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- 2184 Boosting CO₂ Electroreduction to CH₄ via Tuning Neighboring Single-Copper Sites.
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- 2180 Computational Design of Non-natural Sugar Alcohols to Increase Thermal Storage Density: Beyond Existing Organic Phase Change Materials.
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- 2176 Rare Examples of Fe(IV) Alkyl-Imide Migratory Insertions: Impact of FeC Covalency in (Me2IPr)Fe(NAd)R2 (R = neoPe, 1nor).
- 2175 Silicon and Oxygens Bond of Affection: An Acyclic Three-Coordinate Silanone and Its Transformation to an Iminosiloxysilylene.
- 2174 Dynamics and Reactions of Molecular Ru Catalysts at Carbon Nanotube/Water Interfaces.
- 2173 Cp* Noninnocence Leads to a Remarkably Weak CH Bond via Metallocene Protonation.
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- 2171 .
- 2170 Ligand Redox Noninnocence in [CoIII(TAML)]0/ Complexes Affects Nitrene Formation.
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2158 .

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2156 .

2155 Cyclombandakamines A1 and A2, Oxygen-Bridged Naphthylisoquinoline Dimers from a Congolese Ancistrocladus Liana.

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2145 Site-Selective Carbene-Induced CH Functionalization Catalyzed by Dirhodium Tetrakis(triarylcyclopropanecarboxylate) Complexes.

2144 Intramolecular Hydrogen Bond Activation: Thiourea-Organocatalyzed Enantioselective 1,3-Dipolar Cycloaddition of Salicylaldehyde-Derived Azomethine Ylides with Nitroalkenes.

2143 Highly Chemo- and Stereoselective Transfer Semihydrogenation of Alkynes Catalyzed by a Stable, Well-Defined Manganese(II) Complex.

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2141 Comparison of Reactivity and Enantioselectivity between Chiral Bimetallic Catalysts: BismuthRhodium- and Dirhodium-Catalyzed Carbene Chemistry.

- 2140 Catalytic Enantioselective Cyclopropanation of Fluoroacrylates: An Experimental and Theoretical Study.
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- 2136 Activation of H₂ over the RuZn Bond in the Transition Metal-Lewis Acid Heterobimetallic Species [Ru(IPr)₂(CO)ZnEt]⁺.
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- 2132 A Strategy to Synthesize Molecular Knots and Links Using the Hydrophobic Effect.
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- 2127 Nickel-Catalyzed [5+2] Cycloaddition of 10-Electron Aromatic Benzothiophenes with Alkynes To Form Thermally Metastable 12-Electron Nonaromatic Benzothiepinines.
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- 2125 .
- 2124 Robust Metal-Triazolate Frameworks for CO₂ Capture from Flue Gas.
- 2123 Effects of Ortho-halogen Substituents on Nitrate Binding in Urea-Based Silver(I) Coordination Polymers.

2122	How Do Ring Size and Donating Thiolate Ligands Affect Redox-Active, IminoNheterocycle Ligand Activation?.		
2121	Cycloosmathioborane Compounds: Other Manifestations of the Huckel Aromaticity.		
2120	Introducing NHeterocyclic Borylenes: Theoretical Prediction of Stable, Neutral, Monomeric Boron(I) Carbenoids.		
2119	A Dinuclear Copper Complex Featuring a Flexible Linker as Water Oxidation Catalyst with an Activity Far Superior to Its Mononuclear Counterpart.		
2118	Overcoming systematic DFT errors for hydrocarbon reaction energies. 2010 , 127, 429-442		45
2117	Theoretical treatment of the electronic excited states of the DMSO molecule: A challenge for current theoretical methods. 2010 , 377, 136-141		2
2116	Local response dispersion method. II. Generalized multicenter interactions. <i>Journal of Chemical Physics</i> , 2010 , 133, 194101	3.9	82
2115	Correcting for dispersion interaction and beyond in density functional theory through force matching. <i>Journal of Chemical Physics</i> , 2010 , 133, 174115	3.9	23
2114	Importance of London dispersion effects for the packing of molecular crystals: a case study for intramolecular stacking in a bis-thiophene derivative. 2010 , 12, 8500-4		100
2113	Assessment of TD-DFT methods and of various spin scaled CIS(D) and CC2 versions for the treatment of low-lying valence excitations of large organic dyes. <i>Journal of Chemical Physics</i> , 2010 , 132, 184103	3.9	282
2112	Adsorption of small aromatic molecules on the (111) surfaces of noble metals: A density functional theory study with semiempirical corrections for dispersion effects. <i>Journal of Chemical Physics</i> , 2010 , 132, 224701	3.9	201
2111	Two- and three-body interatomic dispersion energy contributions to binding in molecules and solids. <i>Journal of Chemical Physics</i> , 2010 , 132, 234109	3.9	180
2110	First-Principles-Based Dispersion Augmented Density Functional Theory: From Molecules to Crystals. 2010 , 1, 2550-2555		36
2109	The Relevance of Dispersion Interactions for the Stability of Oxide Phases. 2010 , 114, 22718-22726		55
2108	Nonlocal van der Waals density functional: the simpler the better. <i>Journal of Chemical Physics</i> , 2010 , 133, 244103	3.9	799
2107	Water Adsorption on Coordinatively Unsaturated Sites in CuBTC MOF. 2010 , 1, 3354-3359		142
2106	n-Alkane isodesmic reaction energy errors in density functional theory are due to electron correlation effects. 2010 , 12, 4670-3		51
2105	Molecular Crystals: A Test System for Weak Bonding \square 2010 , 114, 20523-20530		14

2104	Probing the hydration structure of polarizable halides: a multiedge XAFS and molecular dynamics study of the iodide anion. 2010 , 114, 12926-37	68
2103	A System-Dependent Density-Based Dispersion Correction. 2010 , 6, 1990-2001	118
2102	Thermochemical benchmarking of hydrocarbon bond separation reaction energies: Jacob's ladder is not reversed!. 2010 , 108, 2655-2666	45
2101	DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction. 2010 , 114, 20801-20808	261
2100	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. 2010 , 35, 435-442	244
2099	Improved description of the structure of molecular and layered crystals: ab initio DFT calculations with van der Waals corrections. 2010 , 114, 11814-24	737
2098	Validation of dispersion-corrected density functional theory calculations for the crystal structure prediction of molecular salts: a crystal structure prediction study of pyridinium chloride. 2010 , 12, 3827	12
2097	Stability of noble-gas hydrocarbons in an organic liquid-like environment: HXeCCH in acetylene. 2011 , 13, 19601-6	26
2096	On the dimerization of chlorophyll in photosystem II. 2011 , 13, 16022-7	15
2095	Binding modes of oxalate in UO ₂ (oxalate) in aqueous solution studied with first-principles molecular dynamics simulations. Implications for the chelate effect. 2011 , 40, 11192-9	11
2094	Heating a bowl of single-molecule-soup: structure and desorption energetics of water-encapsulated open-cage [60] fullerene anions in the gas-phase. 2011 , 13, 9818-23	29
2093	Dissolution thermochemistry of alkali metal dianion salts (M ₂ X ₁ , M = Li ⁺ , Na ⁺ , and K ⁺ with X = CO ₃ ²⁻ , SO ₄ ²⁻ , C ₈ H ₈ ²⁻ , and B ₁₂ H ₁₂ ²⁻). 2011 , 50, 11412-22	10
2092	Free energy of reaction by density functional theory: oxidative addition of ammonia by an iridium complex with PCP pincer ligands. 2011 , 1, 1526	39
2091	Conformer interconversion in a switchable porous organic cage. 2011 , 13, 20081-5	16
2090	Crystal-structure prediction of pyridine with four independent molecules. 2011 , 13, 7135	27
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2088	On the PES for the interaction of an H atom with an H chemisorbate on a graphenic platelet. 2011 , 13, 17579-87	13
2087	Multiscale modelling in computational heterogeneous catalysis. 2012 , 307, 69-107	39

2086	Polarized Molecular Orbital Model Chemistry. II. The PMO Method. 2011 , 7, 857-867	24
2085	Application of the Quantum Cluster Equilibrium (QCE) model for the liquid phase of primary alcohols using B3LYP and B3LYP-D DFT methods. 2011 , 115, 3936-41	19
2084	Improved DFT description of intrastrand cross-link formation by inclusion of London dispersion corrections. 2011 , 115, 15138-44	21
2083	Electronic structure of a weakly antiferromagnetically coupled Mn(II)Mn(III) model relevant to manganese proteins: a combined EPR, ⁵⁵ Mn-ENDOR, and DFT study. 2011 , 50, 8238-51	46
2082	Transition metal-alkane π -complexes with oxygen donor co-ligands. 2011 , 133, 13806-9	33
2081	Isotopic hydration of cellobiose: vibrational spectroscopy and dynamical simulations. 2011 , 115, 9498-509	25
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2079	Density Functional Theoretical Study of Perfluoropentacene/Noble Metal Interfaces with van der Waals Corrections: Adsorption States and Vacuum Level Shifts. 2011 , 115, 5767-5772	22
2078	Novel substrate-based inhibitors of human glutamate carboxypeptidase II with enhanced lipophilicity. 2011 , 54, 7535-46	18
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2076	Aurophilic Interactions from Wave Function, Symmetry-Adapted Perturbation Theory, and Rangehybrid Approaches. 2011 , 7, 2399-407	34
2075	Nuclear shieldings with the SSB-D functional. 2011 , 115, 1250-6	16
2074	Stability of Hydrocarbons of the Polyhedrane Family: Convergence of ab Initio Calculations and Corresponding Assessment of DFT Main Approximations. 2011 , 7, 2761-5	3
2073	Reaction of aminodihydropentalenes with HB(C ₆ F ₅) ₂ : the crucial role of dihydrogen elimination. 2011 , 133, 3480-91	14
2072	Effect of nitrogen adsorption on the mid-infrared spectrum of water clusters. 2011 , 115, 6218-25	22
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2070	Proton ordering in cubic ice and hexagonal ice; a potential new ice phase--Xlc. 2011 , 13, 19788-95	55
2069	VOPO ₄ ·H ₂ O: a stacking faults structure studied by X-ray powder diffraction and DFT-D calculations. 2011 , 50, 4378-83	11

2068	Heat-to-connect: surface commensurability directs organometallic one-dimensional self-assembly. 2011 , 5, 9093-103	62
2067	Hydrogen bonds and van der waals forces in ice at ambient and high pressures. 2011 , 107, 185701	181
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2065	Understanding the interaction of the porphyrin macrocycle to reactive metal substrates: structure, bonding, and adatom capture. 2011 , 5, 1831-8	55
2064	On the Mechanism of Iridium-Catalyzed Asymmetric Hydrogenation of Imines and Alkenes: A Theoretical Study. 2011 , 30, 2483-2497	107
2063	Charge Transfer in Molecular Complexes with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ): A Density Functional Theory Study. 2011 , 23, 5149-5159	87
2062	Adsorption of Gases in Microporous Organic Molecular Crystal, a Multiscale Computational Investigation. 2011 , 115, 4935-4942	13
2061	Density functional theory study of pyrophyllite and M-montmorillonites (M = Li, Na, K, Mg, and Ca): role of dispersion interactions. 2011 , 115, 9695-703	55
2060	Cation-cation "attraction": when London dispersion attraction wins over Coulomb repulsion. 2011 , 50, 2619-28	112
2059	A step beyond the Feltham-Enemark notation: spectroscopic and correlated ab initio computational support for an antiferromagnetically coupled M(II)-(NO)- description of Tp*M(NO) (M = Co, Ni). 2011 , 133, 18785-801	83
2058	Weak Molecular Interactions Studied with Parallel Implementations of the Local Pair Natural Orbital Coupled Pair and Coupled Cluster Methods. 2011 , 7, 76-87	127
2057	Computational Insights into Palladium-Mediated Allylic Substitution Reactions. 2011 , 65-93	22
2056	Electronic structure and chemical bond in naphthalene and anthracene. 2011 , 13, 5679-86	45
2055	BiomaterialBiomolecule Interaction: DFT-D Study of Glycine Adsorption on Cr2O3. 2011 , 115, 719-727	26
2054	Dynamics of carbene cycloadditions. 2011 , 133, 17848-54	56
2053	Van der Waals effects in ab initio water at ambient and supercritical conditions. <i>Journal of Chemical Physics</i> , 2011 , 135, 154503	3,9 127
2052	Directional Dependence of Hydrogen Bonds: a Density-based Energy Decomposition Analysis and Its Implications on Force Field Development. 2011 , 7, 4038-4049	33
2051	The calculation of intermolecular interaction energies. 2011 , 107, 148	24

2050	Parameterization of a B3LYP specific correction for non-covalent interactions and basis set superposition error on a gigantic dataset of CCSD(T) quality non-covalent interaction energies. 2011 , 7, 658-668	59
2049	Evaluation of a combination of local hybrid functionals with DFT-D3 corrections for the calculation of thermochemical and kinetic data. 2011 , 115, 8990-6	25
2048	Electronic structures of silver oxides. 2011 , 84,	51
2047	Accuracy of Density Functionals in the Prediction of Electronic Proton Affinities of Amino Acid Side Chains. 2011 , 7, 3898-908	35
2046	The directive of the protein: how does cytochrome P450 select the mechanism of dopamine formation?. 2011 , 133, 7977-84	200
2045	The reactivity of endohedral fullerenes. What can be learnt from computational studies?. 2011 , 13, 3585-603	117
2044	The polymorphism of ice: five unresolved questions. 2011 , 13, 18468-80	163
2043	Geometry Optimization of the Active Site of a Large System with the Fragment Molecular Orbital Method. 2011 , 2, 282-288	60
2042	Preparation, Structure, and Ether Cleavage of a Mixed Hapticity Allyl Compound of Calcium. 2011 , 30, 5291-5296	24
2041	Protein-ligand interaction energies with dispersion corrected density functional theory and high-level wave function based methods. 2011 , 115, 11210-20	73
2040	Density functional theory studies of interactions of ruthenium-arene complexes with base pair steps. 2011 , 115, 11293-302	21
2039	A Parameter-Free Density Functional That Works for Noncovalent Interactions. 2011 , 2, 983-989	124
2038	Predictive Modeling of Molecular Properties: Can We Go beyond Interpretation?. 2011 , 91-106	1
2037	Density Functional Theory for Transition Metal Chemistry: The Case of a Water-Splitting Ruthenium Cluster. 2011 , 137-163	2
2036	Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications. 2011 , 1-16	1
2035	A Transferable Non-bonded Pairwise Force Field to Model Zinc Interactions in Metalloproteins. 2011 , 7, 433-443	43
2034	Does DFT-D estimate accurate energies for the binding of ligands to metal complexes?. 2011 , 40, 11176-83	72
2033	Redox noninnocence of nitrosoarene ligands in transition metal complexes. 2011 , 50, 5763-76	49

2032	Noncanonical hydrogen bonding in nucleic acids. Benchmark evaluation of key base-phosphate interactions in folded RNA molecules using quantum-chemical calculations and molecular dynamics simulations. 2011 , 115, 11277-92		25
2031	The Nature of the Binding of Au, Ag, and Pd to Benzene, Coronene, and Graphene: From Benchmark CCSD(T) Calculations to Plane-Wave DFT Calculations. 2011 , 7, 3743-3755		90
2030	Relativity and the mercury battery. 2011 , 13, 16510-2		13
2029	Organometallic reactivity: the role of metal-ligand bond energies from a computational perspective. 2011 , 40, 11184-91		48
2028	Solvation and crystal effects in bilirubin studied by NMR spectroscopy and density functional theory. 2011 , 115, 11696-714		8
2027	Palladium and platinum complexes of a benzannulated N-heterocyclic plumblyene with an unusual bonding mode. 2011 , 133, 11118-20		58
2026	Theoretical evaluation of structural models of the S ₂ state in the oxygen evolving complex of Photosystem II: protonation states and magnetic interactions. 2011 , 133, 19743-57		249
2025	Epitaxial growth of polymorphic systems: The case of sulfathiazole. 2011 , 13, 5903		16
2024	Analytic energy gradient for second-order Møller-Plesset perturbation theory based on the fragment molecular orbital method. <i>Journal of Chemical Physics</i> , 2011 , 135, 044110	3-9	44
2023	Elastic properties of poly(vinylidene fluoride) (PVDF) crystals: A density functional theory study. 2011 , 109, 093514		26
2022	Biomolecule-biomaterial interaction: a DFT-D study of glycine adsorption and self-assembly on hydroxylated Cr ₂ O ₃ surfaces. 2011 , 27, 2747-60		37
2021	Dispersion corrections essential for the study of chemical reactivity in fullerenes. 2011 , 115, 3491-6		108
2020	On the influence of density functional approximations on some local Bader's atoms-in-molecules properties. 2011 , 115, 5505-15		47
2019	Interplay of Correlation and Relativistic Effects in Correlated Calculations on Transition-Metal Complexes: The (Cu ₂ O ₂) ²⁺ Core Revisited. 2011 , 7, 1511-23		85
2018	Structural and electronic properties of the graphene/Al/Ni(111) intercalation system. 2011 , 13, 113028		95
2017	A correlation-based predictor for pair-association in ionic liquids. 2011 , 13, 12138-45		23
2016	Tin Monoxide: Structural Prediction from First Principles Calculations with van der Waals Corrections. 2011 , 115, 19916-19924		79
2015	One product, two pathways: initially divergent radical reactions reconverge to form a single product in high yield. 2011 , 133, 16270-6		28

