Molecular insights into the complex formation between dodecamethylcucurbit[6]uril and phenylenediamine isomers. **2022**, 102, 637-651 0
- 460 How Robust Is the Reversible Steric Shielding Strategy for Photoswitchable Organocatalysts?. **2022**, 87, 8849-8857 1
- 459 Supramolecular cis-Bis(Chelation) of [M(CN)₆]³⁻ (M = Cr^{III}, Fe^{III}, Co^{III}) by Phloroglucinol (H₃PG). **2022**, 27, 4111
- 458 Modeling Heme Peroxidase: Heme Saddling Facilitates Reactions with Hyperperoxides to Form High-Valent Fe(IV)=Oxo Species. 1
- 457 Secondary ligand engineering of nanoclusters: Effects on molecular structures, supramolecular aggregates, and optical properties.
- 456 Bonding situations in tricoordinated beryllium phenyl complexes. *Journal of Computational Chemistry*, 3.5 1
- 455 On The Nature of the Chemical Bond in Valence Bond Theory. 3
- 454 Theoretical Investigation of Catalytic Water Splitting by the Arene-Anchored Actinide Complexes. 0
- 453 What Determines the Drastic Reactivity of Nbn⁺ Clusters with Nitric Oxide under Thermalized Conditions?. 1
- 452 Chemical looping combustion characteristics and kinetic behaviour of Sr-doped perovskite-type CaFeO₃ oxygen carriers: theoretical and experimental investigations.

- 451 Methoxyl-Substituted Phosphine Ligand Properties and a Case Study of Formation Adducts to Indium(III) Bromide by DFT Calculations. **2022**, 116043
- 450 Methyl Substitution Destabilizes Alkyl Radicals.
- 449 3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives. **2022**, 13, 5
- 448 Anisotropic Charge Transfer Mobility Properties of Systems with Large Conjugation Core and Peripheral Phenyl Rings.
- 447 Design of a ZnO@Plant Polyphenol/Poly(vinyl alcohol) Film via Plant Polyphenol-Induced Cross-Linking and Its Enhanced UV Shielding and Antibacterial Performance. 2
- 446 Origin of Catalysis and Selectivity in Lewis Acid-Promoted Diels-Alder Reactions Involving Vinylazaarenes as Dienophiles. **2022**, 87, 9307-9315 1
- 445 Mixed-Ligand Mandelato-Phosphine Copper(I) Complexes as Active Catalysts in Carbene Transfer Reactions. **2022**, 7,
- 444 Au₂₀(t-Bu₃P)₈: A highly symmetric metalloid gold cluster in oxidation state 0. 0
- 443 Au₂₀(t-Bu₃P)₈: A highly symmetric metalloid gold cluster in oxidation state 0.
- 442 Host-guest binding selectivity of ethylated pillar[5]arene (EtP5A) towards octane, 1,7-octadiene, and 1,7-octadiyne: a computational investigation.
- 441 The Interaction of Deep Eutectic Solvents with Pristine Carbon Nanotubes and Their Associated Defects: A Density Functional Theory Study. **2022**, 119855 0
- 440 Anisotropic Band-Edge Absorption of Millimeter-Sized Zn(3-ptz)₂ Single-Crystal Metal-Organic Frameworks. **2022**, 7, 24432-24437
- 439 Methyl Substitution Destabilizes Alkyl Radicals. 2
- 438 Molecular dynamics study of crystal lattice effect on mechanical properties of SiO₂: A density functional tight binding investigation. **2022**, 203, 111305 0
- 437 Relativistic and vibrational effects on the electronic structure of isopropyl iodide. **2022**, 562, 111650
- 436 More than 25,000h device lifetime in blue phosphorescent organic light-emitting diodes via fast triplet up-conversion of n-type hosts with sub-ns triplet exciton lifetime. **2022**, 450, 137974 0
- 435 Molecular and Electronic Structure of Isolated Platinum Sites Enabled by the Expedient Measurement of ¹⁹⁵Pt Chemical Shift Anisotropy. 1
- 434 Oxygen and Proton Transport in Flooded Graphene Pores with N-Dopants and Defects. **2022**, 126, 11447-11456

433 Multimetallic Permethylpentalene Hydride Complexes.

432 Tuning the Ground- and Excited-State Redox Potentials of Octahedral Hexanuclear Rhenium(III) Complexes by the Combination of Terminal Halide and N-Heteroaromatic Ligands. 0

431 Structural Features of the Cu(II) Complex with 5-Phenyltetrazolate Anion and 4,4'-Dimethyl-2,2'-bipyridine. **2022**, 67, 575-580

430 Rational Tuning of the Reactivity of Three-Membered Heterocycle Ring-Openings via SN2 Reactions. 0

429 Synthesis and Chemistry of Ammonioethenyl and Phosphonioethenyl Ligands in Zwitterionic Dirhenium Carbonyl Complexes. 0

428 Relationship between structure and cytotoxicity of vanadium and molybdenum complexes with pyridoxal derived ligands. **2022**, 235, 111937 2

427 Theoretical studies on boron dimesityl-based thermally activated delayed fluorescence organic emitters: excited-state properties and mechanisms. **2022**, 46, 15678-15685 0

426 Electronic effects on the mechanism of the NAD⁺ coenzyme reduction catalysed by a non-organometallic ruthenium(II) polypyridyl amine complex in the presence of formate. **2022**, 12, 21191-21202 0

425 A Quantum Chemical Deep-Dive into the π -Interactions of 3-Methylindole and Its Halogenated Derivatives π -towards an Improved Ligand Design and Tryptophan Stacking. **2022**, 15, 935 1

424 Rational Amphiphilic Ligand Engineering Enables Enhanced Stability and Efficiency of CsPbBr₃ Nanocrystals Based Light Emitting Diodes. 2201176 1

423 Density Functional Theory Study on Magnetic character and Mn Crystal Field Split Levels in Mn-doped SnO Monolayer.

422 Advancing the Am Extractant Design through the Interplay among Planarity, Preorganization, and Substitution Effects. **2022**, 61, 11556-11570 2

421 Discovery of Polythioplattinate(II) [Pt₃S₂(SO₃)₆]₁₀ and Study of Its Solution and Catalytic Properties. **2022**, 61, 11529-11538 0

420 Molecular Structures of the Silicon Pyridine-2-(thi)olates Me₃Si(pyX), Me₂Si(pyX)₂ and Ph₂Si(pyX)₂ (py = 2-Pyridyl, X = O, S), and Their Intra- and Intermolecular Ligand Exchange in Solution. **2022**, 12, 1054 0

419 Bonding Nature of Ibnic Carbenes In [M₃(β -H₂)]-Containing Compounds: The Covalent Interaction. **2022**, 61, 12349-12355

418 Complexation of Astatine(III) with Ketones: Roles of NO₃⁻ Counterion and Exploration of Possible Binding Modes. **2022**, 61, 12087-12096 0

417 DFT study of common anions adsorption at graphene surface due to anion- π interaction. **2022**, 28, 1

416 Uncovering the hidden reactivity of benzyne/aryne precursors utilized under milder condition: Bonding and stability studies by EDA-NOCV analyses. **2022**, 43, 1543-1560

- 415 Ligand accommodation causes altered reactivity of silver clusters with iodomethane: superatomic stability of Ag₉I₂⁺ in mimicking XeF₂. **2022**, 65, 1594-1600 0
- 414 Rational Design of Bimetallic Metal Chalcogenide Clusters for CO₂ Dissociation. 0
- 413 Substituted Cyclopentannulated Tetraazapentacenes. 0
- 412 Unusually Large Effects of Charge-assisted C≡N...F Hydrogen Bonds to Anionic Fluorine in Organic Solvents: Computational Study of 19 F NMR Shifts versus Thermochemistry. 1
- 411 Cycloaddition Reactivities Analyzed by Energy Decomposition Analyses and the Frontier Molecular Orbital Model. 4
- 410 Extending machine learning beyond interatomic potentials for predicting molecular properties. 3
- 409 Computational Prediction of Tc-99 NMR Chemical Shifts in Technetium Complexes with Radiopharmaceutical Applications. **2022**, 126, 5434-5448
- 408 Electronegativity Equilibration. **2022**, 126, 5472-5482
- 407 Bonding Situation of E≡E Complexes in Transition Metal and Main Group Compounds. 0
- 406 N-Heterocyclic carbene-based C-centered Au(I)-Ag(I) clusters with intense phosphorescence and organelle-selective translocation in cells. **2022**, 13, 1
- 405 Cationic Gold(II) Complexes: Experimental and Theoretical Study. 0
- 404 Structural and Electronic Properties of SnO Downscaled to Monolayer. **2022**, 15, 5578 0
- 403 Insights into the Coordination Behavior of Methyl-Substituted Phosphinic Acids with Actinides. **2022**, 61, 13047-13057
- 402 Coupling between Plasmonic and Molecular Excitations: TDDFT Investigation of an Ag-Nanorod/BODIPY Dye Interaction. 0
- 401 Unraveling the Origin of the Regioselectivity of a Supramolecular Hydroformylation Catalyst. 0
- 400 Hydrogen-Bond-Assisted Adsorption of Nitric Oxide on Various Metal-Loaded ZSM-5 Zeolites. 0
- 399 Iodine Gauche Effect Induced by an Intramolecular Hydrogen Bond. 0
- 398 Towards the description of charge transfer states in solubilised LHCII using subsystem DFT. 0