2014	tert-Butyl cation affinities of main-group-element hydrides: effect of methyl substituents at the protophilic center. 2011 , 115, 8310-5	13
2013	GGA versus van der Waals density functional results for mixed gold/mercury molecules and pure Au and Hg cluster properties. 2011 , 13, 20863-70	26
2012	Evaluation of theoretical approaches for describing the interaction of water with linear acenes. 2011 , 115, 5955-64	23
2011	Growth and organization of an organic molecular monolayer on TiO ₂ : catechol on anatase (101). 2011 , 133, 7816-23	93
2010	Accurate description of argon and water adsorption on surfaces of graphene-based carbon allotropes. 2011 , 115, 11387-93	63
2009	On the physisorption of water on graphene: a CCSD(T) study. 2011 , 13, 12041-7	152
2008	Nitrogen atom transfer from iron(IV) nitrido complexes: a dual-nature transition state for atom transfer. 2011 , 50, 9508-17	57
2007	Synthesis and molecular structure of gold triarylcorroles. 2011 , 50, 12844-51	91
2006	A Multibox Splitting Scheme: Robust Approximation For ab Initio Molecular Dynamics. 2011 , 7, 3872-83	2
2005	Accurate Interaction Energies for Problematic Dispersion-Bound Complexes: Homogeneous Dimers of NCCN, P ₂ , and PCCP. 2011 , 7, 2842-51	41
2004	Obtaining Good Performance With Triple- ζ Type Basis Sets in Double-Hybrid Density Functional Theory Procedures. 2011 , 7, 2852-63	52
2003	Electronic structure of 2,2'-bipyridine organotransition-metal complexes. Establishing the ligand oxidation level by density functional theoretical calculations. 2011 , 50, 9773-93	146
2002	Accurate Prediction of Methane Adsorption in a Metal-Organic Framework with Unsaturated Metal Sites by Direct Implementation of an ab Initio Derived Potential Energy Surface in GCMC Simulation. 2011 , 115, 23074-23080	82
2001	Assessment of Theoretical Methods for Complexes of Gold(I) and Gold(III) with Unsaturated Aliphatic Hydrocarbon: Which Density Functional Should We Choose?. 2011 , 7, 4002-11	101
2000	Van der Waals interactions in ionic and semiconductor solids. 2011 , 107, 245501	131
1999	A DFT comparison of the neutral and cationic Heck pathways. 2011 , 40, 11308-14	31
1998	DSD-PBEP86: in search of the best double-hybrid DFT with spin-component scaled MP2 and dispersion corrections. 2011 , 13, 20104-7	304
1997	Hierarchical interactions and their influence upon the adsorption of organic molecules on a graphene film. 2011 , 133, 9208-11	55

1996	A unique transition metal-stabilized silicon cation. 2011 , 133, 12442-4		64
1995	Interactions of the N3 dye with the iodide redox shuttle: quantum chemical mechanistic studies of the dye regeneration in the dye-sensitized solar cell. 2011 , 13, 15148-57		28
1994	Validation of electronic structure methods for isomerization reactions of large organic molecules. 2011 , 13, 13683-9		67
1993	Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionals-Evaluation with the Extended GMTKN30 Database for General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. 2011 , 7, 291-309		841
1992	Real-world predictions from ab initio molecular dynamics simulations. 2012 , 307, 109-53		74
1991	Dispersion interactions in density-functional theory: an adiabatic-connection analysis. <i>Journal of Chemical Physics</i> , 2011 , 135, 194109	3.9	18
1990	Adventitious formation of a new oxopentadienyl Mn(I) tricarbonyl complex: Structural study and bonding investigation of (B-CH ₂ C(Fc)CHC(Fc)O)Mn(CO) ₃ . 2011 , 696, 3268-3273		2
1989	Sterically Governed Selectivity in Palladium-Assisted Allylic Alkylation. 2011 , 30, 230-238		14
1988	Nature of adhesion of condensed organic films on platinum by first-principles simulations. 2011 , 13, 11827-37	7	
1987	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. 2011 , 7, 3567-77		322
1986	Physisorption of Hydrophobic and Hydrophilic 1-Alkyl-3-methylimidazolium Ionic Liquids on the Graphenes. 2011 , 115, 5626-5636		72
1985	Interaction of metal ions with biomolecular ligands: how accurate are calculated free energies associated with metal ion complexation?. 2011 , 115, 11394-402		36
1984	What Makes for a Bad Catalytic Cycle? A Theoretical Study on the Suzuki-Miyaura Reaction within the Energetic Span Model. 2011 , 1, 246-253		106
1983	Chimeric GNA/DNA metal-mediated base pairs. 2011 , 47, 11041-3		29
1982	Adsorption behavior of 4-methoxypyridine on gold nanoparticles. 2011 , 27, 7258-64		16
1981	Theoretical investigation of gold clusters supported on graphene sheets. 2011 , 35, 2153		26
1980	Further evidences of the quality of double-hybrid energy functionals for π -conjugated systems. <i>Journal of Chemical Physics</i> , 2011 , 134, 234102	3.9	6
1979	Performance of the van der Waals Density Functional VV10 and (hybrid)GGA Variants for Thermochemistry and Noncovalent Interactions. 2011 , 7, 3866-71		175

1978	Comparison of the performance of dispersion-corrected density functional theory for weak hydrogen bonds. 2011 , 13, 13942-50	119
1977	Intermolecular vs molecule-substrate interactions: A combined STM and theoretical study of supramolecular phases on graphene/Ru(0001). 2011 , 2, 365-73	34
1976	Shielding: Overview of Theoretical Methods. 2011 ,	
1975	The ground states of iron(III) porphines: role of entropy-enthalpy compensation, Fermi correlation, dispersion, and zero-point energies. 2011 , 105, 1286-92	24
1974	Conventional and density-fitting local Møller-Plesset theory calculations of C60 and its endohedral H ₂ @C60 and 2H ₂ @C60 complexes. 2011 , 513, 236-240	8
1973	Raman and infrared spectra of cellobiose in the solid state: What can be learned from single-molecule calculations?. 2011 , 514, 284-290	12
1972	2D vs. 3D titanium dioxide: Role of dispersion interactions. 2011 , 516, 72-75	18
1971	Computational organic chemistry. 2011 , 107, 349	3
1970	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. 2011 , 13, 6670-88	1347
1969	Assessment of the Performance of DFT and DFT-D Methods for Describing Distance Dependence of Hydrogen-Bonded Interactions. 2011 , 7, 88-96	342
1968	Semiempirical self-consistent polarization description of bulk water, the liquid-vapor interface, and cubic ice. 2011 , 115, 6046-53	21
1967	Optical rotation calculated with time-dependent density functional theory: the OR45 benchmark. 2011 , 115, 10930-49	97
1966	Electronic Control of Frustrated Lewis Pair Behavior: Chemistry of a Geminal Alkylidene-Bridged Per-pentafluorophenylated P/B Pair. 2011 , 30, 4211-4219	88
1965	Modular and predictable assembly of porous organic molecular crystals. 2011 , 474, 367-71	396
1964	A van der Waals density functional study of adenine on graphene: single-molecular adsorption and overlayer binding. 2011 , 23, 135001	40
1963	Pyranoside phosphite-oxazoline ligands for the highly versatile and enantioselective ir-catalyzed hydrogenation of minimally functionalized olefins. A combined theoretical and experimental study. 2011 , 133, 13634-45	147
1962	Density-functional approaches to noncovalent interactions: a comparison of dispersion corrections (DFT-D), exchange-hole dipole moment (XDM) theory, and specialized functionals. <i>Journal of Chemical Physics</i> , 2011 , 134, 084107	3.9 526
1961	π - π and π - π Interactions are equally important: multilayered graphanes. 2011 , 133, 20036-9	65

1960	Dispersion-corrected density functional theory comparison of hydrogen adsorption on boron-nitride and carbon nanotubes. 2011 , 84,	23
1959	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. 2011 , 7, 3944-51	230
1958	Density Functional Theory for Reaction Energies: Test of Meta and Hybrid Meta Functionals, Range-Separated Functionals, and Other High-Performance Functionals. 2011 , 7, 669-676	165
1957	Computational methods to calculate accurate activation and reaction energies of 1,3-dipolar cycloadditions of 24 1,3-dipoles. 2011 , 115, 13906-20	104
1956	Density functional theory with London dispersion corrections. 2011 , 1, 211-228	1645
1955	DNA insertion in and wrapping around carbon nanotubes. 2011 , 1, 902-919	5
1954	Correlated wavefunction methods in bioinorganic chemistry. 2011 , 16, 821-9	41
1953	Computational studies of the interactions of I ⁺ and I ³⁺ with TiO ₂ clusters: implications for dye-sensitized solar cells. 2011 , 129, 199-208	14
1952	Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. 2011 , 130, 251-260	34
1951	The nature of base stacking: a Monte Carlo study. 2011 , 130, 859-870	5
1950	Synthesis, Molecular Structure, and Physical Properties of the Complexes [{PhB(pz) ₂ (CH ₂ SMe)} ₂ M] (M = MnII, FeII; pz = pyrazol-1-yl) Containing a Novel [N,N,S]-Heteroscorpionate Ligand. 2011 , 2011, 1709-1718	8
1949	Chemistry on a Half-Shell: Synthesis and Derivatization of Buckybowls. 2011 , 2011, 1611-1625	223
1948	Selenation/Thionation of α -Amino Acids: Formation and X-ray Structures of Diselenopiperazine and Dithiopiperazine and Related Compounds. 2011 , 2011, 3067-3073	25
1947	On the importance of the dispersion energy for the thermodynamic stability of molecules. 2011 , 12, 1258-61	146
1946	Do metal-water hydrogen bonds hold in solution? Insight from ab initio molecular dynamics simulations. 2011 , 12, 1666-8	21
1945	Adsorption of supramolecular building blocks on graphite: a force field and density functional theory study. 2011 , 12, 2242-5	12
1944	Insights into uranyl chemistry from molecular dynamics simulations. 2011 , 12, 3095-105	49
1943	Assessing spin-component-scaled second-order Møller-plesset theory using anharmonic frequencies. 2011 , 12, 3383-91	6

1942	System-dependent dispersion coefficients for the DFT-D3 treatment of adsorption processes on ionic surfaces. 2011 , 12, 3414-20	188
1941	Empirical hydrogen-bond potential functions--an old hat reconditioned. 2011 , 12, 3131-42	22
1940	Substituent effects on non-covalent interactions with aromatic rings: insights from computational chemistry. 2011 , 12, 3116-30	116
1939	Benchmarking density functional methods against the S66 and S66x8 datasets for non-covalent interactions. 2011 , 12, 3421-33	252
1938	Inter- and intramolecular dispersion interactions. 2011 , 32, 1117-27	32
1937	Sensitivity analysis and uncertainty calculation for dispersion corrected density functional theory. 2011 , 32, 1424-30	39
1936	Effect of the damping function in dispersion corrected density functional theory. 2011 , 32, 1456-65	10429
1935	Accurate quantum-chemical description of gold complexes with pyridine and its derivatives. 2011 , 32, 1839-45	15
1934	Interaction of quinacridone derivatives. 2011 , 32, 2055-63	10
1933	Reaktionen frustrierter Lewis-Paare mit konjugierten Ionen Selektive Hydrierung der Kohlenstoff-Kohlenstoff-Dreifachbindung. 2011 , 123, 7321-7324	65
1932	Capture of NO by a Frustrated Lewis Pair: A New Type of Persistent N-Oxyl Radical. 2011 , 123, 7709-7713	59
1931	The Inherent Competition between Addition and Substitution Reactions of Br ₂ with Benzene and Arenes. 2011 , 123, 6941-6945	1
1930	Sterische Hinderung kann ein labiles Molekül stabilisieren: zur Lösung des Hexaphenylethan-Rätsels. 2011 , 123, 12849-12853	77
1929	Large Self-Assembled Chiral Organic Cages: Synthesis, Structure, and Shape Persistence. 2011 , 123, 10841-10848	38
1928	Struktureller Beweis für ein höheres Polybromidmonoanion: Untersuchung von [N(C ₃ H ₇)][Br ₉]. 2011 , 123, 11732-11736	27
1927	Dispersion and Back-Donation Gives Tetracoordinate [Pd(PPh ₃) ₄]. 2011 , 123, 11998-12001	24
1926	Reaction of frustrated Lewis pairs with conjugated ynones-selective hydrogenation of the carbon-carbon triple bond. 2011 , 50, 7183-6	160
1925	Capture of NO by a Frustrated Lewis Pair: a new type of persistent N-oxyl radical. 2011 , 50, 7567-71	161

1924	The inherent competition between addition and substitution reactions of Br ₂ with benzene and arenes. 2011 , 50, 6809-13	33
1923	Steric crowding can stabilize a labile molecule: solving the hexaphenylethane riddle. 2011 , 50, 12639-42	197
1922	Large self-assembled chiral organic cages: synthesis, structure, and shape persistence. 2011 , 50, 10653-6	109
1921	Structural proof for a higher polybromide monoanion: investigation of [N(C ₃ H ₇) ₄][Br ₉]. 2011 , 50, 11528-32	46
1920	Dispersion and back-donation gives tetracoordinate [Pd(PPh ₃) ₄]. 2011 , 50, 11794-7	70
1919	Modeling the cis-oxo-labile binding site motif of non-heme iron oxygenases: water exchange and oxidation reactivity of a non-heme iron(IV)-oxo compound bearing a tripodal tetradentate ligand. 2011 , 17, 1622-34	97
1918	Dodeka(ethylene)octamine. 2011 , 17, 3575-8	6
1917	CO ₂ and formate complexes of phosphine/borane frustrated Lewis pairs. 2011 , 17, 9640-50	135
1916	Neutral nickel oligo- and polymerization catalysts: the importance of alkyl phosphine intermediates in chain termination. 2011 , 17, 14628-42	15
1915	Palladium-catalyzed allylic sulfinylation and the Mislow-Braverman-Evans rearrangement. 2011 , 17, 13963-5	5
1914	Modellierung von heterogen-katalysierten Reaktionen in porösen Medien. 2011 , 83, 2188-2210	2
1913	Challenges in the first-principles description of reactions in electrocatalysis. 2011 , 165, 129-137	128
1912	The effect of cluster thickness on the adsorption of CH ₄ on Pd. 2011 , 963, 236-244	13
1911	Theoretical study of weak chemical interactions in solid formamide. 2011 , 508, 54-58	10
1910	Computational thermochemistry of iron-platinum carbonyl clusters. 2011 , 509, 158-161	3
1909	Synthesis of a 2-benzocymantrenylpyridine and further mechanistic insights. 2011 , 696, 2101-2107	9
1908	Three-component conformational equilibria of some flexible pyrrolidin-2-(thi)ones in solution by NMR data (¹³ C, ¹ H, and nJHH) and their DFT predictions: a confrontation of different approaches. 2011 , 67, 6901-6916	16
1907	Assessment of Some Density Functional Theory Methods and Force Field Models in Describing Various Interaction Modes of Benzene Dimer. 2011 , 24, 635-639	7

1906	Electrostatic embedding in large-scale first principles quantum mechanical calculations on biomolecules. <i>Journal of Chemical Physics</i> , 2011 , 135, 224107	3.9	44
1905	Evaluation of a density functional with account of van der Waals forces using experimental data of H ₂ physisorption on Cu(111). 2011 , 84,		44
1904	Self-assembled cyclic oligothiophene nanotubes: Electronic properties from a dispersion-corrected hybrid functional. 2011 , 84,		28
1903	Exchange-correlation generalized gradient approximation for gold nanostructures. <i>Journal of Chemical Physics</i> , 2011 , 134, 194112	3.9	33
1902	A generalized-gradient approximation exchange hole model for dispersion coefficients. <i>Journal of Chemical Physics</i> , 2011 , 134, 044117	3.9	211
1901	Dependence of dispersion coefficients on atomic environment. <i>Journal of Chemical Physics</i> , 2011 , 135, 234109	3.9	29
1900	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. 2011 , 108, 19896-900		124
1899	Communication: The effect of dispersion corrections on the melting temperature of liquid water. <i>Journal of Chemical Physics</i> , 2011 , 134, 121105	3.9	135
1898	Self-consistent meta-generalized gradient approximation study of adsorption of aromatic molecules on noble metal surfaces. <i>Journal of Chemical Physics</i> , 2011 , 135, 084704	3.9	34
1897	Communication: efficient counterpoise corrections by a perturbative approach. <i>Journal of Chemical Physics</i> , 2011 , 135, 081105	3.9	9
1896	Recognition of asymmetrically dimethylated arginine by TDRD3. 2012 , 40, 11748-55		33
1895	Pt ₃ and Pt ₄ clusters on graphene monolayers supported on a Ni(111) substrate: relativistic density-functional calculations. <i>Journal of Chemical Physics</i> , 2012 , 137, 044710	3.9	10
1894	Theoretical Investigation of Migration Pathways for Li Diffusion in h-LiTiS ₂ . 2012 , 226, 449-459		5
1893	Pt on graphene monolayers supported on a Ni(111) substrate: relativistic density-functional calculations. <i>Journal of Chemical Physics</i> , 2012 , 136, 074701	3.9	17
1892	Long-range correlation energies from frequency-dependent weighted exchange-hole dipole polarisabilities. <i>Journal of Chemical Physics</i> , 2012 , 136, 014104	3.9	15
1891	The structure of N ₂ adsorbed on the rumpled NaCl(100) surface--a combined LEED and DFT-D study. <i>Journal of Chemical Physics</i> , 2012 , 137, 174705	3.9	10
1890	Dispersion-free component of non-covalent interaction via mutual polarization of fragment densities. <i>Journal of Chemical Physics</i> , 2012 , 136, 204109	3.9	8
1889	Analytic gradient for second order Møller-Plesset perturbation theory with the polarizable continuum model based on the fragment molecular orbital method. <i>Journal of Chemical Physics</i> , 2012 , 136, 204112	3.9	45

1888	Analysis of the basis set superposition error in molecular dynamics of hydrogen-bonded liquids: application to methanol. <i>Journal of Chemical Physics</i> , 2012 , 137, 104506	3.9	3
1887	Effect of dispersion correction on the Au(1 1 1)-H ₂ O interface: a first-principles study. <i>Journal of Chemical Physics</i> , 2012 , 137, 114709	3.9	42
1886	Embedded cluster density functional and second-order Møller-Plesset perturbation theory study on the adsorption of N ₂ on the rutile (110) surface. <i>Journal of Chemical Physics</i> , 2012 , 137, 114705	3.9	6
1885	Extension of local response dispersion method to excited-state calculation based on time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2012 , 137, 124106	3.9	16
1884	Structural, elastic, and vibrational properties of layered titanium dichalcogenides: a van der Waals density functional study. <i>Journal of Chemical Physics</i> , 2012 , 137, 224509	3.9	10
1883	Assessment of dispersion corrections in DFT calculations on large biological systems. 2012 , 110, 3061-3076		8
1882	Phase transition in GeF ₂ driven by change of type of intermolecular interaction. 2012 , 86,		5
1881	Two-dimensional nucleation and growth mechanism explaining graphene oxide structures. 2012 , 86,		33
1880	Semiempirical van der Waals interactions versus ab initio nonlocal correlation effects in the thiophene-Cu(111) system. 2012 , 86,		22
1879	Role of functional groups in surface bonding of planar π -conjugated molecules. 2012 , 86,		62
1878	Accurate and efficient method for many-body van der Waals interactions. 2012 , 108, 236402		920
1877	Nonequilibrium thermodynamics of interacting tunneling transport: variational grand potential, density functional formulation and nature of steady-state forces. 2012 , 24, 424219		10
1876	Structure and stability of weakly chemisorbed ethene adsorbed on low-index Cu surfaces: performance of density functionals with van der Waals interactions. 2012 , 24, 424217		18
1875	Protonated sugars: vibrational spectroscopy and conformational structure of protonated O-methyl β -D-galactopyranoside. 2012 , 110, 1609-1615		16
1874	Surface Modification of a n-Si(111) Electrode through Aldehyde Grafting and Subsequent Metallization: Theory and Experiment. 2012 , 226, 1039-1048		
1873	Theoretische Chemie 2011. 2012 , 60, 323-331		
1872	Dispersion-corrected density functional theory calculations of the molecular binding of n-alkanes on Pd(111) and PdO(101). <i>Journal of Chemical Physics</i> , 2012 , 136, 054702	3.9	56
1871	Azurin as a protein scaffold for a low-coordinate nonheme iron site with a small-molecule binding pocket. 2012 , 134, 19746-57		28

1870	Why the standard B3LYP/6-31G* model chemistry should not be used in DFT calculations of molecular thermochemistry: understanding and correcting the problem. 2012 , 77, 10824-34		298
1869	A geometrical correction for the inter- and intra-molecular basis set superposition error in Hartree-Fock and density functional theory calculations for large systems. <i>Journal of Chemical Physics</i> , 2012 , 136, 154101	3.9	368
1868	JACOB: a dynamic database for computational chemistry benchmarking. 2012 , 52, 3255-62		4
1867	Mechanism of gold(I)-catalyzed rearrangements of acetylenic amine-N-oxides: computational investigations lead to a new mechanism confirmed by experiment. 2012 , 134, 1078-84		89
1866	Making C π Bonds with Gold: Identification of Selective Gold Sites for Homo- and Cross-Coupling Reactions between Iodobenzene and Alkynes. 2012 , 116, 24855-24867		61
1865	Ab initio calculations of the interaction between CO ₂ and the acetate ion. 2012 , 116, 11643-50		48
1864	First-principles investigations of the atomic, electronic, and thermoelectric properties of equilibrium and strained Bi ₂ Se ₃ and Bi ₂ Te ₃ including van der Waals interactions. 2012 , 86,		111
1863	Synthesis, characterization and sorption properties of NH ₂ -MIL-47. 2012 , 14, 15562-70		25
1862	TD-DFT Assessment of Functionals for Optical 0-0 Transitions in Solvated Dyes. 2012 , 8, 2359-72		342
1861	The reaction mechanism of the enantioselective Tsuji allylation: inner-sphere and outer-sphere pathways, internal rearrangements, and asymmetric C-C bond formation. 2012 , 134, 19050-60		89
1860	Synthesis and reactions of the first room temperature stable Li/Cl phosphinidenoid complex. 2012 , 51, 12343-9		45
1859	Observation of a tungsten alkane π complex showing selective binding of methyl groups using FTIR and NMR spectroscopies. 2012 , 134, 8294-7		39
1858	Origin of enantioselectivity in benzotetramisole-catalyzed dynamic kinetic resolution of azlactones. 2012 , 14, 3288-91		117
1857	Pnicogen- π complexes: theoretical study and biological implications. 2012 , 14, 14061-6		93
1856	Performance of dispersion-corrected density functional theory for the interactions in ionic liquids. 2012 , 14, 4875-83		181
1855	Van der Waals forces in the perfluorinated metal-organic framework zinc 1,2-bis(4-pyridyl)ethane tetrafluoroterephthalate. 2012 , 14, 7059-64		16
1854	Detailed QM/MM study of the Electron Paramagnetic Resonance Parameters of Nitrosyl Myoglobin. 2012 , 8, 563-74		22
1853	Electronic regioselectivity of diarylalkynes in cobalt-mediated Pauson-Khand reaction: an experimental and computational study with para- and meta-substituted diarylalkynes and norbornene. 2012 , 77, 9134-47		21

1852	Selective Formation of 1,4-Disubstituted Triazoles from Ruthenium-Catalyzed Cycloaddition of Terminal Alkynes and Organic Azides: Scope and Reaction Mechanism. 2012 , 31, 4904-4915	43
1851	Modifying the fullerene surface using endohedral noble gas atoms: density functional theory based molecular dynamics study of C70O3. 2012 , 116, 3413-9	15
1850	Random-phase approximation and its applications in computational chemistry and materials science. 2012 , 47, 7447-7471	389
1849	Absolute configuration of atropisomeric polychlorinated biphenyl 183 enantiomerically enriched in human samples. 2012 , 116, 9340-6	24
1848	van der Waals Interaction Energies of Small Fragments of P, As, Sb, S, Se, and Te: Comparison of Complete Basis Set Limit CCSD(T) and DFT with Approximate Dispersion. 2012 , 8, 2301-9	5
1847	Configurational Assignment of Cyclic Bisbibenzyls by HPLC-CD and Quantum-Chemical CD Calculations. 2012 , 2012, 6878-6887	12
1846	Advanced Corrections of Hydrogen Bonding and Dispersion for Semiempirical Quantum Mechanical Methods. 2012 , 8, 141-51	336
1845	Quantum Modeling of Water and Oxygen Adsorption on Beryllium Surface. 2012 , 116, 4662-4670	8
1844	Photoswitching of Azobenzene-Functionalized Molecular Platforms on Au Surfaces. 2012 , 116, 25943-25948	49
1843	Antiferromagnetic coupling across a tetrametallic unit through noncovalent interactions. 2012 , 3, 602-609	30
1842	The Binding of Fe(II)-Heme to the Amyloid Beta Peptide of Alzheimer's Disease: QM/MM Investigations. 2012 , 8, 5150-8	9
1841	Elucidation of Strong Cooperative Effects Caused by Dispersion Interactions in a Recognition-Mediated Diels-Alder Reaction. 2012 , 8, 5064-71	9
1840	Second-Order Møller-Plesset Perturbation Theory in the Condensed Phase: An Efficient and Massively Parallel Gaussian and Plane Waves Approach. 2012 , 8, 4177-88	106
1839	A first-principles-based correlation functional for harmonious connection of short-range correlation and long-range dispersion. <i>Journal of Chemical Physics</i> , 2012 , 137, 204121	3.9 6
1838	Can density functional theory describe the NO(X2)-Ar and NO(A2)-Ar van der Waals complexes?. <i>Journal of Chemical Physics</i> , 2012 , 136, 244313	3.9 14
1837	Adsorption studies of C6H6 on Cu (111), Ag (111), and Au (111) within dispersion corrected density functional theory. <i>Journal of Chemical Physics</i> , 2012 , 137, 134703	3.9 36
1836	Binding of noble metal clusters with rare gas atoms: theoretical investigation. 2012 , 116, 12510-7	35
1835	Attenuating Away the Errors in Inter- and Intramolecular Interactions from Second-Order Møller-Plesset Calculations in the Small Aug-cc-pVDZ Basis Set. 2012 , 3, 3592-8	31

1834	Investigation of the Solid-State Polymorphic Transformations of Piracetam. 2012 , 12, 6223-6233		29
1833	Elastic and Vibrational Properties of β - and γ -PbO ₂ . 2012 , 116, 21514-21522		35
1832	Dimensionality transformation through paddlewheel reconfiguration in a flexible and porous Zn-based metal-organic framework. 2012 , 134, 20466-78		73
1831	L-Cysteine Interaction with Au55 Nanoparticle. 2012 , 116, 25816-25823		35
1830	Application of double-hybrid density functionals to charge transfer in N-substituted pentacenequinones. <i>Journal of Chemical Physics</i> , 2012 , 136, 174703	3.9	10
1829	Carbon dioxide insertion into diamines: a computational study of solvent effects. 2012 , 5, 1967-73		10
1828	Molecular recognition in glycolaldehyde, the simplest sugar: two isolated hydrogen bonds win over one cooperative pair. 2012 , 1, 269-75		18
1827	The assessment and application of an approach to noncovalent interactions: the energy decomposition analysis (EDA) in combination with DFT of revised dispersion correction (DFT-D3) with Slater-type orbital (STO) basis set. 2012 , 18, 4577-89		35
1826	Modeling van der Waals Interactions in Zeolites with Periodic DFT: Physisorption of n-Alkanes in ZSM-22. 2012 , 142, 1057-1060		57
1825	Mechanistic insight into the cyclohexene epoxidation with VO(acac) ₂ and tert-butyl hydroperoxide. 2012 , 294, 1-18		34
1824	Crystal Structure Prediction. 2012 ,		1
1823	A theoretical study of metal-metal cooperativity in the homogeneous water gas shift reaction. 2012 , 51, 377-85		22
1822	Prediction of CO ₂ Adsorption Properties in Zeolites Using Force Fields Derived from Periodic Dispersion-Corrected DFT Calculations. 2012 , 116, 10692-10701		107
1821	The interplay of intermolecular interactions, packing motifs and electron transport properties in perylene diimide related materials: a theoretical perspective. 2012 , 22, 20840		55
1820	Molecular redox: revisiting the electronic structures of the group 9 metallocorroles. 2012 , 51, 12473-82		17
1819	Theoretical study on the leaching of palladium in a CO atmosphere. 2012 , 2, 2238		17
1818	Analytic gradient for the embedding potential with approximations in the fragment molecular orbital method. 2012 , 544, 87-93		24
1817	First-principles theoretical study of organic/metal interfaces: Vacuum level shifts and interface dipoles. 2012 , 12, S2-S9		14

1816	Poly-proline-based chiral stationary phases: a molecular dynamics study of triproline, tetraproline, pentaproline and hexaproline interfaces. 2012 , 1265, 70-87	13
1815	Assessment of the performance of MP2 and MP2 variants for the treatment of noncovalent interactions. 2012 , 116, 4159-69	101
1814	On the high-temperature phase of barbituric acid. 2012 , 14, 3046	19
1813	Neutral noble gas compounds exhibiting a Xe-Xe bond: structure, stability and bonding situation. 2012 , 14, 14869-77	39
1812	CRYSCOR: a program for the post-Hartree-Fock treatment of periodic systems. 2012 , 14, 7615-28	111
1811	Electrochemical properties of crystallized dilithium squarate: insight from dispersion-corrected density functional theory. 2012 , 14, 11398-412	22
1810	Computational studies on the mechanism of the gold(I)-catalysed rearrangement of cyclopropenes. 2012 , 10, 4433-40	28
1809	Reduced Pd density of states in Pd/SAM/Au junctions: the role of adsorbed hydrogen atoms. 2012 , 14, 2353-61	8
1808	Evaluating London Dispersion Interactions in DFT: A Nonlocal Anisotropic Buckingham-Hirshfeld Model. 2012 , 8, 125-34	17
1807	Chloroperoxidase-catalyzed epoxidation of cis- β -methylstyrene: distal pocket flexibility tunes catalytic reactivity. 2012 , 116, 12905-14	15
1806	A density functional theory investigation of the molecular and dissociative adsorption of hydrazine on defective copper surfaces. 2012 , 22, 23210	21
1805	Surface state engineering of molecule-molecule interactions. 2012 , 14, 4971-6	52
1804	First-Principles Modeling of Non-Covalent Interactions in Supramolecular Systems: The Role of Many-Body Effects. 2012 , 8, 4317-22	98
1803	Structure and electronic structure of S-doped graphitic C ₃ N ₄ investigated by density functional theory. 2012 , 21, 107101	30
1802	Spin-forbidden hydrogen atom transfer reactions in a cobalt biimidazole system. 2012 , 3, 230-243	31
1801	A sting in the tail of flexible molecules: spectroscopic and energetic challenges in the case of p-aminophenethylamine. 2012 , 14, 9219-29	6
1800	Theoretical analysis of cooperative effects of small molecule activation by frustrated Lewis pairs. 2012 , 41, 9111-8	35
1799	Dipole driven bonding schemes of quinonoid zwitterions on surfaces. 2012 , 48, 7143-5	28

1798	Frustrated Lewis pair addition to conjugated diynes: formation of zwitterionic 1,2,3-butatriene derivatives. 2012 , 41, 9135-42	28
1797	Pathways for C-H bond cleavage of propane π -complexes on PdO(101). 2012 , 14, 12202-12	31
1796	Structural and DFT Studies on the Polymorphism of a Cadmium(II) Dipicolinate Coordination Polymer. 2012 , 12, 456-465	18
1795	Buckyplates and buckybowl: examining the effects of curvature on π - π interactions. 2012 , 116, 11920-6	56
1794	Structural and vibrational properties of β -MoO ₃ from van der Waals corrected density functional theory calculations. 2012 , 85,	42
1793	Volatilities of Actinide and Lanthanide N,N-Dimethylaminodiboranate Chemical Vapor Deposition Precursors: A DFT Study. 2012 , 116, 23194-23200	16
1792	SET Oxidation of Li/X Phosphinidenoid Complexes by TEMPO. 2012 , 31, 3457-3459	15
1791	Molecular Tweezers in Host-Guest Complexes: A Computational Study through a DFT-D Approach. 2012 , 116, 23067-23074	7
1790	Theoretical Electronic Circular Dichroism Spectroscopy of Large Organic and Supramolecular Systems. 2012 , 643-673	16
1789	Ab Initio Molecular Dynamics Study of the AlOOH Boehmite/Water Interface: Role of Steps in Interfacial Grotthuss Proton Transfers. 2012 , 116, 12514-12524	66
1788	Efficient Approach for the Computational Study of Alcohol and Nitrile Adsorption in H-ZSM-5. 2012 , 116, 5499-5508	74
1787	Insight into the Adsorption of Water on the Clean CeO ₂ (111) Surface with van der Waals and Hybrid Density Functionals. 2012 , 116, 13584-13593	99
1786	Symmetrical hydrogen bonds in iridium(III) alkoxides with relevance to outer sphere hydrogen transfer. 2012 , 51, 12313-23	17
1785	Short range DFT combined with long-range local RPA within a range-separated hybrid DFT framework. 2012 , 550, 162-169	28
1784	Synthesis and Application of Strong Brønsted Acids Generated from the Lewis Acid Al(ORF) ₃ and an Alcohol. 2012 , 31, 7485-7491	34
1783	Adsorption of CO ₂ on a PdO(101) Thin Film. 2012 , 116, 3007-3016	20
1782	An Assessment of the vdW-TS Method for Extended Systems. 2012 , 8, 1503-13	95
1781	CF ₃ Bh Reductive Elimination from [(Xantphos)Pd(CF ₃)(Ph)]. 2012 , 31, 1315-1328	79

1780	DFT study with inclusion of the Grimme potential on anatase TiO ₂ : structure, electronic, and vibrational analyses. 2012 , 116, 11731-5		27
1779	As ₂ O ₃ Polymorphs: Theoretical Insight into Their Stability and Ammonia Templated Claudetite II Crystallization. 2012 , 12, 5663-5670		18
1778	Computational Mechanistic Study of C≡C Coupling of Methanol and Allenes Catalyzed by an Iridium Complex. 2012 , 31, 2066-2077		4
1777	Uranyl-peroxide nanocapsules: electronic structure and cation complexation in [(UO ₂) ₂ (EO ₂) ₃ O] ₂₀ . 2012 , 51, 3840-5		33
1776	N,N-addition of frustrated Lewis pairs to nitric oxide: an easy entry to a unique family of aminoxyl radicals. 2012 , 134, 10156-68		147
1775	A benchmark for non-covalent interactions in solids. <i>Journal of Chemical Physics</i> , 2012 , 137, 054103	3.9	260
1774	Ethanol and Water Adsorption on Close-Packed 3d, 4d, and 5d Transition-Metal Surfaces: A Density Functional Theory Investigation with van der Waals Correction. 2012 , 116, 24695-24705		87
1773	Physisorption of nucleobases on graphene: a comparative van der Waals study. 2012 , 24, 424210		72
1772	Influence of water on the electronic structure of metal-supported graphene: Insights from van der Waals density functional theory. 2012 , 85,		61
1771	The π-π stacking interactions between homogeneous dimers of C ₆ F _(x) I _(6-x) (x = 0, 1, 2, 3, 4, and 5): a comparative study with the halogen bond. 2012 , 116, 12486-91		19
1770	New insights into frustrated Lewis pairs: structural investigations of intramolecular phosphane-borane adducts by using modern solid-state NMR techniques and DFT calculations. 2012 , 134, 4236-49		74
1769	A functional [NiFe]-hydrogenase model compound that undergoes biologically relevant reversible thiolate protonation. 2012 , 134, 20745-55		95
1768	Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. 2012 , 85,		852
1767	σ vs π Bonding in Manganese(II) Allyl Complexes. 2012 , 31, 6131-6138		13
1766	Intramolecular aminoalkene hydroamination mediated by a tethered bis(ureate)zirconium complex: computational perusal of various pathways for aminoalkene activation. 2012 , 51, 3786-95		23
1765	Assessment of theoretical procedures for calculating barrier heights for a diverse set of water-catalyzed proton-transfer reactions. 2012 , 116, 4211-21		65
1764	NO _x Reactions on Aqueous Surfaces with Gaseous HCl: Formation of a Potential Precursor to Atmospheric Cl Atoms. 2012 , 3, 3405-10		30
1763	Oxidation of an organic adlayer: a bird's eye view. 2012 , 134, 8817-22		9

1762	Nanostructured diamine-fullerene derivatives: computational density functional theory study and experimental evidence for their formation via gas-phase functionalization. 2012 , 116, 1663-76	14
1761	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. 2012 , 8, 2824-34	58
1760	Experimental fingerprints for redox-active terpyridine in [Cr(tpy) ₂](PF ₆) _n (n = 3-0), and the remarkable electronic structure of [Cr(tpy) ₂] ¹⁻ . 2012 , 51, 3718-32	104
1759	Surface interactions of Au(I) cyclo-trimer with Au(111) and Al(111) surfaces: A computational study. 2012 , 606, 1100-1107	7
1758	Investigation of the complexation behaviour and catalysis of IBiox-[(1R)-menthyl]HOTf. 2012 , 68, 7636-7644	9
1757	The catalytic mechanism of mouse renin studied with QM/MM calculations. 2012 , 14, 12605-13	20
1756	BDE261: a comprehensive set of high-level theoretical bond dissociation enthalpies. 2012 , 116, 4975-86	58
1755	Phonons and electron-phonon interaction at the Sb(111) surface. 2012 , 86,	22
1754	Application of Local Second-Order Møller-Plesset Perturbation Theory to the Study of Structures in Solution. 2012 , 8, 3053-60	4
1753	How critical are the van der Waals interactions in polymer crystals?. 2012 , 116, 9347-52	54
1752	Effects of Dispersion in Density Functional Based Quantum Mechanical/Molecular Mechanical Calculations on Cytochrome P450 Catalyzed Reactions. 2012 , 8, 4637-45	70
1751	Constrained density functional theory. 2012 , 112, 321-70	366
1750	Exploring chemistry with the fragment molecular orbital method. 2012 , 14, 7562-77	284
1749	State-of-the-art and challenges in theoretical simulations of heterogeneous catalysis at the microscopic level. 2012 , 2, 2405	34
1748	Improved Catalytic Activity of Ruthenium-Arene Complexes in the Reduction of NAD ⁺ . 2012 , 31, 5958-5967	54
1747	Anatase TiO ₂ Surface Functionalization by Alkylphosphonic Acid: A DFT+D Study. 2012 , 116, 2819-2828	36
1746	Assessment of weak intermolecular interactions across QM/MM noncovalent boundaries. 2012 , 52, 93-8	4
1745	Origins of stereoselectivities of dihydroxylations of cis-bicyclo[3.3.0]octenes. 2012 , 134, 16054-8	15