- 397 Sn,P-Peri-Substituted Naphthalene as a Ligand for Transition Metals. **2022**, 41, 2327-2341
- 396 Shape Entropy of a Reconfigurable Ising Surface. **2022**, 129,
- 395 Constructing and interpreting volcano plots and activity maps to navigate homogeneous catalyst landscapes. 0
- 394 Structural Aspects and Stability of Interactions between Phenyl-3,3'-Bis(Indolyl)Methanes and β -Cyclodextrin from Density Functional Theory. 1-23 0
- 393 In the Chalcogenoxide Elimination Panorama: Systematic Insight into a Key Reaction. 1
- 392 Janus dione derivatives: Novel high-mobility hole transport materials for perovskite solar cells. **2022**, 32, 104090
- 391 Homoleptic 1-norbornyl complexes of group 4 and manganese: synthesis, structures, volatility, and thermal stability.
- 390 Effective removal of cationic dye on activated carbon made from cactus fruit peels: a combined experimental and theoretical study. 0
- 389 The Labile Nature of Air Stable Ni(II)/Ni(0)-phosphine/Olefin Catalysts/Intermediates: EDA-NOCV Analysis.
- 388 Synthesis and computational characterization of aryl-fluorinated thiazoles: Experimental, DFT and molecular coupling studies. **2022**, 261-262, 110024
- 387 Peripheral group engineering on hole-transporting materials in perovskite solar cells: Theoretical design and experimental research. **2022**, 206, 110604 2
- 386 Opto-Electronic properties of Quasi-Planar boron clusters Δ A DFT investigation. **2022**, 804, 139914
- 385 Ligand-dictated cluster core characteristics in Au₈Se₂ gold selenido. Insights from relativistic DFT. **2022**, 542, 121149
- 384 Microstructural features transformation at various temperature stages and multi-scale atomistic representations of calcined petroleum coke based on HRTEM. **2022**, 330, 125521 0
- 383 Two simple hole-transporting materials for perovskite solar cells: A DFT calculation and experimental study. **2022**, 604, 154603 2
- 382 Vibrational Circular Dichroism from DFT Molecular Dynamics: The AWW Method. 0
- 381 Computational Studies of Super-B as Anodes for AM (Li, Na, and K) Ion Batteries. **2022**, 169, 090514 0
- 380 Polymeric REE coordination compounds based on novel enaminone derivative. **2022**, 227, 116122 0

- 379 Experimental and theoretical study of the physicochemical properties of the novel imidazole-based eutectic solvent. **2023**, 118, 108319 0
- 378 Evolution of the active species of homogeneous Ru hydrodeoxygenation catalysts in ionic liquids. **2022**, 13, 10251-10259 0
- 377 Oxidative addition or Werner coordination complex? Reactivity of μ -diketiminato supported main group and first-row transition metal complexes towards ammonia. **2022**, 51, 13444-13450 0
- 376 Pericyclic reaction benchmarks: hierarchical computations targeting CCSDT(Q)/CBS and analysis of DFT performance. **2022**, 24, 18028-18042 3
- 375 Unravelling the Binding Affinity and Selectivity of Molybdenum (II) Phenanthroline Complexes with DNA G-Quadruplexes by Using Linear-Scaling DFT Studies. The Important Role of the Ancillary Ligands. 0
- 374 Computational aspects to design iridium complexes as emitters for OLEDs. **2022**, 7, 1172-1206 0
- 373 Tuning photoelectron dynamic behavior of thiolate-protected MAu₂₄ nanoclusters via heteroatom substitution. **2022**, 7, 1192-1200 2
- 372 Stable N-heterocyclic borylenes with promising ligand properties: a contribution from theory. 0
- 371 [Fe₄S₄] cubane in sulfite reductases: new insights into bonding properties and reactivity. **2022**, 24, 18543-18551 0
- 370 Advances in understanding and use of NMR scalar couplings. **2022**, 185-254 0
- 369 Industrial applications of quantum dots. **2022**, 771-803 0
- 368 Ni(II)TPA stabilization by hydrogen bond formation on the second coordination sphere: a DFT characterization. **2022**, 51, 12585-12595 0
- 367 Photochromic spiro-indoline naphthoxazines and naphthopyrans in dye-sensitized solar cells. 1
- 366 The smallest 4f-metalla-aromatic molecule of cyclo-PrB₂ with PrB multiple bonds. **2022**, 13, 10082-10094 1
- 365 The spin-orbit effects on platinabenzene: a ring current and electron delocalization approach. **2022**, 46, 16708-16716 0
- 364 NIR-emissive, singlet-oxygen-sensitizing gold tetra(thiocyano)corroles. **2022**, 51, 13236-13245 0
- 363 How reduced are nucleophilic gold complexes?. 1
- 362 Existence of noble gas-inserted phosphorus fluorides: FN_gPF₂ and FN_gPF₄ with N_gB covalent bond (N_g = Ar, Kr, Xe and Rn). **2022**, 24, 20466-20479 0

361	Binding of saturated and unsaturated C6-hydrocarbons to the electrophilic anion [B12Br11]Ba systematic mechanistic study. 2022 , 24, 21759-21772	0
360	DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science.	9
359	Side-chain engineering for high degradation performance of mandrel materials in ICF target fabrication.	0
358	Modeling Metal Ions in Enzyme Catalysis. 2022 ,	0
357	Concentration dependent interfacial chemistry of the NaOH(aq): gibbsite interface. 2022 , 24, 20998-21008	0
356	Why trans and not cis? [Molecular dynamics and DFT study on selective separation of dihaloethene isomers using perethylated pillar[5]arene. 2022 , 24, 21812-21821	1
355	Geometries, interaction energies and bonding in [Po(H2O)n]4+ and [PoCl _n]4 ⁻ complexes.	0
354	Industrial Expectations of a Pure Component Database for Thermodynamic and Transport Properties.	1
353	Modulation of metal carbonyl stretching frequencies in the second coordination sphere through the internal Stark effect.	0
352	What It Takes for Imidazolium Cations to Promote Electrochemical Reduction of CO ₂ . 3439-3446	2
351	Accurate Vertical Excitation Energies of BODIPY/Aza-BODIPY Derivatives from Excited-State Mean-Field Calculations.	0
350	P _n Ring Size Dependence on NHC-Induced Ring Contraction Reactions of [CoCp*(P4)], [Ta(CO)2Cp*(P4)], and [FeCp*(P5)]: A DFT Study.	0
349	Efficient and Stable Perovskite Solar Cells with a High Open-Circuit Voltage Over 1.2V Achieved by a Dual-Side Passivation Layer. 2205268	4
348	Atomistic simulations of B [110](111) grain boundary in diamond: Structure, stability, and properties.	0
347	Purely Predicting the Pharmaceutical Solubility: What to Expect from PC-SAFT and COSMO-RS?.	1
346	[Fp(CH4)]+, [P5-CpRu(CO)2(CH4)]+, and [P5-CpOs(CO)2(CH4)]+: A Complete Set of Group 8 MetalMethane Complexes. 2022 , 144, 17622-17629	2
345	Designing a Four-Ring Tubular Boron Motif through Metal Doping. 2022 , 61, 14553-14559	0
344	Potential-Dependent Pt(111)/Water Interface: Tackling the Challenge of a Consistent Treatment of Electrochemical Interfaces.	0