1744	Reaction Dynamics of ATP Hydrolysis in Actin Determined by ab Initio Molecular Dynamics Simulations. 2012 , 8, 3373-83		8
1743	Collective many-body van der Waals interactions in molecular systems. 2012 , 109, 14791-5		158
1742	Structure, bonding, and catecholase mechanism of copper bispidine complexes. 2012 , 51, 9214-25		53
1741	Benchmark Calculations of Noncovalent Interactions of Halogenated Molecules. 2012 , 8, 4285-92		223
1740	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. <i>Journal of Chemical Physics</i> , 2012 , 136, 174103	3.9	86
1739	Novel characterization of the adsorption sites in large pore metal-organic frameworks: combination of X-ray powder diffraction and thermal desorption spectroscopy. 2012 , 14, 12892-7		11
1738	Two interconvertible structures that explain the spectroscopic properties of the oxygen-evolving complex of photosystem II in the S2 state. 2012 , 51, 9935-40		293
1737	Atomic C 6 dispersion coefficients: a four-component relativistic Kohn-Sham study. 2012 , 110, 2535-2541		13
1736	Rollover cyclometalation pathway in rhodium catalysis: dramatic NHC effects in the C-H bond functionalization. 2012 , 134, 17778-88		139
1735	Towards chemically accurate simulation of molecule-surface reactions. 2012 , 14, 14966-81		73
1734	A Density Functional with Spherical Atom Dispersion Terms. 2012 , 8, 4989-5007		324
1733	Solvation and ion-pairing properties of the aqueous sulfate anion: explicit versus effective electronic polarization. 2012 , 14, 10248-57		62
1732	Ab initio quantum chemistry for protein structures. 2012 , 116, 12501-9		88
1731	Hydrogen-bonding networks from first-principles: exploring the guanidine crystal. 2012 , 116, 4551-9		29
1730	Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. 2012 , 8, 4305-16		34
1729	Computational Methods for the Assignment of Vibrational Modes in Crystalline Materials. 2012 , 151-190		3
1728	How Accurate Can a Local Coupled Cluster Approach Be in Computing the Activation Energies of Late-Transition-Metal-Catalyzed Reactions with Au, Pt, and Ir?. 2012 , 8, 3119-27		53
1727	A benchmark comparison of π - and π -dispersion: the dimers of naphthalene and decalin, and coronene and perhydrocoronene. 2012 , 134, 17520-5		70

1726	Assessment of ten DFT methods in predicting structures of sheet silicates: importance of dispersion corrections. <i>Journal of Chemical Physics</i> , 2012 , 137, 114105	3.9	92
1725	Aerobic epoxidation of propene over silver (111) and (100) facet catalysts. 2012 , 292, 138-147		49
1724	Methylation of benzene by methanol: Single-site kinetics over H-ZSM-5 and H-beta zeolite catalysts. 2012 , 292, 201-212		105
1723	Counter anion binding in the phenoxyimine, salan and metallocene olefin polymerization catalysts activated with perfluorophenylborate. 2012 , 718, 124-130		5
1722	Adsorption of methane on carbon models of coal surface studied by the density functional theory including dispersion correction (DFT-D3). 2012 , 992, 37-47		43
1721	On the ability of periodic dispersion-corrected DFT calculations to predict molecular crystal polymorphism in para-diiodobenzene. 2012 , 541, 12-15		17
1720	Assessment of density functionals on intramolecular dispersion interaction in large normal alkanes. 2012 , 541, 7-11		17
1719	Reducing the scaling of the fragment molecular orbital method using the multipole method. 2012 , 543, 159-165		11
1718	Structures and spectral properties of heteroleptic copper (I) complexes: A theoretical study based on density functional theory. 2012 , 15, 255-266		9
1717	Quantum chemical investigation of attractive non-covalent interactions between halomethanes and rare gases. 2012 , 116, 10621-8		22
1716	Unraveling the Complex Nature of the Hydrated Electron. 2012 , 3, 3071-5		99
1715	Strengthening π Interactions While Suppressing Csp ² H π (T-Shaped) Interactions via Perfluoroalkylation: A Crystallographic and Computational Study That Supports the Beneficial Formation of 1-D Stacked Aromatic Materials. 2012 , 12, 5655-5662		36
1714	Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory. <i>Journal of Chemical Physics</i> , 2012 , 137, 120901	3.9	813
1713	Hydrogen Activation by an Intramolecular Boron Lewis Acid/Zirconocene Pair. 2012 , 124, 8960-8963		13
1712	Binding of Molecular Magnesium Hydrides to a Zirconocene-Alkyne Template. 2012 , 124, 8976-8979		4
1711	Metal-free Catalytic Olefin Hydrogenation: Low-Temperature H ₂ Activation by Frustrated Lewis Pairs. 2012 , 124, 10311-10315		85
1710	Zwei ineinander umwandelbare Strukturen erklären die spektroskopischen Eigenschaften des Wasser oxidierenden Enzyms des Photosystems II im S ₂ -Zustand. 2012 , 124, 10074-10079		25
1709	Synthese, Struktur, Tautomerie und Reaktivität von Methantrisamidinen. 2012 , 124, 11051-11055		4

1708	Metal-free catalytic olefin hydrogenation: low-temperature H ₂ activation by frustrated Lewis pairs. 2012 , 51, 10164-8	200
1707	Synthesis, structure, tautomerism, and reactivity of methanetrissamidines. 2012 , 51, 10893-7	3
1706	Hydrogen-bonding interactions and properties of energetic nitroamino[1,3,5]triazine-based guanidinium salts: DFT-D and QTAIM studies. 2012 , 7, 2577-91	18
1705	Density functional study on UV/VIS spectra of copper-protein active sites: the effect of mutations. 2012 , 9, 1728-38	2
1704	Transition-metal complexes of tetrylones [(CO) ₅ W-E(PPh ₃) ₂] and tetrylenes [(CO) ₅ W-NHE] (E=C-Pb): a theoretical study. 2012 , 18, 12733-48	62
1703	β-Cyclodextrin duplexes that are connected through two disulfide bonds: potent hosts for the complexation of organic molecules. 2012 , 18, 12292-304	9
1702	Relationship between dye-iodine binding and cell voltage in dye-sensitized solar cells: a quantum-mechanical look. 2012 , 33, 2492-7	16
1701	Density functional study of tetraphenylporphyrin long-range exciton coupling. 2012 , 1, 184-94	18
1700	Room temperature tandem hydroamination and hydrosilation/protodesilation catalysis by a tricarbonylchromium-bound iridacycle. 2012 , 48, 10310-2	30
1699	Splitting of dihydrogen by five-membered zirconacycloallene: a novel pathway to conjugated diene zirconocene complexes. 2012 , 48, 11085-7	13
1698	Accurate Hydrogen Positions in Organic Crystals: Assessing a Quantum-Chemical Aide. 2012 , 12, 1014-1021	66
1697	A computational study of the enantioselective addition of n-BuLi to benzaldehyde in the presence of a chiral lithium N,P amide. 2012 , 10, 2807-14	11
1696	Benchmark Assessment of the Accuracy of Several van der Waals Density Functionals. 2012 , 8, 1929-34	90
1695	The accuracy of DFT-optimized geometries of functional transition metal compounds: a validation study of catalysts for olefin metathesis and other reactions in the homogeneous phase. 2012 , 41, 5526-41	346
1694	Accurate evaluation of the resonance energies of benzene and pyridine via cyclic reference state. 2012 , 14, 15888-96	7
1693	Combined Computational and Experimental NMR Study of Calix[4]arene Derivatives. 2012 , 116, 23441-23452	1
1692	Detection of mercury-TpT dinucleotide binding by Raman spectra: a computational study. 2012 , 116, 8313-20	17
1691	Density functional study on the cytochrome-mediated S-oxidation: identification of crucial reactive intermediate on the metabolic path of thiazolidinediones. 2012 , 116, 10441-50	16

1690	Dioxygen Activation by a Non-Heme Iron(II) Complex: Theoretical Study toward Understanding Ferric-Superoxo Complexes. 2012 , 8, 915-26		61
1689	Zero-field splitting in a series of structurally related mononuclear Ni(II)-bispidine complexes. 2012 , 51, 12324-35		33
1688	Accurate Prediction of Noncovalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test Set. 2012 , 8, 2835-43		80
1687	Ab initio and semi-empirical van der Waals study of graphene-boron nitride interaction from a molecular point of view. 2012 , 24, 424214		23
1686	First-Principles Computational Modeling of Fluorescence Resonance Energy Transfer in Co-Sensitized Dye Solar Cells. 2012 , 3, 2146-53		30
1685	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. 2012 , 14, 12554-70		29
1684	Role of different molecular fragments in formation of the supramolecular architecture of the crystal of 1,1-dioxo-tetrahydro-1 β -thiopyran-3-one. 2012 , 14, 8698		14
1683	A DFT-D study of structural and energetic properties of TiO ₂ modifications. 2012 , 24, 424206		44
1682	Improved description of soft layered materials with van der Waals density functional theory. 2012 , 24, 424216		134
1681	The Nature of Transannular Interactions in E ₄ N ₄ and E ₈ (2+) (E = S, Se). 2012 , 8, 4249-58		13
1680	On the formulation of a density matrix functional for Van der Waals interaction of like- and opposite-spin electrons in the helium dimer. <i>Journal of Chemical Physics</i> , 2012 , 137, 204117	3-9	7
1679	Ligand effects on rates and regioselectivities of Rh(I)-catalyzed (5 + 2) cycloadditions: a computational study of cyclooctadiene and dinaphthocyclooctatetraene as ligands. 2012 , 134, 11012-25		106
1678	Dimer self-association via hydrogen bonding: Measurement and comparison of binding constants with 2-amidopyrimidine derivatives. 2012 , 547, 24-29		2
1677	Density functional theory with fractional orbital occupations. <i>Journal of Chemical Physics</i> , 2012 , 136, 154104	3-9	99
1676	Substituted Benzene Derivatives on the Cu(111) Surface. 2012 , 116, 12636-12643		26
1675	A discrete interaction model/quantum mechanical method for simulating surface-enhanced Raman spectroscopy. <i>Journal of Chemical Physics</i> , 2012 , 136, 214103	3-9	49
1674	Correction to DFT interaction energies by an empirical dispersion term valid for a range of intermolecular distances. 2012 , 14, 3414-24		8
1673	A pass too far: dissociation of internal energy selected paracyclophane cations, theory and experiment. 2012 , 14, 11920-9		14

- 1672 Propene Epoxidation with H₂/H₂O/O₂ Mixtures Over Gold Atoms Supported on Defective Graphene: A Theoretical Study. **2012**, 116, 19355-19362 23
- 1671 Accurate Computation of Gas Uptake in Microporous Organic Molecular Crystals. **2012**, 116, 8865-8871 38
- 1670 Ab initio molecular dynamics study of water at constant pressure using converged basis sets and empirical dispersion corrections. *Journal of Chemical Physics*, **2012**, 137, 044506 3.9 73
- 1669 The performance of density functional based methods in the description of selected biological systems and processes. **2012**, 14, 14943-53 27
- 1668 The inhibition of iridium-promoted water oxidation catalysis (WOC) by cucurbit[n]urils. **2012**, 41, 12233-43 12
- 1667 Possible dimers of hypochlorous acid (HOCl) arising from hydrogen- and halogen-bond interactions. **2012**, 999, 48-54 9
- 1666 Comment on Thioformyl chloride dimer: An excellent model system for the assessment of new computational methods[Comput. Theoret. Chem. 983 (2012) 8387]. **2012**, 999, 152-153
- 1665 One catalyst for both enantiomers: uncovering the inversion of enantioselectivity in cinchona-mediated desymmetrization of glutaric meso-anhydrides. **2012**, 68, 8311-8317 10
- 1664 The role of van der Waals interactions in the adsorption of noble gases on metal surfaces. **2012**, 24, 424211 35
- 1663 Room temperature metalation of 2H-TPP monolayer on iron and nickel surfaces by picking up substrate metal atoms. **2012**, 6, 10800-7 58
- 1662 Mild and efficient nickel-catalyzed Heck reactions with electron-rich olefins. **2012**, 134, 443-52 115
- 1661 Fluorine-fluorine interactions in the solid state: an experimental and theoretical study. **2012**, 116, 1435-44 117
- 1660 Mechanisms of organocatalytic amidation and trans-esterification of aromatic esters as a model for the depolymerization of poly(ethylene) terephthalate. **2012**, 116, 12389-98 55
- 1659 Benchmarking van der Waals density functionals with experimental data: potential-energy curves for H₂ molecules on Cu(111), (100) and (110) surfaces. **2012**, 24, 424213 33
- 1658 Theoretical investigation of hydrogen adsorption in all-metal aromatic clusters. **2012**, 2, 2914 34
- 1657 Reliable DFT-based estimates of cohesive energies of organic solids: the anthracene crystal. *Journal of Chemical Physics*, **2012**, 137, 194311 3.9 12
- 1656 Charge Transfer between Water Molecules As the Possible Origin of the Observed Charging at the Surface of Pure Water. **2012**, 3, 107-111 86
- 1655 The significance of the alkene size and the nature of the metal ion in metal-alkene complexes: a theoretical study. **2012**, 41, 4965-75 38

1654	Van der Waals interactions in solids using the exchange-hole dipole moment model. <i>Journal of Chemical Physics</i> , 2012 , 136, 174109	3.9	154
1653	Highlights on Anthocyanin Pigmentation and Copigmentation: A Matter of Flavonoid π -Stacking Complexation To Be Described by DFT-D. 2012 , 8, 2034-43		58
1652	Ab Initio Parametrized Force Field for the Flexible Metal-Organic Framework MIL-53(Al). 2012 , 8, 3217-31		58
1651	How Many Ligands Can Be Bound by Magnesium-Porphyrin? A Symmetry-Adapted Perturbation Theory Study. 2012 , 8, 2972-82		17
1650	The effect of side-chain length on the solid-state structure and optoelectronic properties of fluorene-alt-benzothiadiazole based conjugated polymers--a DFT study. 2012 , 116, 10597-606		18
1649	Structural evolution of amino acid crystals under stress from a non-empirical density functional. 2012 , 24, 424209		48
1648	Combined Density Functional Theory and Monte Carlo Analysis of Monomolecular Cracking of Light Alkanes Over H-ZSM-5. 2012 , 116, 23408-23417		50
1647	Shock Hugoniot calculations of polymers using quantum mechanics and molecular dynamics. <i>Journal of Chemical Physics</i> , 2012 , 137, 204901	3.9	30
1646	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. 2012 , 86,		227
1645	Like-Charge Ion Pairing in Water: An Ab Initio Molecular Dynamics Study of Aqueous Guanidinium Cations. 2012 , 3, 2021-2024		49
1644	Stereodynamics in eight-coordination; a 2D NMR spectroscopic and computational study of the exchange process in $\text{ThCl}_4(\text{Me}_2\text{NCH}_2\text{CH}_2\text{NMe}_2)_2$. 2012 , 51, 10141-7		2
1643	Polarization charge densities provide a predictive quantification of hydrogen bond energies. 2012 , 14, 955-63		43
1642	A practical guide to modelling enzyme-catalysed reactions. 2012 , 41, 3025-38		124
1641	Can two T-shaped isomers of $\text{OCS}\cdots\text{H}_2$ van der Waals complex exist?. 2012 , 549, 6-11		14
1640	MOLECULAR BIOLOGY AT THE QUANTUM LEVEL: CAN MODERN DENSITY FUNCTIONAL THEORY FORGE THE PATH?. 2012 , 02, 1230006		7
1639	van der Waals interactions in density functional theory using Wannier functions: Improved C6 and C3 coefficients by a different approach. 2012 , 85,		33
1638	Computational studies of protonated β -D-galactose and its hydrated complex: structures, interactions, proton transfer dynamics, and spectroscopy. 2012 , 116, 4851-9		15
1637	The Cobalt-Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations. 2012 , 8, 1870-94		78

1636	A Hierarchy of Methods for the Energetically Accurate Modeling of Isomerism in Monosaccharides. 2012 , 8, 2630-45	49
1635	Wavefunction-based electron correlation methods for solids. 2012 , 14, 7605-14	72
1634	DFT Study of Furfural Conversion to Furan, Furfuryl Alcohol, and 2-Methylfuran on Pd(111). 2012 , 2, 2496-2504	84
1633	Investigating inclusion complexes using quantum chemical methods. 2012 , 41, 3119-28	58
1632	Noncovalent interactions in peri-substituted chalconium acenaphthene and naphthalene salts: a combined experimental, crystallographic, computational, and solid-state NMR study. 2012 , 51, 11087-97	33
1631	Advancing Understanding and Design of Functional Materials Through Theoretical and Computational Chemical Physics. 2012 , 209-278	3
1630	Structure-dependent interatomic dispersion coefficients in oxides with maximally localized Wannier functions. 2012 , 24, 475501	3
1629	Rationale for switching to nonlocal functionals in density functional theory. 2012 , 24, 424215	15
1628	Fundamentals of Time-Dependent Density Functional Theory. 2012 ,	277
1627	Adsorption of Organic Electron Acceptors on Graphene-like Molecules: Quantum Chemical and Molecular Mechanical Study. 2012 , 116, 25328-25336	20
1626	The effects of ligand variation on enantioselective hydrogenation catalysed by RuH ₂ (diphosphine)(diamine) complexes. 2012 , 41, 1867-77	14
1625	Explicitly correlated benchmark calculations on C ₈ H ₈ isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. 2012 , 110, 2477-2491	47
1624	Random-phase-approximation correlation method including exchange interactions. 2012 , 85,	55
1623	A hybrid zinc phthalocyanine/zinc oxide system for photovoltaic devices: a DFT and TDDFT theoretical investigation. 2012 , 22, 440-446	29
1622	Noncovalent Interactions in SIESTA Using the vdW-DF Functional: S22 Benchmark and Macrocyclic Structures. 2012 , 8, 281-9	25
1621	Strained cyclophane macrocycles: impact of progressive ring size reduction on synthesis and structure. 2012 , 134, 2127-38	57
1620	The role of surface defects in large organic molecule adsorption: substrate configuration effects. 2012 , 14, 10726-31	16
1619	Electronic structures of the [V(tbpy) ₃] ^z (z = 3+, 2+, 0, 1-) electron transfer series. 2012 , 51, 3707-17	41

1618	First-principles kinetic modeling in heterogeneous catalysis: an industrial perspective on best-practice, gaps and needs. 2012 , 2, 2010		124
1617	Correction of vibrational broadening in molecular dynamics clusters with the normal mode optimization method. 2012 , 116, 336-42		35
1616	Reaction Mechanisms for CO Catalytic Oxidation by N ₂ O on Fe-Embedded Graphene. 2012 , 116, 16992-16998	112	
1615	Synthesis, Characterization, and Fluxional Behavior of a 34 Electron Homochiral Dimetallic Complex with an Unsupported Hydride Bridge between Two Ru Atoms. 2012 , 31, 2821-2828		2
1614	Mechanism of ketone hydrosilylation using NHCCu(I) catalysts: a computational study. 2012 , 131, 1		15
1613	On the unusual weak intramolecular C...C interactions in Ru ₃ (CO) ₁₂ : a case of bond path artifacts introduced by the multipole model?. 2012 , 116, 738-46		17
1612	Structural optimization of molecular clusters with density functional theory combined with basin hopping. <i>Journal of Chemical Physics</i> , 2012 , 137, 134106	3-9	39
1611	Structural and electronic properties of oligo- and polythiophenes modified by substituents. 2012 , 3, 909-19		34
1610	Properties of crystalline coronene: Dispersion forces leading to a larger van der Waals radius for carbon. 2012 , 249, 1438-1444		26
1609	Spin-component-scaled electron correlation methods. 2012 , 2, 886-906		173
1608	Symmetry-adapted perturbation theory of intermolecular forces. 2012 , 2, 254-272		377
1607	Investigation of Polybromide Monoanions of the Series [NAlk ₄][Br ₉] (Alk = Methyl, Ethyl, Propyl, Butyl). 2012 , 638, 553-558		45
1606	Can computational approaches aid in untangling the inherent complexity of practical organic photovoltaic systems?. 2012 , 50, 1071-1089		28
1605	Review and analysis of molecular simulations of methane, hydrogen, and acetylene storage in metal-organic frameworks. 2012 , 112, 703-23		983
1604	Why are the Interaction Energies of Charge-Transfer Complexes Challenging for DFT?. 2012 , 8, 1629-40		141
1603	Anion effects in the scattering of CO ₂ from the room-temperature ionic liquids [bmim][BF ₄] and [bmim][Tf ₂ N]: insights from quantum mechanics/molecular mechanics trajectories. 2012 , 116, 3587-602		26
1602	Computational modelling of inorganic solids. 2012 , 108, 449		2
1601	Reverse cope elimination of hydroxylamines and alkenes or alkynes: theoretical investigation of tether length and substituent effects. 2012 , 134, 2434-41		59

1600	O(N) methods in electronic structure calculations. 2012 , 75, 036503	367
1599	Cationic Gold Catalysis with Pyridine-Tethered Au(III) NHC-Carbenes: An Experimental and DFT Computational Study. 2012 , 31, 4320-4330	35
1598	A B3LYP-DBLOC empirical correction scheme for ligand removal enthalpies of transition metal complexes: parameterization against experimental and CCSD(T)-F12 heats of formation. 2012 , 14, 7724-38	30
1597	Planar P(6)E(6) (E = Se, S) macrocycles incorporating P(2)N(2) scaffolds. 2012 ,	40
1596	Silylium ion-catalyzed challenging Diels-Alder reactions: the danger of hidden proton catalysis with strong Lewis acids. 2012 , 134, 4421-8	87
1595	Challenges for density functional theory. 2012 , 112, 289-320	1521
1594	Calculation of dispersion energies. 2012 , 24, 073201	155
1593	Reactivity and Regioselectivity of Palladium-Catalyzed Direct Arylation in Noncooperative and Cooperative Processes. 2012 , 31, 4631-4634	33
1592	Bonds or not bonds? Pancake bonding in 1,2,3,5-dithiadiazolyl and 1,2,3,5-diselenadiazolyl radical dimers and their derivatives. 2012 , 14, 10713-25	68
1591	Dispersion-Corrected Density Functional Theory and Classical Force Field Calculations of Water Loading on a Pyrophyllite(001) Surface. 2012 , 116, 17134-17141	36
1590	[2.2]Paracyclophane derived bisphosphines for the activation of hydrogen by FLPs: application in domino hydrosilylation/hydrogenation of enones. 2012 , 41, 9056-60	51
1589	Stable alkanes containing very long carbon-carbon bonds. 2012 , 134, 13641-50	153
1588	The anion dependence of the interaction strength between ions in imidazolium-based ionic liquids probed by far-infrared spectroscopy. 2012 , 116, 9507-11	48
1587	Accuracy of Several Wave Function and Density Functional Theory Methods for Description of Noncovalent Interaction of Saturated and Unsaturated Hydrocarbon Dimers. 2012 , 8, 2282-92	47
1586	DFT investigation of the molybdenum cofactor in periplasmic nitrate reductases: structure of the Mo(V) EPR-active species. 2012 , 51, 3409-19	30
1585	Fully ab initio protein-ligand interaction energies with dispersion corrected density functional theory. 2012 , 33, 1730-9	60
1584	Computational investigations on covalent dimerization/oligomerization of polyacenes: is it relevant to soot formation?. 2012 , 33, 1762-72	14
1583	M(O)V(I)P(AC): vibrational spectroscopy with a robust meta-program for massively parallel standard and inverse calculations. 2012 , 33, 2186-98	50

1582	Implementation of empirical dispersion corrections to density functional theory for periodic systems. 2012 , 33, 2023-31	107
1581	Binding energies of five molecular pincers calculated by explicit and implicit solvent models. 2012 , 33, 2310-7	12
1580	Halogen Bonding versus Hydrogen Bonding: A Molecular Orbital Perspective. 2012 , 1, 96-105	149
1579	The Reactions of Thianthrene and Selenanthrene with AlCl ₃ : Coordination Complexes, Radical Ions, and Investigations on the Unique Triple-Decker Molecule (Thianthrene) ₃ 2 ⁺ . 2012 , 2012, 3625-3635	15
1578	Accurate Computation of Structures and Strain Energies of Cyclophanes with Modern DFT Methods. 2012 , 52, 180-192	32
1577	Assessment of ab initio MP2 and density functionals for characterizing the potential energy profiles of the S _N 2 reactions at N center. 2012 , 33, 1347-52	11
1576	Universal Correction of Density Functional Theory to Include London Dispersion (up to Lr, Element 103). 2012 , 3, 360-3	41
1575	Tuned Range-Separated Time-Dependent Density Functional Theory Applied to Optical Rotation. 2012 , 8, 245-56	92
1574	Nanodiamonds in sugar rings: an experimental and theoretical investigation of cyclodextrin-nanodiamond inclusion complexes. 2012 , 10, 4524-30	42
1573	Comparing van der Waals Density Functionals for CO ₂ Adsorption in Metal Organic Frameworks. 2012 , 116, 16957-16968	63
1572	Comparison of the relative stability of zinc and lithium-boron zeolitic imidazolate frameworks. 2012 , 14, 374-378	43
1571	On the Adsorption of Formaldehyde and Methanol on a Water-Covered Pt(111): a DFT-D Study. 2012 , 116, 15484-15492	32
1570	Modeling Ruthenium-Dye-Sensitized TiO ₂ Surfaces Exposing the (001) or (101) Faces: A First-Principles Investigation. 2012 , 116, 18124-18131	52
1569	Nukleophile Addition von Enolen und Enaminen an β,β -ungesättigte Acylazoliumionen: Mechanistische Studien. 2012 , 124, 5325-5329	34
1568	Niederfrequente Schwingungsmoden protischer geschmolzener Salze und ionischer Flüssigkeiten: Nachweis und Quantifizierung von Wasserstoffbrücken. 2012 , 124, 6340-6344	26
1567	Nucleophilic addition of enols and enamines to β,β -unsaturated acylazoliums: mechanistic studies. 2012 , 51, 5234-8	90
1566	Low-frequency vibrational modes of protic molten salts and ionic liquids: detecting and quantifying hydrogen bonds. 2012 , 51, 6236-40	92
1565	Hydrogen activation by an intramolecular boron Lewis acid/zirconocene pair. 2012 , 51, 8830-3	43

1564	Binding of molecular magnesium hydrides to a zirconocene-enyne template. 2012 , 51, 8846-9	23
1563	Mechanistic studies on the Pd-catalyzed direct C-H arylation of 2-substituted thiophene derivatives with arylpalladium bipyridyl complexes. 2012 , 7, 1256-60	57
1562	Transmetallation versus β -hydride elimination: the role of 1,4-benzoquinone in chelation-controlled arylation reactions with arylboronic acids. 2012 , 18, 4714-22	36
1561	Synthesis of planar chiral iridacycles by cationic metal π -coordination: facial selectivity, and conformational and stereochemical consequences. 2012 , 18, 6063-78	17
1560	Metal-ligand cooperation in catalytic intramolecular hydroamination: a computational study of iridium-pyrazolato cooperative activation of aminoalkenes. 2012 , 18, 7248-62	21
1559	Investigating the halochromic properties of azo dyes in an aqueous environment by using a combined experimental and theoretical approach. 2012 , 18, 8120-9	35
1558	The exohedral Diels-Alder reactivity of the titanium carbide endohedral metallofullerene Ti ₂ C ₂ @D(3h)-C ₇₈ : comparison with D(3h)-C ₇₈ and M ₃ N@D(3h)-C ₇₈ (M=Sc and Y) reactivity. 2012 , 18, 7141-54	47
1557	Theoretical approach towards the understanding of asymmetric additions of dialkylzinc to enals and iminals catalysed by [2.2]paracyclophane-based N,O-ligands. 2012 , 18, 8377-85	10
1556	Correlating DFT-calculated energy barriers to experiments in nonheme octahedral Fe(IV)O species. 2012 , 18, 10444-53	20
1555	Iron borohydride pincer complexes for the efficient hydrogenation of ketones under mild, base-free conditions: synthesis and mechanistic insight. 2012 , 18, 7196-209	172
1554	Silver and gold complexes with a new 1,10-phenanthroline analogue N-heterocyclic carbene: a combined structural, theoretical, and photophysical study. 2012 , 18, 5506-9	47
1553	Supramolecular binding thermodynamics by dispersion-corrected density functional theory. 2012 , 18, 9955-64	974
1552	Hydride ligands make the difference: density functional study of the mechanism of the Murai reaction catalyzed by [Ru(H) ₂ (H ₂) ₂ (PR ₃) ₂] (R=cyclohexyl). 2012 , 18, 11449-58	16
1551	Effect of dispersion on the structure and dynamics of the ionic liquid 1-ethyl-3-methylimidazolium thiocyanate. 2012 , 13, 1845-53	75
1550	Force fields for studying the structure and dynamics of ionic liquids: a critical review of recent developments. 2012 , 13, 1625-37	218
1549	Comment on: "On the accuracy of DFT methods in reproducing ligand substitution energies for transition metal complexes in solution: the role of dispersive interactions" by H. Jacobsen and L. Cavallo. 2012 , 13, 1407-9; author reply 1405-6	40
1548	Three types of induced tryptophan optical activity compared in model dipeptides: theory and experiment. 2012 , 13, 2748-60	15
1547	Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized Tröger's Base Derivatives: Part II. 2012 , 77, 396-403	24

1546	Aggregation and Solvation of Chiral N,P-Amide Ligands in Coordinating Solvents: A Computational and NMR Spectroscopic Study. 2012 , 77, 799-806		10
1545	Heptabismuthate [Bi ₇ I ₂₄]·3H ₂ O: a main group element anderson-type structure and its relationships with the polyoxometalates. 2012 , 51, 1562-8		39
1544	Computational organic chemistry. 2012 , 108, 334		3
1543	Weak Intermolecular Interactions: A Supramolecular Approach. 2012 , 443-466		9
1542	Assessment of density functional theory to calculate the phase transition pressure of ice. 2012 , 14, 11484-90	20	
1541	Preparation and characterization of stable aqueous higher-order fullerenes. 2012 , 23, 055705		18
1540	Graphane/fluorographene bilayer: considerable C-H...F-C hydrogen bonding and effective band structure engineering. 2012 , 134, 11269-75		100
1539	Electric field induced phase transitions in polymers: a novel mechanism for high speed energy storage. 2012 , 108, 087802		37
1538	Communication: Density functional theory overcomes the failure of predicting intermolecular interaction energies. <i>Journal of Chemical Physics</i> , 2012 , 136, 161102	3.9	56
1537	Carbon monoxide activation via O-bound CO using decamethylscandocinium-hydridoborate ion pairs. 2012 , 134, 10843-51		83
1536	Theoretical investigation on DNA/RNA base pairs mediated by copper, silver, and gold cations. 2012 , 41, 1816-23		19
1535	A (Nearly) Universally Applicable Method for Modeling Noncovalent Interactions Using B3LYP. 2012 , 3, 1738-44		99
1534	Computational Investigation of Dye-Dye Interactions in Organic Dye-Sensitized Solar Cells. 2012 , 116, 5965-5973		82
1533	Removal of Bisphenol A and 17 β -Estradiol by Single-Walled Carbon Nanotubes in Aqueous Solution: Adsorption and Molecular Modeling. 2012 , 223, 3281-3293		69
1532	Computational ¹⁹ F NMR. 1. General features. 2012 , 131, 1		15
1531	Range-separated density functional theory: A 4-component relativistic study of the rare gas dimers He ₂ , Ne ₂ , Ar ₂ , Kr ₂ , Xe ₂ , Rn ₂ and Uuo ₂ . 2012 , 395, 54-62		34
1530	DFT investigation of endohedral boron oxide nanocapsules: Encapsulation of He, Ne, Ar, H, N, and Cl atoms. 2012 , 393, 86-95		6
1529	DFT study of salicylaldehyde semicarbazone derivatives interaction with copper and the effect of aminic substituent. 2012 , 384, 29-36		3

1528	A theoretical spectroscopy investigation of oxosumanenes. 2012 , 519-520, 49-53	13
1527	A DFT-D evaluation of the complexation of a molecular tweezer with small aromatic molecules. 2012 , 522, 11-16	16
1526	Hydration of cellobiose: Structure and dynamics of cellobiose $(\text{H}_2\text{O})_n$, $n=5-25$. 2012 , 531, 52-58	15
1525	Extending the applicability of the PBE0-DH double-hybrid model to weak interactions. 2012 , 535, 136-139	10
1524	Seeking for reliable double-hybrid density functionals without fitting parameters: The PBE0-2 functional. 2012 , 538, 121-125	92
1523	A periodic hybrid DFT approach (including dispersion) to MgCl_2 -supported Ziegler-Natta catalysts \square 1: TiCl_4 adsorption on MgCl_2 crystal surfaces. 2012 , 286, 103-110	90
1522	Electronic structure of a single MoS_2 monolayer. 2012 , 152, 909-913	421
1521	Assessment of a variety of dispersion-corrected density functional theory calculations used in molecular crystal structure prediction. 2012 , 4,	0
1520	Performance of dispersion-corrected density functional theory for thermochemistry and non-covalent interactions. 2012 , 4,	2
1519	tBu or not tBu?. 2012 , 18, 1640-9	33
1518	Carboxylation of arene C-H bonds with CO_2 : a DFT-based approach to catalyst design. 2012 , 18, 170-7	55
1517	Alder-ene reaction: aromaticity and activation-strain analysis. 2012 , 33, 509-16	83
1516	Dispersive interactions in water bilayers at metallic surfaces: a comparison of the PBE and RPBE functional including semiempirical dispersion corrections. 2012 , 33, 695-701	119
1515	Ab initio molecular dynamics study of water oxidation reaction pathways in mono-Ru catalysts. 2012 , 13, 140-6	45
1514	Combined theoretical and experimental investigation of CO adsorption on coordinatively unsaturated sites in CuBTC MOF. 2012 , 13, 488-95	38
1513	A DFT study of the interaction between microhydrated anions and naphthalendiimides. 2012 , 13, 570-7	7
1512	On the accuracy of DFT methods in reproducing ligand substitution energies for transition metal complexes in solution: the role of dispersive interactions. 2012 , 13, 562-9	53
1511	Di-, Tetra-, Penta- and Polynuclear Zinc Complexes Supported by a Flexible Tetradentate Schiff Base Ligand. 2012 , 2012, 1130-1138	14

1510	Toward ab initio refinement of protein X-ray crystal structures: interpreting and correlating structural fluctuations. 2012 , 131, 1	7
1509	An improved theoretical approach to the empirical corrections of density functional theory. 2012 , 26, 199-213	2
1508	Theoretical study of electronic absorptions in aminopyridines - TCNE CT complexes by quantum chemical methods, including solvent. 2013 , 19, 4639-50	5
1507	Aromatic interactions as control elements in stereoselective organic reactions. 2013 , 46, 979-89	183
1506	Probing the relation between charge transport and supramolecular organization down to Ångström resolution in a benzothiadiazole-cyclopentadithiophene copolymer. 2013 , 25, 1939-47	79
1505	Large-scale DFT calculations in implicit solvent: A case study on the T4 lysozyme L99A/M102Q protein. 2013 , 113, 771-785	29
1504	Self-consistent field treatment and analytical energy gradient of local response dispersion method. 2013 , 113, 257-262	16
1503	Interactions between Methane and Polycyclic Aromatic Hydrocarbons: A High Accuracy Benchmark Study. 2013 , 9, 370-89	30
1502	Convergence of the Interaction Energies in Noncovalent Complexes in the Coupled-Cluster Methods Up to Full Configuration Interaction. 2013 , 9, 3420-8	32
1501	Ab initio molecular dynamics studies on the growth of ammonium chloride clusters. 2013 , 132, 1	3
1500	Hexagonal boron nitride on transition metal surfaces. 2013 , 132, 1	85
1499	Dispersion-corrected Rung 3.5 density functionals. 2013 , 132, 1	1
1498	Accurate ranking of CH ₄ [(H ₂ O) ₂₀] clusters with the density functional theory supplemental potential approach. 2013 , 132, 1	8
1497	In silico studies toward understanding the interactions of DNA base pairs with protonated linear/cyclic diamines. 2013 , 117, 9840-50	3
1496	Theoretical Insights into the Nature of Divalent Lanthanide-Ligand Interactions. 2013 , 32, 1265-1271	28
1495	Redox-dependent structural transformations of the [4Fe-3S] proximal cluster in O ₂ -tolerant membrane-bound [NiFe]-hydrogenase: a DFT study. 2013 , 135, 11809-23	25
1494	Electronic Structures of Antimony Oxides. 2013 , 117, 14759-14769	62
1493	Why Mercury Prefers Soft Ligands. 2013 , 4, 2317-2322	40