- 343 Uranium-Doped Zinc, Copper, and Nickel Oxides for Enhanced Catalytic Conversion of Furfural to Furfuryl Alcohol: A Relativistic DFT Study. **2022**, 27, 6094 0
- 342 DFT Insights into the Variety in the Coordination Modes of the Equatorial Halides in $[Au_{13}Ag_{12}(PR_3)_{10}X_8]+[X=Cl/Br]$ Clusters. 0
- 341 Enhancing Effects of the Cyano Group on the C-X \cdots H Hydrogen or Halogen Bond in Complexes of X-Cyanomethanes with Trimethyl Amine: $CH_3\bar{B}(CN)_nX\bar{B}Me_3$, ($n = 0\bar{B}$; X = H, Cl, Br, I). **2022**, 23, 11289 1
- 340 Inhomogeneity Effects on Reactions in Supercritical Fluids: A Computational Study on the Pyrolysis of n-Decane. **2022**, 2, 2081-2088 0
- 339 Cheap Turns Superior: A Linear Regression-Based Correction Method to Reaction Energy from the DFT. 0
- 338 Environmental Control of the Magnetic Behavior of Transition Metal Complexes: Density Functional Theory Study of Zeolite Y Embedded Complexes $[M(bpy)_3]^{2+}@Y$ (M = Fe²⁺, Co²⁺). **2022**, 126, 6221-6235 0
- 337 Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**. 2
- 336 In silico studies of Mpro and PLpro from SARS-CoV-2 and a new class of cephalosporin drugs containing 1,2,4-thiadiazole. 0
- 335 The reactivity of the trapping reaction of the benzene-bridged boron/phosphorus-based frustrated Lewis pair with difluorocarbene and its group 14 analogs: A theoretical investigation. **2022**, 43, 1783-1792 2
- 334 Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**. 10
- 333 Super-Excimer: Anomalous Bonding in a Metastable Excited-State Dimer of Superatomic Dimers. **2022**, 13, 8455-8461 0
- 332 Explaining the High Catalytic Activity in Bis(indenyl) Methyl Zirconium Cation Using Combined EDA-NOCV/QTAIM Approach. 0
- 331 Sandwich, Triple-Decker and Other Sandwich-like Complexes of Cyclopentadienyl Anions with Lithium or Sodium Cations. **2022**, 27, 6269 0
- 330 Electronic Structures and Unusual Chemical Bonding in Actinyl Peroxide Dimers $[An_2O_6]^{2+}$ and $[(An_2O_6)(12\text{-crown-4 ether})_2]^{2+}$ (An = U, Np, and Pu). **2022**, 61, 15589-15599 2
- 329 Stability and bonding of carbon(0)-iron \bar{N} 2 complexes relevant to nitrogenase co-factor: EDA-NOCV analyses. 0
- 328 Frozen-Density Embedding for Including Environmental Effects in the Dirac-Kohn-Sham Theory: An Implementation Based on Density Fitting and Prototyping Techniques. 0
- 327 Synthesis, Structure, and Bonding Analysis of Lewis Base and Lewis Acid/Base-Stabilized Phosphanyl gallanes. 1
- 326 Magic Numbers in Octahedral Ligated Metal-Chalcogenide Superatoms. 0

325	Filling Chlorine Vacancy with Bromine: A Two-Step Hot-Injection Approach Achieving Defect-Free Hybrid Halogen Perovskite Nanocrystals.	0
324	Theoretical investigation of the effect of $O^*M=\{Ti,Zr,\dots\}$. 2022 , 108341	0
323	Helicate versus Mesocate in Quadruple-Stranded Lanthanide Cages: A Computational Insight. 2022 , 23, 10619	1
322	Ligand-stabilized heteronuclear diatomics of group 13 and 15. 2022 , 43, 1964-1977	0
321	ZORA Gaussian basis sets for Fr, Ra, and Ac. 2022 , 28,	0
320	EF24, a schistosomicidal curcumin analog: Insights from its synthesis and phenotypic, biochemical and cytotoxic activities. 2022 , 110191	0
319	A computational approach for modeling electronic circular dichroism of solvated chromophores.	3
318	Quasiparticle Self-Consistent GW-Bethe-Salpeter Equation Calculations for Large Chromophoric Systems.	2
317	Synthesis and Characterization of Ir-(η -NSi) Species Active toward the Solventless Hydrolysis of HSiMe(OSiMe ₃) ₂ .	1
316	Development of a novel ReaxFF reactive potential for organochloride molecules.	0
315	Experimental and Theoretical Evaluation of Four NLO-Active Divalent Transition Metal Complexes Supported by an Enantiomerically Pure Tetradentate Schiff Base Ligand.	0
314	Biofuel Additives: Thermodynamic Studies of Glycerol Ethers.	0
313	The Raman Active Vibrational Modes of Anthraquinones. 2022 , 22, 1165-1175	1
312	Understanding electronic structures, chemical bonding, and fluxional behavior of Lu ₂ @C _{2n} (2n = 76 - 88) by a theoretical study.	1
311	Influence of stereoelectronic interactions on the ¹³ C NMR chemical shift in iodine-containing molecules. 2022 , 12-13, 100080	0
310	Theoretical insights into the separation of Am(III)/Eu(III): designing ligands based on a preorganization strategy.	0
309	Theoretical seeking of the charge transport materials with inherent mobility higher than 2,6-Diphenyl anthracene: three isomers of 2,6-Dipyridyl anthracene.	0
308	Basis Set Convergence and Extrapolation of Connected Triple Excitation Contributions (T) in Computational Thermochemistry: The W4-17 Benchmark with Up to k Functions. 2022 , 467-496	0

- 307 Thermodynamic properties of high energy amine borane adducts. **2022**, 0
- 306 Molecular structural dataset of lignin macromolecule elucidating experimental structural compositions. **2022**, 9, 0
- 305 Descriptors of Aromaticity: Energetic Criteria. **2022**, 111-130 0
- 304 Effects of Diglyme on Au Nanocluster Formation: Mechanism, ¹H NMR, and Bonding. **2022**, 126, 7598-7605 1
- 303 Charge Transport Capabilities of Dibenzo[n]phenacenes (n = 5-7): Influence of Trap States and Molecular Packing. 0
- 302 Superstrong Chemical Bonding of Noble Gases with Oxidoboron (BO⁺) and Sulfidoboron (BS⁺). **2022**, 126, 7888-7900 0
- 301 Thermodynamics of the Metal Carbonates and Bicarbonates of Mn, Co, Ni, Cu, and Zn Relevant to Mineral Energetics. **2022**, 126, 7874-7887 1
- 300 Twist-Bent Bonds Revisited: Adiabatic Ionization Potentials Demystify Enhanced Reactivity. **2022**, 7, 37917-37921 1
- 299 CAT: A Compound Attachment Tool for the Construction of Composite Chemical Compounds. 0
- 298 The Distortivity of π Electrons. **2022**, 223-239 0
- 297 Porphyrine. 0
- 296 Ab Initio Study of H-Bond Dynamics in Three-Component Crystals Comprising (DABCOH⁺)_n Polycationic Chains. 0
- 295 The Role of Quadruple Bonding in the Electron Transport through a Dimolybdenum Tetraacetate Molecule. **2022**, 27, 6912 0
- 294 The abnormally long and weak methylidyne C \equiv H bond. 0
- 293 Structure-Optical Property Relationship of Carbon Dots with Molecular-like Blue-Emitting Centers. **2022**, 126, 18170-18176 0
- 292 Mononuclear Oxidovanadium(IV) Complexes with BIAN Ligands: Synthesis and Catalytic Activity in the Oxidation of Hydrocarbons and Alcohols with Peroxides. **2022**, 12, 1168 0
- 291 Theoretical Study on the Thermal Degradation Process of Nylon 6 and Polyhydroxybutyrate. **2022**, 2, 334-346 1
- 290 Understanding the Reactivity, Selectivity, and Deactivation of Frustrated Lewis Pairs for Semihydrogenation of Acetylene. 0

- 289 The Question of the Redox Site in Metal-Metal Multiple-Bonded Metalloporphyrin Dimers. 0
- 288 Predicting Solvent Effects on SN2 Reaction Rates: Comparison of QM/MM, Implicit, and MM Explicit Solvent Models. 2
- 287 Fast Charge Separation in Distant Donor-Acceptor Dyads Driven by Relaxation of a Hot Excited State. 1
- 286 DFT Study of Heteronuclear (TMFeO₃)_x Molecular Clusters (Where TM = Sc, Ti, Fe and x = 2, 4, 8) for Photocatalytic and Photovoltaic Applications. **2022**, 15, 7253 0
- 285 Can a chemical bond be exclusively covalent or ionic?. **2022**, 134, 1
- 284 Understanding chemical enhancements of surface-enhanced Raman scattering using a Raman bond model for extended systems. 0
- 283 Pnictide-Capped Butterfly Cluster in the Crystal Structure of Nb₄PnX₁₁ (Pn = N, P; X = Cl, Br, I). 0
- 282 A new design of Borax-Cannabinol nanomaterial used to strengthen concrete structures: Non-Scc-GFN₁xTB model. **2022**, 114995 0
- 281 Red shift in optical excitations on layered copper perovskites under pressure: role of the orthorhombic instability. 0
- 280 Optical response properties of some metal cluster supported host-guest systems. **2023**, 123-137 0
- 279 M(L)₈ complexes (M = Ca, Sr, Ba; L = PH₃, PF₃, N₂, CO): Act of an alkaline-earth metal as a conventional transition metal. **2023**, 157-171 0
- 278 ¹H Chemical Shift Anisotropy: A High Sensitivity Solid-State NMR Dynamics Probe for Surface Studies?. 1
- 277 Actinide-doped boron clusters: from borophenes to borospherenes. 0
- 276 Uranium(IV) alkyl cations: synthesis, structures, comparison with thorium(IV) analogues, and the influence of arene-coordination on thermal stability and ethylene polymerization activity. 0
- 275 Biosorption of zinc (II) from synthetic wastewater by using *Inula viscosa* leaves as a low-cost biosorbent: Experimental and molecular modeling studies. **2023**, 326, 116742 0
- 274 A theoretical study on the influence of N-containing heterocyclic ligands on the luminescence mechanisms (phosphorescence or TADF) of Au (III) complexes. **2023**, 113, 106676 0
- 273 Understanding the influence of alkali cations and halogen anions on the cooperativity of cyclic hydrogen-bonded rosettes in supramolecular stacks. 0
- 272 Study of Electronic, Structural and Magnetic Properties of Electrodeposited Co₂MnSn Heusler Alloy Thin Films. **2022**, 0

- 271 How Bases Catalyze Diels-Alder Reactions. 0
- 270 Thioxanthone-containing blue thermally activated delayed fluorescent emitter. 0
- 269 Assessing the Quality of QM/MM Approaches to Describe Vacuo-to-Water Solvatochromic Shifts. 1
- 268 Azaarenes: 13 Rings in a Row by Cyclopentannulation. 0
- 267 C(spⁿ) π (n = 1B) Bond Activation by Iron. 0
- 266 Speciation and Structures in Pt Surface Sites Stabilized by N-Heterocyclic Carbene Ligands Revealed by Dynamic Nuclear Polarization Enhanced Indirectly Detected ¹⁹⁵Pt NMR Spectroscopic Signatures and Fingerprint Analysis. 1
- 265 Octahedral Rhenium Cluster Complexes with 1,2-Bis(4-pyridyl)ethylene and 1,3-Bis(4-pyridyl)propane as Apical Ligands. **2022**, 27, 7874 0
- 264 Mechanism Analysis of Ethanol Production from Cellulosic Insulating Paper Based on Reaction Molecular Dynamics. **2022**, 14, 4918 0
- 263 Current density functional framework for spin-orbit coupling. 1
- 262 Ab initio calculation based solvent system selection in silico for counter-current chromatography: separation of resibufogenin glycosylation products. **2022**, 463649 0
- 261 Chalcogen Bond as a Factor Stabilizing Ligand Conformation in the Binding Pocket of Carbonic Anhydrase IX Receptor Mimic. **2022**, 23, 13701 2
- 260 Azaarenes: 13 Rings in a Row by Cyclopentannulation. 0
- 259 Synthesis of Trapen Ligand-Based U(IV) and Th(IV) 2-Phosphaethynolate Complexes and Comparison of Covalency with Corresponding Ti(IV) Analogues. **2022**, 61, 17993-18001 0
- 258 Theoretical Study of Reaction Mechanisms of Carbon Dioxide with E π H₂ π -Type Frustrated Lewis Pairs (E = C π B π ; Z = N π i). 0
- 257 Bond Bundle Analysis of Ketosteroid Isomerase. 1
- 256 Activation of Alkynes by a Redox-Active Carboranyl Diphosphine and Formation of Boron-Containing Phosphacycles. 0
- 255 Thioxanthone-containing blue thermally activated delayed fluorescent emitter. 0
- 254 Computationally rational design of metal-involving halogen bonds with π covalency: Structures and bonding analysis. 0

- 253 Synthesis and Structural Characterization of Multi-Molybdenum-Substituted Preyssler-type Phosphotungstates. ○
- 252 Nature and Role of Formal Charge of the ion Inclusion in Hexanuclear Platinum(II) Host-Guest Species. Insights from Relativistic DFT Calculations. **2022**, 121298 ○
- 251 Understanding the Impact of Composition on the Geometry, Electronic Structure and Spectroscopic Profile of an Atomically Precise Gold-Phosphine Cluster. ○
- 250 Mn₂ Dimers Encapsulated in Silicon Cages: A Complex Challenge to MC-SCF Theory. **2022**, 27, 7544 ○
- 249 Predictions on Structural and Electronic Properties to Synthesize Bismuth-Carbon Compounds in Different Periodicities. **2022**, 15, 8150 ○
- 248 Growth mechanism study of boron nitride atomic layer deposition by experiment and density functional theory. **2023**, 217, 111919 ○
- 247 Unraveling the complexation effect of electron transporting materials with Liq on the charge transport properties: A theoretical perspective. **2022**, 140207 ○
- 246 Radical-like reactivity for dihydrogen activation by coinage metal-alumanyl complexes: computational evidence inspired by experimental main group chemistry. ○
- 245 Chemical bonding analysis on MgEH₁₅ (E = Sc and Y), highly stable clusters for hydrogen storage. **2023**, 811, 140240 ○
- 244 Molecular self-assembling structure and formation mechanism of lubricating grease: A computational simulation approach. **2023**, 179, 108150 ○
- 243 Placing gold on a β -surface: ligand design and impact on reactivity. ○
- 242 Accurate quantum-chemical fragmentation calculations for ion-water clusters with the density-based many-body expansion. **2022**, 25, 736-748 ○
- 241 Highly oxidized U(vi) within the smallest fullerene: gas-phase synthesis and computational study of boron-doped U@C₂₇B. 1
- 240 Physical image of amino acid interaction on graphene surface: Scientific fundamental for biological identification and detection from first-principles. **2023**, 131, 109571 ○
- 239 Relativistic Modulation of Supramolecular Halogen/Copper Interactions and Phosphorescence in Cu(I) Pyrazolate Cyclotrimers. ○
- 238 Spectroscopic evidence of a Xe-Xe bond in the linear Xe₂Au⁺Xe ion. **2022**, 59, 179-182 ○
- 237 Theoretical study on the structure and properties of Au-Au interlocking gold(I) thiolate [2]catenanes. ○
- 236 Computational designing of Au-decorated buckled bismuthene and its application as a humidity gas sensor. **2023**, 295, 127174 ○

- 235 Ultrasound-excited temozolomide sonosensitization induces necroptosis in glioblastoma. **2023**, 554, 216033 ○
- 234 Experimental and theoretical insight into biphasic extractive mass transfer of thorium into ionic liquid phase using chloroamide ligands. **2023**, 371, 121074 ○
- 233 Thermodynamics of hydrogen storage: Equilibrium study of the LOHC system indole/octahydroindole. **2023**, 335, 127025 1
- 232 Adsorption behavior of methylene blue on graphene and hexagonal boron nitride monolayers in aqueous solution: A first-principles treatment. **2023**, 174, 111151 ○
- 231 Insight into the effect of alkyl chain length and substituent bulkiness on the mobility anisotropy of benzothieno[3,2-b][1]benzothiophenes. **2022**, 10, 18423-18432 ○
- 230 Composition and Thickness Effect of TiAlN-Type Nanocoatings on the Strength of Their Bond with Iron: Quantum Chemical Analysis. **2022**, 43, 286-292 ○
- 229 Molecular enhancement factors for the P,T -violating electric dipole moment of the electron in BaCH₃ and . **2022**, 106, ○
- 228 Self-Assembled Monolayers of Molecular Conductors with Terpyridine-Metal Redox Switching Elements: A Combined AFM, STM and Electrochemical Study. **2022**, 27, 8320 ○
- 227 A TD-DFT study of optical properties of TiSiO₄ clusters. **2023**, 55, ○
- 226 The Halogen Effect on the Magnetic Behaviour of Dimethylformamide Solvates in [Fe(halide-salEen)₂]BPh₄. **2022**, 8, 162 ○
- 225 Mechanistic Insights into Oxidation-Induced Size Conversion of [Au₆(dppp)₄]²⁺ to [Au₈(dppp)₄Cl₂]²⁺. **2022**, 61, 19773-19779 ○
- 224 Occurrence and stability of anion-π interactions between phosphate and nucleobases in functional RNA molecules. **2022**, 50, 11455-11469 ○
- 223 Copper and Zinc Complexes of 2,7-Bis(6-methyl-2-pyridyl)-1,8-naphthyridine-A Redox-Active, Dinucleating Bis(bipyridine) Ligand. **2022**, 61, 19333-19343 ○
- 222 On the Nature of Three-Atom Metal Cluster Catalysis for N₂ Reduction to Ammonia. **2022**, 12, 14964-14975 1
- 221 Realistic simulation of thermoelectric characteristics of organic semiconductors based on electronic structure calculations. ○
- 220 Isomerism effects in relaxation dynamics of Au₂₄(SR)₁₆ thiolate-protected gold nanoclusters. **2023**, 34, 105701 ○
- 219 Hybrid Molecular Magnets with Lanthanide- and Countercation-Mediated Interfacial Electron Transfer between Phthalocyanine and Polyoxovanadate. 1
- 218 Electronic Structure of Re₂(O₂CR)₄Cl₂ Complexes (R = H, CMe₃) and Reassignment of the Electronic Absorption Spectrum of Re₂(O₂CCMe₃)₄Cl₂. **2022**, 7, 48600-48605 ○