1492	A conformationally flexible dinuclear Pt(II) complex with differential behavior of its two states toward quadruplex DNA. 2013 , 19, 11429-38		13
1491	Oxidative Activation of AryldiynylIron Complexes: Regioselective Dimerization. 2013 , 32, 1866-1875		15
1490	Computational Investigation of Brook-Type Silabenzenes and Their Possible Formation through [1,3]-Si-O Silyl Shifts. 2013 , 32, 16-28		10
1489	Relevance of thermal effects in the formation of endohedral metallofullerenes: the case of Gd ₃ N@C(s)(39663)-C ₈₂ and other related systems. 2013 , 52, 1954-9		21
1488	A novel correction scheme for DFT: a combined vdW-DF/CCSD(T) approach. <i>Journal of Chemical Physics</i> , 2013 , 139, 034115	3.9	17
1487	The shape of Au ₈ : gold leaf or gold nugget?. 2013 , 5, 6445-57		36
1486	Effects of metal coordination on the ESR spectrum of the 2,5-bis-((pyrrolidino)-methyl)-pyrrole pincer ligand. 2013 , 52, 9539-48		22
1485	Density functional theory study of fullerene-barbene Lewis acid-base adducts: critical role of dispersion interactions. 2013 , 3, 10177		6
1484	A modified cyclen azaxanthone ligand as a new fluorescent probe for Zn ²⁺ . 2013 , 42, 12157-64		21
1483	Error estimates for (semi-)empirical dispersion terms and large biomacromolecules. 2013 , 11, 6515-9		8
1482	Many-body dispersion interactions from the exchange-hole dipole moment model. <i>Journal of Chemical Physics</i> , 2013 , 138, 054103	3.9	59
1481	Dynamic ¹ H NMR spectroscopic study of hindered internal rotation in selected N,N-dialkyl isonicotinamides: an experimental and DFT analysis. 2013 , 69, 8147-8154		13
1480	Towards [NiFe]-hydrogenase biomimetic models that couple H ₂ binding with functionally relevant intramolecular electron transfers: a quantum chemical study. 2013 , 42, 13845-54		7
1479	Atomic structure and electronic properties of folded graphene nanoribbons: A first-principles study. 2013 , 113, 173506		13
1478	Chiral recognition in contact ion-pairs; observation, characterization and analysis. 2013 , 4, 3140		17
1477	The structures of two aldazines: [1,1'-(1E,1'E)-hydrazine-1,2-diylidenebis(methan-1-yl-1-ylidene)dinaphthalen-2-ol] (Lumogen) and 2,2'-(1E,1'E)-hydrazine-1,2-diylidenebis(methan-1-yl-1-ylidene)diphenol (salicylaldazine) in the solid state. 2013 , 51, 530-10		5
1476	Density-Functional Theory with Dispersion-Correcting Potentials for Methane: Bridging the Efficiency and Accuracy Gap between High-Level Wave Function and Classical Molecular Mechanics Methods. 2013 , 9, 3342-9		9
1475	Tests of Exchange-Correlation Functional Approximations Against Reliable Experimental Data for Average Bond Energies of 3d Transition Metal Compounds. 2013 , 9, 3965-77		82

1474	A continuum solvent model of the multipolar dispersion solvation energy. 2013 , 117, 9412-20	61
1473	Effects of London dispersion correction in density functional theory on the structures of organic molecules in the gas phase. 2013 , 15, 16031-42	188
1472	Theoretical spectroscopy of the Ni(II) intermediate states in the catalytic cycle and the activation of [NiFe] hydrogenases. 2013 , 14, 1898-905	48
1471	Unidirectional molecular stacking of tribenzotriquinacenes in the solid state: a combined X-ray and theoretical study. 2013 , 19, 9930-8	41
1470	Analysis of supramolecular complex energetics in artificial replicators. 2013 , 4, 3591	6
1469	Exploiting multivalent nanoparticles for the supramolecular functionalization of graphene with a nonplanar recognition motif. 2013 , 19, 9843-8	15
1468	Chiroptical properties of carbo[6]helicene derivatives bearing extended π -conjugated cyano substituents. 2013 , 25, 455-65	31
1467	Toxic effects of cephalosporins with specific functional groups as indicated by zebrafish embryo toxicity testing. 2013 , 26, 1168-81	29
1466	Performance of conventional and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. 2013 , 15, 12821-8	101
1465	Using the DFT-D method to describe dispersion interactions in systems of weakly-bonded Xe-aromatic molecules. 2013 , 87, 1342-1348	8
1464	A Phosphine-Accelerated Ar-F Chloride Bond Activation Process by Palladium. 2013 , 32, 3074-3082	3
1463	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. 2013 , 34, 2079-90	27
1462	Noble Gas Separation using PG-ESX (X = 1, 2, 3) Nanoporous Two-Dimensional Polymers. 2013 , 117, 393-402	51
1461	Long-range corrected density functionals combined with local response dispersion: A promising method for weak interactions. 2013 , 34, 2353-9	5
1460	Synthesis, structures, and dearomatization by deprotonation of iron complexes featuring bipyridine-based PNN pincer ligands. 2013 , 52, 9636-49	47
1459	Van der Waals interactions in density functional theory by combining the quantum harmonic oscillator-model with localized Wannier functions. <i>Journal of Chemical Physics</i> , 2013 , 139, 054106	3-9 33
1458	Aromatic interactions in asymmetric catalysis: control of enantioselectivity in Diels-Alder reactions catalysed by camphor-derived hydrazides. 2013 , 11, 5226-32	9
1457	Convergence of QM/MM and Cluster Models for the Spectroscopic Properties of the Oxygen-Evolving Complex in Photosystem II. 2013 , 9, 3832-42	50

1456	Nonlocal van der Waals Approach Merged with Double-Hybrid Density Functionals: Toward the Accurate Treatment of Noncovalent Interactions. 2013 , 9, 3437-43		46
1455	The accuracy of quantum chemical methods for large noncovalent complexes. 2013 , 9, 3364-3374		223
1454	On the formation of the formate anion: Insights from population analyses. 2013 , 1012, 8-13		1
1453	Understanding the role of vibrations, exact exchange, and many-body van der Waals interactions in the cohesive properties of molecular crystals. <i>Journal of Chemical Physics</i> , 2013 , 139, 024705	3.9	222
1452	Qualitative change of character of dispersive interaction with intermolecular distance. <i>Journal of Chemical Physics</i> , 2013 , 139, 044103	3.9	2
1451	From hydrogen bond donor to acceptor: the effect of ethanol fluorination on the first solvating water molecule. 2013 , 15, 16065-73		42
1450	Toward the microscopic identification of anions and cations at the ionic liquid Ag(111) interface: a combined experimental and theoretical investigation. 2013 , 7, 7773-84		84
1449	Adsorption and decomposition of NH ₃ on Ir(111): A density functional theory study. 2013 , 616, 29-35		10
1448	A simple non-empirical procedure for spin-component-scaled MP2 methods applied to the calculation of the dissociation energy curve of noncovalently-interacting systems. 2013 , 15, 15485-93		13
1447	Role of van der Waals corrections for the PtX ₂ (X=O, S, Se) compounds. 2013 , 88,		23
1446	Chiral, Racemic, and Meso-Lithium Tartrate Framework Polymorphs: A Detailed Structural Analysis. 2013 , 13, 3705-3715		23
1445	6-Trifluoromethyl-phenanthridines through radical trifluoromethylation of isonitriles. 2013 , 52, 10792-5		284
1444	Reactivity of dicoordinated stannylenes (Sn ⁰) versus stannylenes (Sn ^{II}): an investigation using DFT-based reactivity indices. 2013 , 14, 3233-47		6
1443	Density Functional Investigation of the Adsorption of Ethanol/Water Mixture on the Pt(111) Surface. 2013 , 117, 16942-16952		25
1442	Impact of functionalized linkers on the energy landscape of ZIFs. 2013 , 15, 9603		25
1441	Molecular level simulation of the adsorption of bisphenol A and 17 β -ethinyl estradiol onto carbon nanomaterials. 2013 , 116, 471-478		26
1440	Geometrical correction for the inter- and intramolecular basis set superposition error in periodic density functional theory calculations. 2013 , 117, 9282-92		100
1439	Porous Graphene and Nanomeshes. 2013 , 129-151		1

1438	Role of water in Mukaiyama-Aldol reaction catalyzed by lanthanide lewis acid: a computational study. 2013 , 135, 13972-9	39
1437	Assessment of binding energies of atmospherically relevant clusters. 2013 , 15, 16442-5	103
1436	Assessment of Coupled Cluster Theory and more Approximate Methods for Hydrogen Bonded Systems. 2013 , 9, 4403-13	39
1435	Correlation effects on the relative stabilities of alkanes. 2013 , 135, 13008-14	30
1434	Hydrogen Storage in Graphene. 2013 , 371-391	3
1433	Free energies of binding from large-scale first-principles quantum mechanical calculations: application to ligand hydration energies. 2013 , 117, 9478-85	39
1432	Nature of noncovalent interactions in catenane supramolecular complexes: calibrating the MM3 force field with ab initio, DFT, and SAPT methods. 2013 , 117, 7918-27	34
1431	Theoretical study of molecular interactions of sulfur ylide with HF, HCN, and HN ₃ . 2013 , 24, 271-277	7
1430	Energies of the adsorption of functional groups to calcium carbonate polymorphs: the importance of -OH and -COOH groups. 2013 , 29, 11062-73	58
1429	An improved treatment of empirical dispersion and a many-body energy decomposition scheme for the explicit polarization plus symmetry-adapted perturbation theory (XSAPT) method. <i>Journal of Chemical Physics</i> , 2013 , 139, 034107	3,9 52
1428	Synthesis and ligand non-innocence of thiolate-ligated (N ₄ S) Iron(II) and nickel(II) bis(imino)pyridine complexes. 2013 , 52, 10467-80	20
1427	DFT study of the ExBox ² aromatic hydrocarbon host-guest complex. 2013 , 117, 8484-91	30
1426	Reaction of Li/Cl phosphinidenoid complexes with a phosphite substituted ketone: access to complexes with a novel mixed-valence polycyclic P,C-ligand system. 2013 , 42, 10510-4	7
1425	Predicting the stability constants of metal-ion complexes from first principles. 2013 , 52, 10347-55	41
1424	Understanding the reactivity of Pd(0)/PR ₃ -catalyzed intermolecular C(sp ³)-H bond arylation. 2013 , 135, 14206-14	71
1423	Magnetic hardening induced by nonmagnetic organic molecules. 2013 , 111, 106805	74
1422	What factors control O ₂ binding and release thermodynamics in mononuclear ruthenium water oxidation catalysts? A theoretical exploration. 2013 , 52, 5088-96	17
1421	Synthesis and DFT calculations of spirooxaphosphirane complexes. 2013 , 42, 8897-906	23

1420	Reactivity in nucleophilic vinylic substitution (S(N)V):S(N)V versus S(N)V mechanistic dichotomy. 2013 , 78, 8574-84	31
1419	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. 2013 , 1-57	1
1418	Stabilizing factors of the molecular structure in silicon-based peptidomimetics in gas-phase and water solution. Assessment of the correlation between different descriptors of hydrogen bond strength. 2013 , 19, 4293-304	1
1417	Modeling the physisorption of bisphenol A on graphene and graphene oxide. 2013 , 19, 3569-80	37
1416	Effects of local protein environment on the binding of diatomic molecules to heme in myoglobins. DFT and dispersion-corrected DFT studies. 2013 , 19, 3307-23	6
1415	ETS-NOCV description of σ hole bonding. 2013 , 19, 2747-58	35
1414	Theoretical study on electronic spectra and interaction in [Au ₃]-L-[Au ₃] (L = C ₆ F ₆ , Ag ⁺) complexes. 2013 , 19, 1973-9	7
1413	Ab initio molecular dynamics simulation on the formation process of He@C ₆₀ synthesized by explosion. 2013 , 19, 1705-10	2
1412	Quantum chemical study of silanediols as metal binding groups for metalloprotease inhibitors. 2013 , 19, 1819-34	5
1411	Machine-learning approach for one- and two-body corrections to density functional theory: Applications to molecular and condensed water. 2013 , 88,	148
1410	Computational Modeling of Isoindigo-Based Polymers Used in Organic Solar Cells. 2013 , 117, 17940-17954	27
1409	Spin-component-scaled double hybrids: An extensive search for the best fifth-rung functionals blending DFT and perturbation theory. 2013 , 34, 2327-44	200
1408	Quantum chemical studies on adsorption of CO ₂ on nitrogen-containing molecular segment models of coal. 2013 , 616, 85-92	28
1407	Fe(III)-Heme Complexes with the Amyloid Beta Peptide of Alzheimer's Disease: QM/MM Investigations of Binding and Redox Properties of Heme Bound to the His Residues of A β (1-42). 2013 , 9, 4233-42	7
1406	Oxygen monomers and dimers at gas-phase and Ag(111)-supported nanographenes: A density functional theory study. 2013 , 113, 114307	5
1405	Contribution of van der Waals interactions to the adsorption energy of C ₂ H ₂ , C ₂ H ₄ , and C ₆ H ₆ on Si(100). 2013 , 557, 159-162	10
1404	Noncovalent interaction and its influence on excited-state behavior: A theoretical study on the mixed coaggregates of dicyanonaphthalene and pyrazoline. 2013 , 556, 230-236	12
1403	Revealing the nature of intermolecular interaction and configurational preference of the nonpolar molecular dimers (H ₂ N ₂) and (H ₂ N ₂) 2013 , 19, 5387-95	78

1402	Evaluating London Dispersion Force Corrections in Crystalline Nitroguanidine by Terahertz Spectroscopy. 2013 , 3, 281-287	18
1401	The effects of alkalinity and acidity of process water and hydrochar washing on the adsorption of atrazine on hydrothermally produced hydrochar. 2013 , 93, 1989-96	44
1400	CO-Induced Methyl Migration in a Rhodium Thiophosphoryl Pincer Complex and Its Comparison with Phosphine-Based Complexes: The Divergent Effects of S and P Donor Ligands. 2013 , 32, 7163-7180	16
1399	Study of ligand effects in aurophilic interactions using local correlation methods. 2013 , 15, 18115-22	30
1398	On the role of noncovalent interactions in electrocatalysis. Two cases of mediated reductive dehalogenation. 2013 , 110, 619-627	6
1397	Signatures in vibrational and UV-visible absorption spectra for identifying cyclic hydrocarbons by graphene fragments. 2013 , 5, 12178-84	15
1396	Theoretical study on the mechanism and stereochemistry of the cinchona-thiourea organocatalytic hydrophosphonylation of an α -ketoester. 2013 , 11, 7497-506	10
1395	Theoretical calculation of reorganization energy for electron self-exchange reaction by constrained density functional theory and constrained equilibrium thermodynamics. 2013 , 117, 8017-25	32
1394	Oxazoline-based organocatalyst for enantioselective strecker reactions: a protocol for the synthesis of levamisole. 2013 , 19, 14224-32	16
1393	Functionalization of Monolayer h-BN by a Metal Support for the Oxygen Reduction Reaction. 2013 , 117, 21359-21370	93
1392	Electronic Structure Assessment: Combined Density Functional Theory Calculations and Ru L2,3-Edge X-ray Absorption Near-Edge Spectroscopy of Water Oxidation Catalyst. 2013 , 117, 18994-19001	7
1391	A dispersion-corrected density functional theory case study on ethyl acetate conformers, dimer, and molecular crystal. 2013 , 132, 1	15
1390	Transition polarizability model of induced resonance Raman optical activity. 2013 , 34, 2152-8	20
1389	Stannylyene-Based Lewis Pairs. 2013 , 32, 6785-6791	51
1388	A Computational Investigation of a Molecular Switch. 2013 , 90, 1528-1532	8
1387	Molecular Dynamics Kinetic Study on the Zeolite-Catalyzed Benzene Methylation in ZSM-5. 2013 , 3, 2556-2567	73
1386	CH ₄ dissociation on NiM(111) (M=Co, Rh, Ir) surface: A first-principles study. 2013 , 617, 149-155	27
1385	Anomalous frequency trends in MoS ₂ thin films attributed to surface effects. 2013 , 88,	91

1384	Structure-activity relationships and identification of optimized CC-chemokine receptor CCR1, 5, and 8 metal-ion chelators. 2013 , 53, 2863-73	2
1383	Terahertz vibrations of crystalline acyclic and cyclic diglycine: benchmarks for London force correction models. 2013 , 117, 10504-12	17
1382	Proton affinity of the histidine-tryptophan cluster motif from the influenza A virus from molecular dynamics. 2013 , 422, 156-164	11
1381	Manipulating liquid-crystal properties using a pH activated hydrazone switch. 2013 , 52, 10734-9	64
1380	Hemichelation, a way to stabilize electron-unsaturated complexes: the case of T-shaped Pd and Pt metallacycles. 2013 , 135, 17839-52	27
1379	Computational studies of the electronic absorption spectrum of [(2,2';6',2''-terpyridine)-Pt(II)-OH] [7,7,8,8-tetracyanoquinodimethane] complex. 2013 , 117, 12363-73	3
1378	Accurate Computation of Cohesive Energies for Small to Medium-Sized Gold Clusters. 2013 , 9, 1964-70	37
1377	Novel carbazole-phenothiazine dyads for dye-sensitized solar cells: a combined experimental and theoretical study. 2013 , 5, 9635-47	85
1376	Lattice-matched versus lattice-mismatched models to describe epitaxial monolayer graphene on Ru(0001). 2013 , 88,	30
1375	High-resolution molybdenum K-edge X-ray absorption spectroscopy analyzed with time-dependent density functional theory. 2013 , 15, 20911-20	58
1374	Insight in the activity and diastereoselectivity of various Lewis acid catalysts for the citronellal cyclization. 2013 , 305, 118-129	45
1373	A very stable complex of a modified marine cyclopeptide with chloroform. 2013 , 4, 2945	18
1372	Theoretical insights into the adsorption of neutral, radical and anionic thiophenols on gold(111). 2013 , 15, 20363-70	22
1371	Remarkable behavior of a bifunctional alkynylborane zirconocene complex toward donor ligands and acetylenes. 2013 , 135, 17444-56	26
1370	Importance of dispersion in density functional calculations of cesium chloride and its related halides. 2013 , 88,	26
1369	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. 2013 , 9, 355-63	62
1368	Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory. 2013 , 4, 3753-3759	117
1367	Electrochromic Platinum(II) Complexes Derived from Azobenzene and Zwitterionic Quinonoid Ligands: Electronic and Geometric Structures. 2013 , 32, 7366-7375	36