217	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
216	Can the Fluxionality in Borospherene Influence the Confinement-Induced Bonding between Two Noble Gas Atoms?. 2022 , 27, 8683	0
215	New perspectives and insights into direct epoxidation of propylene using O ₂ and silver-based catalysts. 2022 , 119002	0
214	From Molecule to Device: Prediction and Validation of the Optical Orientation of Iridium Phosphors in Organic Light-Emitting Diodes.	0
213	Bimetallic Nickel Complexes Supported by a Planar Macrocyclic Diphosphanide Ligand.	0
212	Improved Vapor Pressure Prediction from PR + COSMOSAC EOS using Normal Boiling Temperature.	0
211	Periodic Trends in the Infrared and Optical Absorption Spectra of Metal Chalcogenide Clusters.	0
210	Unveiling novel reactivity of P/Al frustrated Lewis pair: ring size-dependent activation of cyclic ethers/thioethers and CO ₂ insertion therein. 2022 , 134,	0
209	Synthesis and Characterization of Yttrium Methanediide Silanide Complexes.	0
208	Theoretical Photoelectron Spectroscopy of Low-Valent Carbon Species: A ~6 eV Range of Ionization Potentials among Carbenes, Ylides, and Carbodiphosphanes.	0
207	Halogen Bonds between Diiodotetrafluorobenzenes and Halide Anions: Theoretical Analysis.	1
206	Relativistic density functional investigation of the mono-lanthanum silicide clusters LaSi _n (n=1-6): geometries, electronic properties and IR spectra. 2022 , 2393, 012023	0
205	Photocatalytic study of TiO ₂ Thin Films Modified with Anderson-Type Polyoxometalates (Cr, Co and Ni): Experimental and DFT study. 2022 , 116253	1
204	Geometry of Charge Density as a Reporter on the Role of the Protein Scaffold in Enzymatic Catalysis: Electrostatic Preorganization and Beyond.	2
203	Behavior of HF and (HF) ₂ inside a fullerene cage: An in silico study using different density functionals.	0
202	Holy Water: Photo-Brightening in Quasi-2D Perovskite Films under Ambient Enables Highly Performing Light-Emitting Diodes. 2209249	0
201	Quantum Chemical Prediction of the Acidities of Sulfonamide Inhibitors of Carbonic Anhydrase. 2022 , 126, 9207-9217	0
200	Experimental and Computational Studies of Ruthenium Complexes Bearing Z-Acceptor Aluminum-Based Phosphine Pincer Ligands. 2022 , 61, 20690-20698	0


- 199 Replenishment in the Family of Rhenium Chalcobromides; Synthesis and Structure of Molecular $\{\text{Re}_4\text{S}_4\}\text{Br}_8(\text{TeBr}_2)_4$, Dimeric $[\{\text{Re}_4\text{S}_4\}\text{Br}_8(\text{TeBr}_2)_3]_2$, and Polymeric $\{\text{Re}_4\text{S}_4\}\text{Br}_8$ Compounds Based on the $\{\text{Re}_4\text{S}_4\}^{8+}$ Tetrahedral Cluster Core. **2022**, 61, 20472-20479 1
- 198 Ambipolar Nickel Dithiolene Complex Semiconductors: From One- to Two-Dimensional Electronic Structures Based upon Alkoxy Chain Lengths. 0
- 197 C-D Bond Activation in Mononuclear Lanthanide Oxocarbonyl Complexes $\text{OLn}(\text{E}-\text{CO})$ ($\text{Ln} = \text{La}, \text{Ce}, \text{Pr}, \text{and Nd}$). 0
- 196 Complexation of N-Heterocyclic Substituted 1,10-Phenanthroline-2,9-diamide with $\text{Am}^{3+}/\text{Eu}^{3+}$ Ions for Nuclear Waste Water Treatment. **2022**, 7, 0
- 195 The subsystem quantum chemistry program Serenity. 0
- 194 Influence of Number of Ligands and Point Group on the Electronic Structure of Co^{2+} Aqua-Complexes. **2022**, 61, 20743-20756 0
- 193 Unraveling the Efficiency of Thioxanthone Based Triplet Sensitizers: A Detailed Theoretical Study. 0
- 192 Absolute Hydration Free Energy of Small Anions and the Aqueous pK_a of Simple Acids. **2022**, 126, 9190-9206 0
- 191 Unveiling the gemcitabine drug complexation with cucurbit[n]urils ($n=6-8$): A computational analysis. 0
- 190 Rb^+ -Metalated aryl iodides in Diels-Alder cycloaddition reactions: mode of activation and catalysis. 0
- 189 Attachment Chemistry of 4-Fluorophenylboronic Acid on TiO_2 and Al_2O_3 Nanoparticles. **2022**, 34, 10659-10669 0
- 188 Origins of the Reactivity in 1,3-Dipolar Cycloadditions of Acyl Isocyanide Ylides. 0
- 187 ReaxFF-based nonadiabatic dynamics method for azobenzene derivatives. **2022**, 157, 244101 0
- 186 Bonding of isovalent homologous actinide and lanthanide pairs with chalcogenide donors: effect of metal f-orbital participation and donor softness. 0
- 185 Mechanistic Study of Alkyne Insertion into Cu-Al and Au-Al Bonds: A Paradigm Shift for Coinage Metal Chemistry. **2022**, 61, 21095-21106 0
- 184 Characterization of Excited States in Time-Dependent Density Functional Theory Using Localized Molecular Orbitals. 0
- 183 Synthesis and Characterization of $[\text{Fe}_3(\text{As}_3)_3\text{As}_4]_3$ Binary Fe/As Zintl Cluster With an Fe_3 Core. 0
- 182 Effects of relativity on the superheavy dimers M_2 , $\text{M} = \text{Nh-Og}$. 0

- 181 Reductive Coupling of Nitric Oxide by Cu(I): Stepwise Formation of Mono- and Dinitrosyl Species En Route to a Cupric Hyponitrite Intermediate. ○
- 180 Thermodynamics of Hydrogen Storage: Equilibrium Study of Liquid Organic Hydrogen Carrier System 1-Methylindole/octahydro-1-methylindole. **2023**, 3, 45-63 ○
- 179 Shedding Light on the Physical Nature of Ion Pair Interactions Involving Carba-closo-dodecacaborate Anions. Insights from Computation. ○
- 178 Theoretical Insights into NH₃ Absorption Mechanisms with Imidazolium-based Protic Ionic Liquids. ○
- 177 Terminal and bridging ligand effects on M(I)M(I) multiple bonding: A DFT investigation of the coordination in (X)₂[M₂Cl]₂L₂ complexes (M = Cr, Fe). ○
- 176 Comparative Study of a Decadentate Acyclic Chelate, HOPO-O10, and Its Octadentate Analogue, HOPO-O8, for Radiopharmaceutical Applications. ○
- 175 Quantitative Descriptions of Dewar-Chatt-Duncanson Bonding Model: A Case Study of Zeise and Its Family Ions. ○
- 174 Density functional theory study on sensing properties of g-C₃N₄ sheet to atmospheric gasses: Role of zigzag and armchair edges. ○
- 173 The Halogen Bond in Weakly Bonded Complexes and the Consequences for Aromaticity and Spin-Orbit Coupling. **2023**, 28, 772 ○
- 172 The Search for Enhanced σ -Donor Ligands to Stabilize Boron-Boron Multiple Bonds. ○
- 171 Mechanistic Insights into Multisilver-Mediated Synergistic Activation of Terminal Alkynes. ○
- 170 Factors contributing to halogen bond strength and stretch or contraction of internal covalent bond. 1
- 169 Long-range Corrected Fragment Molecular Orbital Density-Functional Tight-binding Method for Excited States in Large Molecular Systems. 1
- 168 Modulating the Extent of Anisotropic Cuprophilicity via High Pressure with Piezochromic Luminescence Sensitization. 508-515 ○
- 167 Crystal Structure and Chemical Bonds in [CuII(TolF)4(MeOH)2]·2MeOH. **2023**, 24, 1745 ○
- 166 Synthesis and Characterization of [Fe3(As3)3As4]3, a Binary Fe/As Zintl Cluster With an Fe₃ Core. ○
- 165 SQMBox: Interfacing a semiempirical integral library to modular ab initio electronic structure enables new semiempirical methods. ○
- 164 An Unusual Core Engineering on A Copper Hydride Nanoball. ○