1366	Carbonylation reactions of intramolecular vicinal frustrated phosphane/borane Lewis pairs. 2013 , 135, 18567-74	83
1365	Critical Importance of van der Waals Stabilization in Strongly Chemically Bonded Surfaces: Cu(110):O. 2013 , 9, 5578-84	10
1364	Cooperative Ge-N Bond Activation in Hydrogallation Products of Alkynyl(diethylamino)germanes (Et ₂ N) _n Ge(C≡CtBu) _{4-n} . 2013 , 32, 6770-6779	23
1363	Performance of Density Functionals for Activation Energies of Zr-Mediated Reactions. 2013 , 9, 4735-43	54
1362	The protonation states of oxo-bridged Mn(IV) dimers resolved by experimental and computational Mn K pre-edge X-ray absorption spectroscopy. 2013 , 52, 12904-14	41
1361	Dispersion force stabilized two-coordinate transition metal-amido complexes of the -N(SiMe ₃)Dipp (Dipp = C ₆ H ₃ -2,6-Pr(i) ₂) ligand: structural, spectroscopic, magnetic, and computational studies. 2013 , 52, 13584-93	80
1360	Competition between Icosahedral Motifs in AgCu, AgNi, and AgCo Nanoalloys: A Combined Atomistic/DFT Study. 2013 , 117, 26405-26413	110
1359	Copper(I) nitrosyls from reaction of copper(II) thiolates with S-nitrosothiols: mechanism of NO release from RSNOs at Cu. 2013 , 135, 16746-9	30
1358	Activation of nitriles by metal ligand cooperation. Reversible formation of ketimido- and enamido-rhenium PNP pincer complexes and relevance to catalytic design. 2013 , 135, 17004-18	89
1357	Metal-dependent activity of Fe and Ni acireductone dioxygenases: how two electrons reroute the catalytic pathway. 2013 , 425, 3007-18	30
1356	Interaction of Pyridine Derivatives with a Gold (111) Surface as a Model for Adsorption to Large Nanoparticles. 2013 , 117, 4470-4479	36
1355	Structural and electronic properties of perylene from first principles calculations. <i>Journal of Chemical Physics</i> , 2013 , 138, 094509	3.9 30
1354	Easy methods to study the smart energetic TNT/CL-20 co-crystal. 2013 , 19, 4909-17	51
1353	Preparation of non-aggregating aqueous fullerenes in highly saline solutions with a biocompatible non-ionic polymer. 2013 , 24, 395602	13
1352	Binding of O ₂ and NO to heme in heme-nitric oxide/oxygen-binding (H-NOX) proteins. A theoretical study. 2013 , 117, 10103-14	16
1351	Hexamers and witchamers: Which hex do you choose?. 2013 , 1021, 70-83	13
1350	5-Aminotetrazole induces spin crossover in iron(III) pentadentate Schiff base complexes: experimental and theoretical investigations. 2013 , 42, 16279-88	13
1349	Liquid Methanol from DFT and DFT/MM Molecular Dynamics Simulations. 2013 , 9, 106-18	44

1348	New Functionalized Metal-Organic Frameworks MIL-47-X (X = Cl, Br, CH ₃ , CF ₃ , OH, DCH ₃): Synthesis, Characterization, and CO ₂ Adsorption Properties. 2013 , 117, 22784-22796		72
1347	Antioxidant properties of phenolic Schiff bases: structure-activity relationship and mechanism of action. 2013 , 27, 951-64		63
1346	An improved AMBER force field for β , β -dialkylated peptides: intrinsic and solvent-induced conformational preferences of model systems. 2013 , 15, 17395-407		15
1345	Understanding the defect chemistry of tin monoxide. 2013 , 1, 8194		59
1344	Strategies to Simultaneously Enhance the Hydrostability and the Alcohol-Water Separation Behavior of Cu-BTC. 2013 , 117, 20706-20714		21
1343	On the role of halides and thiols in additive-assisted copper electroplating. 2013 , 89, 537-548		39
1342	A scaling PNO-MP2 method using a hybrid OSV-PNO approach with an iterative direct generation of OSVs. 2013 , 111, 2463-2476		55
1341	Spectroscopic signatures of the carbon buckyonions C ₆₀ @C ₁₈₀ and C ₆₀ @C ₂₄₀ : a dispersion-corrected DFT study. 2013 , 15, 18030-8		18
1340	Semilocal and hybrid density embedding calculations of ground-state charge-transfer complexes. <i>Journal of Chemical Physics</i> , 2013 , 138, 124112	3.9	13
1339	L-edge X-ray absorption spectroscopy and DFT calculations on Cu ₂ O ₂ species: direct electrophilic aromatic attack by side-on peroxo bridged dicopper(II) complexes. 2013 , 135, 17417-31		39
1338	Dichotomous hydrogen atom transfer vs proton-coupled electron transfer during activation of X-H bonds (X = C, N, O) by nonheme iron-oxo complexes of variable basicity. 2013 , 135, 17090-104		176
1337	X ₂ Y ₂ isomers: tuning structure and relative stability through electronegativity differences (X = H, Li, Na, F, Cl, Br, I; Y = O, S, Se, Te). 2013 , 52, 2458-65		11
1336	Uranium(III) complexes with bulky aryloxy ligands featuring metal-arene interactions and their reactivity toward nitrous oxide. 2013 , 52, 10552-8		46
1335	Accurate non-covalent interactions with basis-set corrections from interference-corrected perturbation theory: comparison with the S22B database. 2013 , 111, 2299-2305		14
1334	Ammonium adsorption on Brønsted acidic centers on low-index vanadium pentoxide surfaces. 2013 , 19, 4487-501		10
1333	The role of solvent exclusion in the interaction between D124 and the metal site in SOD1: implications for ALS. 2013 , 18, 931-8		6
1332	Insights into the hydrolytic chemistry of molybdocene dichloride based on a theoretical mechanistic study. 2013 , 132, 1		3
1331	Effect of pillar modules and their stoichiometry in 3D porous frameworks of Zn(II) with [Fe(CN) ₆] ³⁻ : high CO ₂ /N ₂ and CO ₂ /CH ₄ selectivity. 2013 , 52, 11385-97		22

1330	On the Short-Range Behavior of Correlated Pair Functions from the Adiabatic-Connection Fluctuation-Dissipation Theorem of Density-Functional Theory. 2013 , 9, 4382-95	14
1329	Trends in Adsorption Characteristics of Benzene on Transition Metal Surfaces: Role of Surface Chemistry and van der Waals Interactions. 2013 , 117, 20572-20583	129
1328	Sterically directed functionalization of the redox-active bis(imino)acenaphthene ligand class: an experimental and theoretical investigation. 2013 , 135, 13939-46	10
1327	Endohedral and exohedral complexes of substituted benzenes with carbon nanotubes and graphene. <i>Journal of Chemical Physics</i> , 2013 , 139, 094703	3.9 19
1326	A complete guide on the influence of metal clusters in the Diels-Alder regioselectivity of I(h)-C80 endohedral metallofullerenes. 2013 , 19, 14931-40	36
1325	How strong is hydrogen bonding in ionic liquids? Combined X-ray crystallographic, infrared/Raman spectroscopic, and density functional theory study. 2013 , 117, 9094-105	119
1324	Co-C bond energies in adenosylcobinamide and methylcobinamide in the gas phase and in silico. 2013 , 135, 13648-51	40
1323	Gas storage of simple molecules in boron oxide nanocapsules. 2013 , n/a-n/a	
1322	Benzyl Cation Stabilized by Metal Complexation. Relative Stability of Coordinated Methylen Arenium, β Benzylic, and β Benzylic Structures. 2013 , 32, 4813-4819	6
1321	Coordination of CO to low-valent phosphorus centres and other related $P\pi$ bonding situations. A theoretical case study. 2013 , 4, 4309	24
1320	A theoretical study on ethylenediamine catalyzed decarboxylation of oxaloacetic acid. 2013 , 1022, 29-34	4
1319	From bis(silylene) and bis(germylene) pincer-type nickel(II) complexes to isolable intermediates of the nickel-catalyzed Sonogashira cross-coupling reaction. 2013 , 135, 15617-26	189
1318	Enhancement in the Stability of 36-Atom Fullerene through Encapsulation of a Uranium Atom. 2013 , 117, 17859-17869	24
1317	Improved Density Dependent Correction for the Description of London Dispersion Forces. 2013 , 9, 4293-9	138
1316	Comparison of molecular mechanics, semi-empirical quantum mechanical, and density functional theory methods for scoring protein-ligand interactions. 2013 , 117, 8075-84	47
1315	Decafluorocyclohex-1-ene at 4.2 K - crystal structure and theoretical analysis of weak interactions. 2013 , 69, 395-404	4
1314	Bis(carbazolyl)ureas as selective receptors for the recognition of hydrogenpyrophosphate in aqueous media. 2013 , 78, 9725-37	28
1313	Manipulating Liquid-Crystal Properties Using a pH Activated Hydrazone Switch. 2013 , 125, 10934-10939	16

1312	Interatomic methods for the dispersion energy derived from the adiabatic connection fluctuation-dissipation theorem. <i>Journal of Chemical Physics</i> , 2013 , 138, 074106	3.9	109
1311	Photodynamics of Lys+Trp protein motifs: hydrogen bonds ensure photostability. 2013 , 163, 189-203; discussion 243-75		6
1310	Conformational preference of glycinamide in solution: an answer derived from combined experimental and computational studies. 2013 , 46, 52-8		1
1309	Charged stacks of dithiin, diselenin, thianthrene and selenanthrene radical cations: long range multicenter bonds. 2013 , 15, 18702-9		9
1308	Highly strained phenylene bicyclophanes. 2013 , 52, 12086-90		33
1307	First principles derived, transferable force fields for CO ₂ adsorption in Na-exchanged cationic zeolites. 2013 , 15, 12882-94		58
1306	Solid-State Structures of Trialkylbismuthines BiR ₃ (R = Me, i-Pr). 2013 , 32, 5445-5450		22
1305	Mechanism of the gold(III)-catalyzed isomerization of substituted allenes to conjugated dienes: a DFT study. 2013 , 78, 9715-24		21
1304	Unexpected strong stacking interactions between the homogeneous dimers of C ₆ F _x I(6-x) (x=0, 1, 2, 3, 4 and 5). 2013 , 1023, 88-94		12
1303	Spin Crossover during β -Hydride Elimination in High-Spin Iron(II) and Cobalt(II) Alkyl Complexes. 2013 , 32, 4741-4751		55
1302	Reaction Pathways for Addition of H ₂ to Amido-Ditetrylynes R ₂ NBEER ₂ (E = Si, Ge, Sn). A Theoretical Study. 2013 , 32, 6666-6673		34
1301	What controls regiochemistry in 1,3-dipolar cycloadditions of malchones with nitrostyrenes?. 2013 , 15, 5218-21		41
1300	Quantum chemical challenges for the binding of simple alkanes to supramolecular hosts. 2013 , 117, 13409-17		23
1299	Shape Prediction for Supramolecular Organic Nanostructures: [4 + 4] Macrocyclic Tetrapods. 2013 , 13, 4993-5000		32
1298	Adsorption of β -D-glucose and cellobiose on kaolinite surfaces: Density functional theory (DFT) approach. 2013 , 71, 73-81		58
1297	Electronic structures of homoleptic [tris(2,2'-bipyridine)M] _n complexes of the early transition metals (M = Sc, Y, Ti, Zr, Hf, V, Nb, Ta; n = 1+, 0, 1-, 2-, 3-): an experimental and density functional theoretical study. 2013 , 52, 2242-56		47
1296	Cobalt catalysis in the gas phase: experimental characterization of cobalt(I) complexes as intermediates in regioselective Diels-Alder reactions. 2013 , 78, 10485-93		55
1295	Thermal isomerization of the chromoprotein asFP595 and its kindling mutant A143G: QM/MM molecular dynamics simulations. 2013 , 117, 13507-14		7

1294	Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. 2013 , 15, 14581-94	79
1293	Transition metal complexes with 2,6-Di-tert-butyl-p-quinone 1?-phthalazinyldiazone. 2013 , 83, 1928-1936	5
1292	When a proton attacks cellobiose in the gas phase: ab initio molecular dynamics simulations. 2013 , 15, 15382-91	3
1291	Crown-linked dipyridylamino-triazine ligands and their spin-crossover iron(II) derivatives: magnetism, photomagnetism and cooperativity. 2013 , 42, 16494-509	25
1290	Chirality-dependent balance between hydrogen bonding and London dispersion in isolated (-)-1-indanol clusters. 2013 , 15, 10167-80	32
1289	Impact of long-range van der Waals forces on chiral recognition in a Cinchona alkaloid chiral selector system. 2013 , 15, 6113-21	6
1288	Benchmark study of the performance of density functional theory for bond activations with (ni,pd)-based transition-metal catalysts. 2013 , 2, 115-24	118
1287	Dispersion corrected hartree-fock and density functional theory for organic crystal structure prediction. 2014 , 345, 1-23	61
1286	Communication: Analytic gradients in the random-phase approximation. <i>Journal of Chemical Physics</i> , 2013 , 139, 081101	3.9 34
1285	Predicting anisotropic displacement parameters using molecular dynamics: density functional theory plus dispersion modelling of thermal motion in benzophenone. 2013 , 46, 656-662	13
1284	Interaction energies between metal ions (Zn ²⁺ and Cd ²⁺) and biologically relevant ligands. 2013 , 113, 2554-2562	13
1283	Autocatalytic cathodic dehalogenation triggered by dissociative electron transfer through a C-H...O hydrogen bond. 2013 , 15, 17522-36	7
1282	Oxygen activation by homoprotocatechuate 2,3-dioxygenase: a QM/MM study reveals the key intermediates in the activation cycle. 2013 , 4, 3624	56
1281	Reactions of phosphorus/boron frustrated Lewis pairs with SO ₂ . 2013 , 4, 213-219	132
1280	Synthetic and computational study of geminally bis(supermesityl) substituted phosphorus compounds. 2013 , 42, 1437-50	11
1279	Exploring suitable oligoamines for phantom ring-closing condensation polymerization with guanidine hydrochloride. 2013 , 4, 707-716	5
1278	Evaluation of the heats of formation of corannulene and C ₆₀ by means of high-level theoretical procedures. 2013 , 117, 1834-42	42
1277	Assessment of Kohn-Sham density functional theory and Møller-Plesset perturbation theory for ionic liquids. 2013 , 15, 13664-75	85

1276	Anharmonic vibrations of N-H in Cl ⁻ (N-methylacetamide) ₁ (H ₂ O) ₍₀₋₂₎ Ar ₂ cluster ions. Combined IRPD experiments and BOMD simulations. 2013 , 15, 16736-45	12
1275	Ab initio simulations of scanning-tunneling-microscope images with embedding techniques and application to C ₅₈ -dimers on Au(111). 2013 , 15, 6684-90	11
1274	Solution dynamics of agostic interactions in T-shaped Pt(II) complexes from ab initio molecular dynamics simulations. 2013 , 42, 12165-72	22
1273	Weakly bound PTCDI and PTCDA dimers studied by using MP2 and DFT methods with dispersion correction. 2013 , 15, 13978-90	5
1272	Consistent descriptions of metal–ligand bonds and spin-crossover in inorganic chemistry. 2013 , 257, 196-209	153
1271	Face-to-face stacks of trinuclear gold(I) trihalides with benzene, hexafluorobenzene, and borazine: impact of aromaticity on stacking interactions. 2013 , 52, 1047-60	9
1270	A systematic approach to identify cooperatively bound homotrimers. 2013 , 117, 174-82	15
1269	Vibrational Sum Frequency Generation Spectroscopy of the Water Liquid-Vapor Interface from Density Functional Theory-Based Molecular Dynamics Simulations. 2013 , 4, 83-7	128
1268	Cationic, neutral, and anionic allyl magnesium compounds: unprecedented ligand conformations and reactivity toward unsaturated hydrocarbons. 2013 , 135, 811-21	29
1267	XH/π(X = C, Si) Interactions in Graphene and Silicene: Weak in Strength, Strong in Tuning Band Structures. 2013 , 4, 269-75	79
1266	Principles and applications of halogen bonding in medicinal chemistry and chemical biology. 2013 , 56, 1363-88	792
1265	Analysis of the performance of DFT-D, M05-2X and M06-2X functionals for studying π interactions. 2013 , 557, 170-175	59
1264	Halogen bonding from a hard and soft acids and bases perspective: investigation by using density functional theory reactivity indices. 2013 , 19, 519-30	102
1263	Hydration structure of salt solutions from ab initio molecular dynamics. <i>Journal of Chemical Physics</i> , 2013 , 138, 014501	3.9 128
1262	The application of quantum mechanics in structure-based drug design. 2013 , 8, 263-76	53
1261	Topology switching in [32]heptaphyrins controlled by solvent, protonation, and meso substituents. 2013 , 19, 1617-28	45
1260	Electron at the Surface of Water: Dehydrated or Not?. 2013 , 4, 338-43	45
1259	Self-assembled tetragonal prismatic molecular cage highly selective for anionic guests. 2013 , 19, 1445-56	29