- 163 Structure, stability, electronic and optical properties of TMDC/coinage metal composites: Vertical atomically thin Self-assembly of Au₆ cluster. ○
- 162 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 ○
- 161 Atomistic insight into the effects of electrostatic fields on hydrocarbon reaction kinetics. ○
- 160 ConvPred : A Deep Learning-based Framework for Predictions of Potential Organic Reactions. ○
- 159 An Active Bio-Based Food Packaging Material of ZnO@Plant Polyphenols/Cellulose/Polyvinyl Alcohol: DESIGN, Characterization and Application. **2023**, 24, 1577 ○
- 158 Relativistic Quantum Calculations to Understand the Contribution of f-type Atomic Orbitals and Chemical Bonding of Actinides with Organic Ligands. ○
- 157 Understanding the enhanced reactivity of strained intermolecular Frustrated Lewis Pairs. ○
- 156 Manipulating Organic Semiconductor Morphology with Visible Light. 2212835 ○
- 155 Thioxanthone-containing blue thermally activated delayed fluorescent emitter. ○
- 154 Exploring depolymerization mechanism and complex reaction networks of aromatic structures in chemical looping combustion via ReaxFF MD simulations. **2023**, 107, 101180 ○
- 153 Fluoro, Trifluoromethyl, and Trifluoroacetyl Substituent Effects on Cycloaddition Reactivities: Computations and Analysis. **2023**, 88, 893-900 ○
- 152 Theoretical Studies on Thermally Activated Delayed Fluorescence Mechanism of Au(III) Complexes in Films: Insights from Quantum Mechanics/Molecular Mechanics Simulations. **2023**, 127, 672-681 ○
- 151 Do mono- or diphenol substitutions in phenanthroline-based ligands serve in effective separation of Am³⁺/Eu³⁺ ions?- Insights from DFT calculations. **2023**, 58, 627-641 ○
- 150 Carbonylmetallates as versatile 2-, 4- or 6-Electron Donor Metalloligands in Transition-Metal Complexes and Clusters: A Global Approach. ○
- 149 Molecular adsorption on coinage metal subnanoclusters: A DFT + D3 investigation. ○
- 148 Spin-State Splittings in 3d Transition-Metal Complexes Revisited: Toward a Reliable Theory Benchmark. **2023**, 19, 97-108 1
- 147 Widening the landscape of small molecule activation with gold-alumanyl complexes: a systematic study of E-H (E=O,N) bond, SO₂ and N₂O activation. ○
- 146 Azobenzene-Based Amino Acids for the Photocontrol of Coiled-Coil Peptides. ○

- 145 Functionalization of carbon and graphene quantum dots. **2023**, 335-381 ○
- 144 Structure effects of Pt₁₅ clusters for the oxygen reduction reaction: first-principles calculations. **2023**, 25, 4764-4772 ○
- 143 Insights into the Reactivity of the Ring-Opening Reaction of Tetrahydrofuran by Intramolecular Group-13/P- and Al/Group-15-Based Frustrated Lewis Pairs. ○
- 142 Theoretical Insights into the Optical and Excited State Properties of Donor-Benzylic Bridge-Acceptor Containing Through-Space Charge Transfer Molecules. **2023**, 127, 886-893 ○
- 141 Low-Temperature Luminescence in Organic Helicenes: Singlet versus Triplet State Circularly Polarized Emission. **2023**, 14, 1073-1081 ○
- 140 Five-Membered N-Heterocyclic Beryllium(I) Compounds: Fluctuating Electronic Structure with Ambiphilic Reactivity. ○
- 139 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 ○
- 138 Enhance Hydrogen Isotopes Separation by Alkali Earth Metal Dopant in Metal-Organic Framework. **2023**, 14, 1198-1207 1
- 137 Single-Atom Catalysis Enabled by High-Energy Metastable Structures. ○
- 136 A bond bundle case study of Diels-Alder catalysis using oriented electric fields. **2023**, 407-430 ○
- 135 Are Ar₃SbCl₂ Species Lewis Acidic? Exploration of the Concept and Pnictogen Bond Catalysis Using a Geometrically Constrained Example. ○
- 134 XPu(CO)_n (X = B, Al, Ga; n = 2 to 4): Back-Bonding in Heterodinuclear Plutonium Boron Group Compounds with an End-On Carbonyl Ligand. **2023**, 127, 1233-1243 ○
- 133 Cobalt complexes with multi-dentate N-donor ligands: Redox, X-ray photoelectron spectroscopic and theoretical study. **2023**, 5, 100818 ○
- 132 Type Tilted Quasi-One-Dimensional Assembly of Actinide-Embedded Coinage Metal Near-Plane Superatoms and Their Optical Properties. 2206899 ○
- 131 Theoretical Investigation of Single-Molecule-Magnet Behavior in Mononuclear Dysprosium and Californium Complexes. **2023**, 62, 1649-1658 ○
- 130 Switching between Fluorescence and Room Temperature Phosphorescence in Carbon Dots: Key Role of Heteroatom Functionalities. **2023**, 127, 2430-2439 ○
- 129 A Reactive Molecular Dynamics Study of Chlorinated Organic Compounds. Part I: Force Field Development. ○
- 128 Gradient bundles. **2023**, 359-373 ○

- 127 Facile modification of phosphole-based aggregation-induced emission luminogens with sulfonyl isocyanates. ○
- 126 Prediction of Donor-Acceptor Type Novel Noble Gas Complexes in the Triplet Electronic State. ○
- 125 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 ○
- 124 Unveiling the gemcitabine drug complexation with cucurbit[n]urils (n = 6B): a computational analysis. ○
- 123 Synthesis, characterization, in-vitro biological evaluation and theoretical studies of 1,2,3-triazoles derived from triclosan as difenconazole analogues. **2023**, 1280, 135053 ○
- 122 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 ○
- 121 Calculation of electric field gradients in Cd(II) model complexes of the CueR protein metal site. ○
- 120 Halogen bonds with carbenes acting as Lewis base units: complexes of imidazol-2-ylidene: theoretical analysis and experimental evidence. **2023**, 25, 9636-9647 ○
- 119 Monocarboxylate-Protected Two-Electron Superatomic Silver Nanoclusters with High Photothermal Conversion Performance. ○
- 118 Spark Discharge Doping Achieving Unprecedented Control over Aggregate Fraction and Backbone Ordering in Poly(3-hexylthiophene) Solutions. 2207537 ○
- 117 Theoretical Insights into the Substitution Effect of Phenanthroline Derivatives on Am(III)/Eu(III) Separation. **2023**, 62, 2705-2714 ○
- 116 Conjugated Imine Polymer Synthesized via Step-Growth Metathesis for Highly Stable Silicon Nanoparticle Anodes in Lithium-Ion Batteries. **2023**, 13, ○
- 115 A study of the oxidation mechanism of the organic pigment indigo in grottoes murals by ozone under dark conditions. **2023**, 11, ○
- 114 Long-Alkyl Chain Functionalized Imidazo[1,5-a]pyridine Derivatives as Blue Emissive Dyes. **2023**, 2, 179-193 ○
- 113 Alanine boronic acid functionalized UiO -66 MOF as a nanoreactor for the conversion of CO₂ into formic acid. ○
- 112 Remote substituent effects on catalytic activity of metal-organic frameworks: a linker orbital energy model. **2023**, 9, ○
- 111 The coupling of graphene, graphitic carbon nitride and cellulose to fabricate zinc oxide-based sensors and their enhanced activity towards air pollutant nitrogen dioxide. **2023**, 324, 138325 ○
- 110 Synthesis, spectra, crystal, DFT, molecular docking and in vitro cholinesterase inhibition evaluation on two novel symmetrical Azine Schiff bases. **2023**, 1281, 135171 ○

- 109 Unraveling the role of the external electric field on the photo-physical properties of thermally activated delayed fluorescence. **2023**, 30, 101515 ○
- 108 The interplay between spin states, geometries and biological activity of Fe(III) and Mn(II) complexes with thiosemicarbazone. **2023**, 237, 116389 ○
- 107 Structure, stability, and properties of cyclo[18]carbon-Zinc super sandwich complexes (C18-Zn-C18). **2023**, 991, 122668 ○
- 106 Computational approach to establish molecularly imprinted polymers interaction of functional monomer methacrylic acid and template norfloxacin. **2023**, 1224, 114124 ○
- 105 Exploring the solvation of water molecules around radioactive elements in nuclear waste water treatment. **2023**, ○
- 104 The design of push-pull substituted coronene molecules for optoelectronic applications. **2023**, 301, 127631 ○
- 103 Thermodynamics of hydrogen storage: LOHC system 1-alkyl-indole/octahydro-1-alkyl-indole. **2023**, 344, 128079 ○
- 102 Exploring Mg decorated antimonene for promising hydrogen storage material: A DFT outlook. **2023**, 161, 107471 ○
- 101  **2022**, 59-65 ○
- 100 DFT perspective of gas sensing properties of Fe-decorated monolayer antimonene. **2023**, 616, 156520 ○
- 99 Computational investigations on the 4-*pyridine* adsorbed on ZnO/graphene oxide nanocomposite toward the efficient performance of surface-enhanced Raman scattering. **2023**, 133, 109693 ○
- 98 Simulation strategies for ReaxFF molecular dynamics in coal pyrolysis applications: A review. **2023**, 170, 105882 ○
- 97 Anion recognition using enhanced halogen bonding through intramolecular hydrogen bonds: A computational insight. **2023**, 47, 4439-4447 ○
- 96 Electronic circular dichroism from real-time propagation in state space. **2023**, 158, 084102 ○
- 95 On the Cation-Binding Capabilities of Infitene: Evaluation of bonding and circular dichroism properties for Infitene-Ag(I)_n (n = 1-4) complexes from relativistic DFT calculations. **2023**, 234, 116323 ○
- 94 Palladium-catalyzed activation of Hn-AHn bonds (AHn = CH₃, NH₂, OH, F). **2023**, ○
- 93 The Raman Active Vibrations of Flavone and Quercetin: The Impact of Conformers and Hydrogen Bonding on Fingerprint Modes. **2023**, 127, 1387-1394 ○
- 92 Theoretical screening of M₃(btc)₂ metal-organic frameworks for ethylene and 1-methylcyclopropene storage. **2023**, 5, 100831 ○

- 91 From 8- to 18-Cluster Electrons Superatoms: Evaluation via DFT Calculations of the Ligand-Protected W@Au₁₂(dppm)₆ Cluster Displaying Distinctive Electronic and Optical Properties. **2023**, 62, 3047-3055 ○
- 90 The 8-Hydroxyquinolinium Cation as a Lead Structure for Efficient Color-Tunable Ionic Small Molecule Emitting Materials. **2023**, 4, 2200279 ○
- 89 Computational and experimental studies on spectra and bonding of cyclohexane linked tris-hydroxyquinoline flexible tripodal chelator and its complexes. ○
- 88 Torsional Rotation in Ditopic Receptor Host and its Complex Formation with Resorcinol Guest: A Computational Study. ○
- 87 The transition state region in nonsynchronous concerted reactions. **2023**, 158, 084109 ○
- 86 Understanding the Coordination Chemistry of Am^{III}/Cm^{III} in the DOTA Cavity: Insights from Energetics and Electronic Structure Theory. **2023**, 62, 3229-3237 ○
- 85 Electronic Structure and Magneto-Structural Correlations Study of Cu₂UL Trinuclear Schiff Base Complexes: A 3d⁹f⁹d Case. **2023**, 127, 1475-1490 ○
- 84 Encapsulation of xenon by bridged resorcinarene cages with high ¹²⁹Xe NMR chemical shift and efficient exchange dynamics. **2023**, 4, 101281 ○
- 83 Theoretical simulations on metal nanocluster systems. **2023**, 201-231 ○
- 82 Unusual Square Pyramidal Chalcogenide Mo₅ Cluster with Bridging Pyrazolate-Ligands. **2023**, 24, 3440 ○
- 81 The disposition of bridge hydrogen bond in the homopolar-diborane and its derivatives. **2023**, 1222, 114071 ○
- 80 First-Principles Calculation of Ligand Field Parameters for L-Edge Spectra of Transition Metal Sites of Arbitrary Symmetry. **2023**, 15, 472 ○
- 79 Unicorns, Rhinoceroses and Chemical Bonds. **2023**, 28, 1746 ○
- 78 Thiol modifier effects of diphenyl diselenides: insight from experiment and DFT calculations. **2023**, 47, 5796-5803 ○
- 77 The combination of polyphenols and phospholipids as an efficient platform for delivery of natural products. **2023**, 13, ○
- 76 Cd Atom Goes into the Interior of Cluster Induced by Directional Consecutive Assembly of Tetrahedral Units on an Icosahedron Kernel. ○
- 75 Modeling Adsorption of CO₂ in Rutile Metallic Oxide Surfaces: Implications in CO₂ Catalysis. **2023**, 28, 1776 ○
- 74 Oxo-Bridged Zr Dimers as Well-defined Models of Oxygen Vacancies on ZrO₂. ○

- 73 Manganese(III) complexes with tetradentate O⁺C⁺C⁺O ligands: Synthesis, characterization and catalytic studies on the CO₂ cycloaddition with epoxides. **2023**, 538, 113006 ○
- 72 Improving the TADF in Corannulene-Based Emitters via Tuning the Strength of Donor and Acceptor Groups. **2023**, 6, ○
- 71 Mg(i)Be(II) and Mg(0)Mg(i) covalent bonding in the Mg_nFe(CO)₄(n = 1, 2) anion complexes: an infrared photodissociation spectroscopic and theoretical study. **2023**, 25, 7697-7703 ○
- 70 Carbon-free sandwich compounds based on arsenic and antimony with icosahedral metal cores. ○
- 69 Molecular structures, chemical descriptors and pancreatic lipase (1LPB) inhibition by natural products: A DFT investigation and molecular docking prediction. ○
- 68 Weak Interactions Initiate C-H and C-C Bond Dissociation of Ethane on Nb_n + Clusters. ○
- 67 Revealing reactive mechanism and nitrogen transformation of HSW coal combustions at molecule and particle scales. **2023**, 419, 118368 ○
- 66 Enantioselective Total Synthesis of (±)-Himalensine A via a Palladium and 4-Hydroxyproline Co-catalyzed Desymmetrization of Vinyl-bromide-tethered Cyclohexanones. **2023**, 145, 5422-5430 ○
- 65 Molecular and electronic structures, bonding analysis, and UV-Vis spectra predictions of quinolino[3,2-b]benzodiazepine and quinolino[3,2-b]benzoxazepine metal transition M(L)₂Cl₂ and M(L)Cl₂ complexes. ○
- 64 Unveiling Structural Diversity of Uranyl Compounds of Aprotic 4,4'-Bipyridine N,N'-Dioxide Bearing O-Donors. **2023**, 8, 8894-8909 ○
- 63 Not antiaromaticity gain, but increased asynchronicity enhances the Diels-Alder reactivity of tropone. **2023**, 59, 3703-3706 ○
- 62 Trapping of Small Molecules within Single or Double Cyclo[18]carbon Rings. **2023**, 28, 2157 ○
- 61 Substituent Effects in Bioorthogonal Diels-Alder Reactions of 1,2,4,5-Tetrazines. ○
- 60 Perfect planar polyynic cyclo[n]carbon complexes [Cs⁺ C₁₈]⁺ and [Na⁺ C₁₄]⁺ with alkaline-metal centers exhibiting record coordination numbers and transition metal behaviors. ○
- 59 Superatomic states under high pressure. **2023**, 26, 106281 ○
- 58 Spin-crossing in heterogeneous ethane dehydrogenation by atomically dispersed Co/SiO₂. **2023**, 3, 100534 ○
- 57 Covalent functionalization of graphene sheets for plasmid DNA delivery: experimental and theoretical study. **2023**, 13, 7000-7008 ○
- 56 Isostructural coordination polymers of the tethering naphthalene anchored bis(2-methylpyridinecarboxamide) ligand: single crystal, XPS, EDS and theoretical studies. **2023**, 47, 5477-5487 ○

- 55 Influence of Group 15 elements on the [3 + 2] cycloaddition reactivity of G15 = G15 π -15-based 1,3-dipoles with cyclooctyne. **2023**, 52, 4796-4807 ○
- 54 Are π Bonds Inside Fullerenes Really Unwilling Bonds?. **2023**, 145, 6710-6718 ○
- 53 Quest for singlet fission of organic sulfur-containing systems in the higher lying singlet excited state: application prospects of anti-Kasha's rule. **2023**, 25, 9115-9122 ○
- 52 Stabilisation and reactivity studies of donor-base ligand-supported gallium-phosphides with stronger binding energy: a theoretical approach. **2023**, 13, 7738-7751 ○
- 51 FIRST EXAMPLE OF RUTHENIUM NITROSO COMPLEXES WITH A NITROXYL RADICAL AS A LIGAND. **2023**, 64, 169-178 ○
- 50 9-Borafluoren-9-yl and diphenylboron tetracoordinate complexes of F- and Cl-substituted 8-quinolinolato ligands: synthesis, molecular and electronic structures, fluorescence and application in OLED devices. **2023**, 52, 4933-4953 ○
- 49 Investigation of electronic and thermal properties of CoCrFe and CoCrFeNi high entropy alloys via extended tight-binding DFT computational method. ○
- 48 Assessments of DFT-based energy decomposition analysis methods for intermolecular interactions. **2023**, 158, 124116 ○
- 47 PromoterPoison Partnership Protects Platinum Performance in Coked Cluster Catalysts. **2023**, 127, 5376-5384 ○
- 46 ScY @ C_{3v}(8)-C₈₂: Metal-Metal π Bond in Mixed Rare-Earth Di-metallofullerenes. ○
- 45 Improved Synthesis of (TBA)₂[W₆Br₁₄] Paving the Way to Further Study of Bromide Cluster Complexes. **2023**, 62, 4934-4946 ○
- 44 Solid-State ¹⁹F NMR Chemical Shift in Square-Planar Nickel(II) Fluoride Complexes Linked by Halogen Bonds. **2023**, 62, 4835-4846 ○
- 43 Investigation of Newly Synthesized Bis-Acyl-Thiourea Derivatives of 4-Nitrobenzene-1,2-Diamine for Their DNA Binding, Urease Inhibition, and Anti-Brain-Tumor Activities. **2023**, 28, 2707 ○
- 42 Theoretical study of the tuning role of π -methylthio or π -methylselenyl on the charge-transport properties of acenedithiophenes derivatives. **2023**, 25, 10313-10324 ○
- 41 The Electronic Nature of Cationic Group 10 Ylidyne Complexes. **2023**, 11, 129 1
- 40 Intramolecular O \cdots H Hydrogen Bonding of Salicylic Acid: Further Insights from O 1s XPS and ¹H NMR Spectra Using DFT Calculations. **2023**, 127, 2705-2716 ○
- 39 Predicting Preferences for Adduct Formation in Electrospray Ionization: The Case Study of Succinic Acid. **2023**, 34, 562-569 ○
- 38 Density Functional Study on the Photopolymerization of Styrene Using Dinuclear Ru(II) and Ir(III) Complexes with Naphthyl-Substituted Ligands. **2023**, 127, 2810-2818 ○

- 37 Converting CO₂ to formic acid by tuning quantum states in metal chalcogenide clusters. **2023**, 6, ○
- 36 Helical allophycocyanin nanotubes absorb far-red light in a thermophilic cyanobacterium. **2023**, 9, ○
- 35 The essential role of symmetry in understanding ³He chemical shifts in endohedral helium fullerenes. **2023**, 25, 10620-10627 ○
- 34 Isolation of a californium(II) crown ether complex. ○
- 33 Imidazolin-2-imine and Imidazolin-2-methylidene Substitutions to Benzene, Pyridine, Phosphine, and N-Heterocyclic Carbene Predict Highly Electron-rich Ligands. **2023**, 42, 571-580 ○
- 32 On the Utmost Importance of the Basis Set Choice for the Calculations of the Relativistic Corrections to NMR Shielding Constants. **2023**, 24, 6231 ○
- 31 Thermal isomerization of phenylazindoles: Inversion or rotation? That is the question. ○
- 30 A first glance into mixed phosphine-tibine moieties as protecting ligands for gold clusters. **2023**, 15, 6934-6940 ○
- 29 Multistimuli-responsive behavior of a phosphorescent Cu₃pyrazolate₃ complex for luminescent logic gates and encrypted information transformation. ○
- 28 Effects of Solvents on Reaction Products: Synthesis of Endohedral Metallofullerene Oxazoline and Epoxide. **2023**, 88, 4234-4243 ○
- 27 Local reactivity descriptors of the important atoms in chelotropic reactions provide insight into their global variants along the reaction path. ○
- 26 A photoelectron spectroscopic investigation of aspirin, paracetamol and ibuprofen in the gas phase. **2023**, 25, 10946-10955 ○
- 25 A facile synthesis and comparative structural characterization with DFT, fluorescence behavior, and anti-microbial activity of O,O'-diethyl-S-(N-phthalimidomethyl) dithiophosphate. 1-9 ○
- 24 Diastereoselective Synthesis of cis-2,6-Disubstituted Dihydropyran Derivatives through a Competitive Silyl-Prins Cyclization versus Alternative Reaction Pathways. **2023**, 28, 3080 ○
- 23 Influencing Bonding Interactions of the Neptunyl (V, VI) Cations with Electron-Donating and -Withdrawing Groups. **2023**, 62, 6055-6064 ○
- 22 Acceleration of Stepwise Carbon-Polygold Bonding Cleavage in Hypercoordinated Carbon-Centered Gold(I) Clusters. **2023**, 62, 6147-6154 ○
- 21 Unveiling the Latent Reactivity of Cp* Ligands (C₅Me₅) toward Carbon Nucleophiles on an Iridium Complex. **2023**, 62, 5961-5971 ○
- 20 Diversity of Chemical Bonding in Zintl Clusters. **2023**, ○

- 19 Structure and stability of a new set of noble gas insertion compounds, $XNgOPO(OH)_2$ ($X = F, Cl, Br$; $Ng = Kr, Xe, Rn$): an in silico investigation. **2023**, 142,
- 18 Genuine quadruple bonds between two main-group atoms. Chemical bonding in AeF_4 ($Ae = Be, Ba$) and isoelectronic EF ($E = B, Si$) and the particular role of d orbitals in covalent interactions of heavier alkaline-earth atoms.
- 17 A Tetraiodomanganate(II) Compound with P,P'-Diprotonated Bis(2-Diphenylphosphinophenyl)Ether Manifesting Unexpected Short Luminescence Lifetime. **2023**, 64, 398-409
- 16 ETS-NOCV and molecular electrostatic potential-based picture of chemical bonding. **2023**,
- 15 Alkali Tin Halides: Exploring the Local Structure of A_2SnX_6 ($A = K, Rb$; $X = Cl, Br, I$) Compounds Using Solid-State NMR and DFT Computations. **2023**, 127, 7284-7298
- 14 A First-Principles Investigation of Structure-Luminescence Activity of Donor-Acceptor-Donor Organic Triad. **2023**, 127, 3330-3338
- 13 Complex with Linear BBB Skeleton Trapped in Dinitrogen Matrix: Matrix Infrared Spectra and Quantum Chemical Calculations.
- 12 Conjugation of a Silver-Based Coordination Polymer with Curcumin: A New Case of an Inorganic Polymeric Co-crystal.
- 11 Structure and aggregation behavior of pertechnetate/perrhenate in organic phase in the extraction by tributyl phosphate.
- 10 Construction of a 3D Onion-like Model of Conductive Carbon Black for Lithium-Ion Batteries and Exploration of the Electrochemical Oxidation Mechanism of CB and Ethylene Carbonate via ReaxFF MD.
- 9 Nonaromatic naphthocorroles.
- 8 Spectroscopical and Molecular Studies of Four Manganese(I) PhotocORMs with Bioinspired Ligands Containing Non-Coordinated Phenol Groups. **2023**, 28, 3439
- 7 Tristhiolato Pseudopeptides Bind Arsenic(III) in an AsS_3 Coordination Environment Imitating Metalloid Binding Sites in Proteins.
- 6 Continuum vs. atomistic approaches to computational spectroscopy of solvated systems.
- 5 Ultrafiltration separation of $Am(VI)$ -polyoxometalate from lanthanides. **2023**, 616, 482-487
- 4 Quantum mechanics/fluctuating charge calculations for absorption spectra of aqueous green fluorescent protein chromophore.
- 3 Theoretical Underpinning of Synergetic Ir/Cu-Metallaphotoredox Catalysis in Multicomponent $C-N$ Cross-Coupling Reactions. 6249-6260
- 2 Dative quadruple bonds between d 10 transition metals and beryllium in $BeM(PMe_3)_2$ and $BeM(CO)_2$ ($M = Ni, Pd$, and Pt).

- 1 Exploring the structure of halomethanes with xenon: An NMR and MD investigation. **2023**, 382, 122011 ○