1258	A Critical Assessment of Two-Body and Three-Body Interactions in Water. 2013 , 9, 1103-14	111
1257	Accurate Noncovalent Interaction Energies Using Truncated Basis Sets Based on Frozen Natural Orbitals. 2013 , 9, 293-9	54
1256	New V(IV)-based metal-organic framework having framework flexibility and high CO ₂ adsorption capacity. 2013 , 52, 113-20	63
1255	Ab initio molecular dynamics. 2013 , 924, 29-42	3
1254	Intricacies of Describing Weak Interactions Involving Halogen Atoms within Density Functional Theory. 2013 , 9, 955-64	21
1253	Ab initio, density functional theory, and semi-empirical calculations. 2013 , 924, 3-27	3
1252	Cluster-Continuum Calculations of Hydration Free Energies of Anions and Group 12 Divalent Cations. 2013 , 9, 555-69	37
1251	Assessment of a Nonlocal Correction Scheme to Semilocal Density Functional Theory Methods. 2013 , 9, 273-83	24
1250	A combined high-field EPR and quantum chemical study on a weakly ferromagnetically coupled dinuclear Mn(III) complex. A complete analysis of the EPR spectrum beyond the strong coupling limit. 2013 , 15, 223-34	18
1249	Dispersion-corrected density functional theory for aromatic interactions in complex systems. 2013 , 46, 916-26	283
1248	Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. 2013 , 9, 263-72	321
1247	Inter- and Intramolecular Interactions in Triptycene-Derived Bisphosphite Hydroformylation Catalysts: Structures, Energies, and Caveats for DFT-Assisted Ligand Design. 2013 , 32, 1044-1052	23
1246	Mechanism of Alcohol/Water Separation in Metal-Organic Frameworks. 2013 , 117, 4124-4130	28
1245	Surface chemistry of late transition metal oxides. 2013 , 113, 4164-215	156
1244	From clusters to liquid: what are the preferred ways for benzene and pyrrole to interact?. 2013 , 132, 1	4
1243	Binding of Polyvinylpyrrolidone to Ag Surfaces: Insight into a Structure-Directing Agent from Dispersion-Corrected Density Functional Theory. 2013 , 117, 1163-1171	82
1242	Iodine (I ₂) as a Janus-faced ligand in organometallics. 2013 , 135, 3262-75	63
1241	Assessment of density functional methods for reaction energetics: iridium-catalyzed water oxidation as case study. 2013 , 34, 870-8	29

1240	Offenschalige Polyhydridokomplexe von 3d-Metallionen mit dem fac-[RuH ₃ (PR ₃) ₃]-Baustein. 2013 , 125, 1352-1357	9
1239	Open-shell first-row transition-metal polyhydride complexes based on the fac-[RuH ₃ (PR ₃) ₃]-building block. 2013 , 52, 1314-8	18
1238	Conformational analysis of β -lactones by DFT calculations: the parent compound and its monomethyl and selected dimethyl derivatives. 2013 , 19, 1288-302	6
1237	"Click" bis-triazoles as neutral C-H \cdots N \cdots H anion-acceptor organocatalysts. 2013 , 19, 1581-5	44
1236	Significant cation effects in carbon dioxide-ionic liquid systems. 2013 , 14, 315-20	71
1235	Ketonic decarboxylation reaction mechanism: a combined experimental and DFT study. 2013 , 6, 141-51	105
1234	Accurate dynamical structure factors from ab initio lattice dynamics: the case of crystalline silicon. 2013 , 34, 346-54	51
1233	Comparison of flux behavior and synthetic organic compound removal by forward osmosis and reverse osmosis membranes. 2013 , 443, 69-82	61
1232	Is There B-N Bond-Length Alternation in 1,2:3,4:5,6-Tris(biphenylene)borazines?. 2013 , 78, 988-994	16
1231	The Role of the Flexible L43-S54 Protein Loop in the CcrA Metallo- β -lactamase in Binding Structurally Dissimilar β -Lactam Antibiotics. 2013 , 9, 730-7	20
1230	Recent Theoretical Advances in Understanding the Mechanism of Aggregation-Induced Emission for Small Organic Molecules. 2013 , 399-418	1
1229	Theoretical and Experimental Investigation of Palladium(II)-Catalyzed Decarboxylative Addition of Arenecarboxylic Acid to Nitrile. 2013 , 32, 490-497	20
1228	The Lewis Acidity of the BO Triple Bond in Methyl(oxo)borane. 2013 , 639, 1199-1204	1
1227	New insights on photocatalytic H ₂ liberation from water using transition-metal oxides: lessons from cluster models of molybdenum and tungsten oxides. 2013 , 135, 17039-51	37
1226	Modeling materials and processes in dye-sensitized solar cells: understanding the mechanism, improving the efficiency. 2014 , 352, 151-236	18
1225	Spin-Crossing in an Organometallic Pt-Benzene Complex. 2013 , 9, 1461-8	18
1224	Assessment of density functional theory for thermochemical approaches based on bond separation reactions. 2013 , 117, 228-43	15
1223	Quantum mechanical force field for water with explicit electronic polarization. <i>Journal of Chemical Physics</i> , 2013 , 139, 054503	3.9 31

1222	Reaction Barriers and Cooperative Effects for the Adsorption of Pyridine on Si(100). 2013 , 117, 26644-26651	9
1221	The Semiempirical Quantum Mechanical Scoring Function for In Silico Drug Design. 2013 , 78, 921-931	70
1220	Asymptotic dispersion energies from distributed polarizabilities. 2013 , 572, 146-149	15
1219	New steroidal 7-azaindole platinum(II) antitumor complexes. 2013 , 128, 48-56	20
1218	Stacked polyphenolic dimers: A case study using dispersion-corrected methods. 2013 , 578, 120-125	11
1217	Contribution analysis of the van der Waals term on electronic structures of carbon related systems. 2013 , 267, 173-176	3
1216	Large face to face tetraphenylporphyrin/fullerene nanoaggregates. A DFT study. 2013 , 14, 2617-2627	17
1215	Trapping of He in intrinsic defects in zirconolite. 2013 , 437, 261-266	6
1214	Helix compactness and stability: Electron structure calculations of conformer dependent thermodynamic functions. 2013 , 563, 80-87	2
1213	The effect of density functional and dispersion interaction on structure and bonding analysis of uranium(VI) nitride complex [NU{N(CH ₂ CH ₂ NSiMe ₃) ₃ }] : A theoretical study. 2013 , 37, 4-6	3
1212	Synthesis, experimental and theoretical investigation of a new type nickel dithiolene complex. 2013 , 62, 208-217	9
1211	Benchmark calculations of density functionals for organothiol adsorption on gold surfaces. 2013 , 1009, 60-69	3
1210	Reactivity of conformationally constrained bispropargyl sulfones: complete preference for 6 π electrocyclicization process. 2013 , 69, 8724-8730	9
1209	Benchmark Study for the Cysteine-Histidine Proton Transfer Reaction in a Protein Environment: Gas Phase, COSMO, QM/MM Approaches. 2013 , 9, 1765-77	33
1208	Angular Distortions at Benzylic Carbons Due to Intramolecular Polarization-Induced Metal-Arene Interactions: A Case Study with Open-Shell Chromium(II) NHC Complexes. 2013 , 32, 1842-1850	13
1207	Density Functional Theory and Molecular Interactions: Dispersion Interactions. 2013 , 65-96	7
1206	Quantum Chemical Methods in the Design of Agrochemicals. 2013 , 43-71	1
1205	Asararenes--a family of large aromatic macrocycles. 2013 , 19, 3860-8	46

1204	Complete Reaction Pathway of Ruthenium-Catalyzed Olefin Metathesis of Ethyl Vinyl Ether: Kinetics and Mechanistic Insight from DFT. 2013 , 32, 2099-2111	55
1203	Noncovalent Interactions of DNA Bases with Naphthalene and Graphene. 2013 , 9, 2090-6	64
1202	Seamless and Accurate Modeling of Organic Molecular Materials. 2013 , 4, 1028-33	107
1201	Efficient and accurate theoretical methods to investigate anion-π interactions in protein model structures. 2013 , 117, 3315-22	23
1200	Hypothetical 3D-periodic covalent organic frameworks: exploring the possibilities by a first principles derived force field. 2013 , 15, 1551	52
1199	Determination of absolute configuration and conformation of a cyclic dipeptide by NMR and chiral spectroscopic methods. 2013 , 117, 1721-36	47
1198	Reliable approach for prediction of heats of formation of polycyclic saturated hydrocarbons using recently developed density functionals. 2013 , 1011, 30-36	17
1197	Assessing the Accuracy of Density Functional and Semiempirical Wave Function Methods for Water Nanoparticles: Comparing Binding and Relative Energies of (H ₂ O) ₁₆ and (H ₂ O) ₁₇ to CCSD(T) Results. 2013 , 9, 995-1006	43
1196	Building multi-component crystals from cations and co-crystals: the use of chaperones. 2013 , 15, 2241-2250	12
1195	Diels-Alder and retro-Diels-Alder cycloadditions of (1,2,3,4,5-pentamethyl)cyclopentadiene to La@C(2v)-C(82): regioselectivity and product stability. 2013 , 19, 4468-79	25
1194	Hydrogen-bonding effects on the reactivity of [X-Fe(III)-O-Fe(IV)?O] (X = OH, F) complexes toward C-H bond cleavage. 2013 , 52, 3976-84	28
1193	Optimization of Crystal Structures of Archetypical Pharmaceutical Compounds: A Plane-Wave DFT-D Study Using Quantum Espresso. 2013 , 13, 2181-2189	20
1192	Prediction of Water Adsorption in Copper-Based Metal-Organic Frameworks Using Force Fields Derived from Dispersion-Corrected DFT Calculations. 2013 , 117, 7519-7525	46
1191	The "catalytic nitrosyl effect": NO bending boosting the efficiency of rhenium based alkene hydrogenations. 2013 , 135, 4088-102	38
1190	Mechanistic study of the Diels-Alder reaction of paramagnetic endohedral metallofullerene: reaction of La@C82 with 1,2,3,4,5-pentamethylcyclopentadiene. 2013 , 135, 5582-7	39
1189	Accurate Reaction Energies in Proteins Obtained by Combining QM/MM and Large QM Calculations. 2013 , 9, 640-9	65
1188	Molecular Scale Modeling of Membrane Water Treatment Processes. 2013 , 249-299	2
1187	Intermolecular Interactions in Dye-Sensitized Solar Cells: A Computational Modeling Perspective. 2013 , 4, 956-74	71

1186	Investigation into the Mechanism of Solution-Mediated Transformation from FI to FIII Carbamazepine: The Role of Dissolution and the Interaction between Polymorph Surfaces. 2013 , 13, 1861-1871	37
1185	Understanding the Nature of the CH \cdots HC Interactions in Alkanes. 2013 , 9, 1977-91	90
1184	Reactivity models of hydrogen activation by frustrated Lewis pairs: synergistic electron transfers or polarization by electric field?. 2013 , 135, 4425-37	162
1183	Catalysis by doped oxides. 2013 , 113, 4391-427	565
1182	Are β -H eliminations or alkene insertions feasible elementary steps in catalytic cycles involving gold(I) alkyl species or gold(I) hydrides?. 2013 , 19, 3954-61	63
1181	Removal of bisphenol A and 17 β -ethinyl estradiol by combined coagulation and adsorption using carbon nanomaterials and powdered activated carbon. 2013 , 107, 37-47	69
1180	Mechanistic Investigation of Palladium-Catalyzed Allylic C-H Activation. 2013 , 3, 294-302	74
1179	Diffusion energy profiles in silica mesoporous molecular sieves modelled with the fragment molecular orbital method. 2013 , 111, 1622-1629	21
1178	Torsional barriers of substituted biphenyls calculated using density functional theory: a benchmarking study. 2013 , 11, 2859-71	47
1177	Diastereoselective synthesis of C60/steroid conjugates. 2013 , 78, 2819-26	18
1176	Computing vibrational spectra from ab initio molecular dynamics. 2013 , 15, 6608-22	298
1175	CO Adsorption on a Mixed-Valence Ruthenium Metal-Organic Framework Studied by UHV-FTIR Spectroscopy and DFT Calculations. 2013 , 117, 5658-5666	41
1174	Joyce and Ulysses: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data. 2013 , 15, 3736-51	69
1173	Silica surface features and their role in the adsorption of biomolecules: computational modeling and experiments. 2013 , 113, 4216-313	414
1172	Control of regioselectivity and stereoselectivity in (4 + 3) cycloadditions of chiral oxyallyls with unsymmetrically disubstituted furans. 2013 , 78, 1753-9	20
1171	An efficient route for the synthesis of phosphorus-selenium macro-heterocycles. 2013 , 49, 2619-2621	20
1170	Are DFT Methods Accurate in Mononuclear Ruthenium-Catalyzed Water Oxidation? An ab Initio Assessment. 2013 , 9, 1872-9	42
1169	Can cyclic HIV protease inhibitors bind in a non-preferred form? An ab initio, DFT and MM-PB(GB)SA study. 2013 , 19, 1125-42	

1168	Mechanistic insights on the ortho-hydroxylation of aromatic compounds by non-heme iron complex: a computational case study on the comparative oxidative ability of ferric-hydroperoxo and high-valent Fe(IV)=O and Fe(V)=O intermediates. 2013 , 135, 4235-49		101
1167	Chemoselectivity in the reductive elimination from high oxidation state palladium complexes—scrambling mechanism uncovered. 2013 , 135, 1978-85		53
1166	DFT studies of trans and cis influences in the homolysis of the Co-C bond in models of the alkylcobalamins. 2013 , 117, 3057-68		17
1165	Computational Evaluation of the Sulfonyl Radical as a Universal Leaving Group for RAFT Polymerisation. 2013 , 66, 308		7
1164	Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations. <i>Journal of Chemical Physics</i> , 2013 , 138, 104109	3.9	65
1163	Assessment of density functional methods for thermochemistry of chromium oxo compounds and their application in a study of chromia-silica system. 2013 , 561-562, 87-91		13
1162	Phenylvinylcobalamin: an alkenylcobalamin featuring a ligand with a large trans influence. 2013 , 42, 7555-61		4
1161	Electronic, geometrical, and thermochemical studies on group-14 element-diruthenaborane cluster compounds: a theoretical investigation. 2013 , 132, 1		8
1160	Strukturbestimmung des Undecabromids [Br ₁₁]. 2013 , 125, 5037-5040		26
1159	Understanding the Metal-Molecule Interface from First Principles. 2013 , 51-89		9
1158	Performance of Non-Local and Atom-Pairwise Dispersion Corrections to DFT for Structural Parameters of Molecules with Noncovalent Interactions. 2013 , 9, 308-15		85
1157	Molecular dynamics simulation of the solid-state topochemical polymerization of S ₂ N ₂ . 2013 , 52, 4648-57		15
1156	A Benchmark Ab Initio and DFT Study of the Structure and Binding of Methane in the Alkane Complex CpRe(CO) ₂ (CH ₄). 2013 , 9, 2199-208		35
1155	New parameterization scheme of DFT-D for graphitic materials. 2013 , 117, 2844-53		12
1154	Theoretical description of halogen bonding - an insight based on the natural orbitals for chemical valence combined with the extended-transition-state method (ETS-NOCV). 2013 , 19, 4681-8		34
1153	Directional Noncovalent Interactions: Repulsion and Dispersion. 2013 , 9, 2264-75		64
1152	Electron-deficient η^1 -Indenyl, η^3 -allylpalladium(II) complexes stabilized by fluxional non-covalent interactions. 2013 , 135, 1715-8		23
1151	Gas doping on the topological insulator Bi ₂ Se ₃ surface. 2013 , 110, 016403		26

1150	Cesium stability in a typical mica structure in dry and wet environments from first-principles. 2013 , 109, 62-73	11
1149	The electronic structure of TEMPO, its cation and anion. 2013 , 111, 2033-2040	12
1148	Molecular simulations to understand and to design porous organic molecules. 2013 , 17, 19-30	37
1147	Quantitative insights into energy contributions of intermolecular interactions in fluorine and trifluoromethyl substituted isomeric N-phenylacetamides and N-methylbenzamides. 2013 , 15, 3711	36
1146	One-pot, two-step, microwave-assisted palladium-catalyzed conversion of aryl alcohols to aryl fluorides via aryl nonaflates. 2013 , 78, 4184-9	30
1145	Cooperative N-Heterocyclic Carbene (NHC) and Ruthenium Redox Catalysis: Oxidative Esterification of Aldehydes with Air as the Terminal Oxidant. 2013 , 355, 1098-1106	102
1144	Accurate quantum chemical energies for tetrapeptide conformations: why MP2 data with an insufficient basis set should be handled with caution. 2013 , 15, 7028-31	57
1143	The role of the Lewis acid/Base properties in the supramolecular association of 1,2,5-chalcogenadiazoles. 2013 , 91, 338-347	31
1142	Carbene formation in ionic liquids: spontaneous, induced, or prohibited?. 2013 , 117, 5898-907	97
1141	Hydrogen activation by frustrated lewis pairs: insights from computational studies. 2013 , 332, 157-211	43
1140	Hierarchy of relative bond dissociation enthalpies and their use to efficiently compute accurate absolute bond dissociation enthalpies for C-H, C-C, and C-F bonds. 2013 , 117, 3666-75	26
1139	Subtle "supramolecular buttressing effects" in Cucurbit[7]uril/guest assemblies. 2013 , 11, 3116-27	9
1138	Quantum chemistry of FLPs and their activation of small molecules: methodological aspects. 2013 , 332, 213-30	25
1137	Regio- and stereocontrolled synthesis of oligostilbenoids: theoretical highlights at the supramolecular level. 2013 , 76, 538-46	13
1136	Structural evidence for undecabromide [Br ₁₁] ⁻ . 2013 , 52, 4937-40	40
1135	A dispersion-corrected density-functional theory study of small molecules adsorbed in alkali-exchanged chabazites. 2013 , 228, 124-133	11
1134	On the magnetic and spectroscopic properties of high-valent Mn ₃ CaO ₄ cubanes as structural units of natural and artificial water-oxidizing catalysts. 2013 , 135, 5726-39	81
1133	Stacking stability, emergence of magnetization and electromechanical nanosensing in bilayer graphene nanoribbons. 2013 , 25, 115303	15

1132	Proton transfer in surface-stabilized chiral motifs of croconic acid. 2013 , 87,	21
1131	What can we learn about dispersion from the conformer surface of n-pentane?. 2013 , 117, 3118-32	51
1130	Why do cycloaddition reactions involving C60 prefer [6,6] over [5,6] bonds?. 2013 , 19, 7416-22	88
1129	Assessment of density functionals for van der Waals complexes of sodium and benzene. 2013 , 111, 1211-1218	5
1128	Gas storage of simple molecules in boron oxide nanocapsules. 2013 , n/a-n/a	1
1127	Origins of stereoselectivities in chiral phosphoric acid catalyzed allyborations and propargylations of aldehydes. 2013 , 78, 1208-15	95
1126	Mechanism and origins of ligand-controlled selectivities in [Ni(NHC)]-catalyzed intramolecular (5 + 2) cycloadditions and homo-ene reactions: a theoretical study. 2013 , 135, 1456-62	63
1125	Noncovalent interactions of metal cations and arenes probed with thallium(I) complexes. 2013 , 52, 5749-56	14
1124	Supramolecular architecture of molecular crystals possessing shearing mechanical properties: columns versus layers. 2013 , 15, 160-167	28
1123	Radical frustrated Lewis pairs. 2013 , 334, 219-38	14
1122	Bond energy decomposition analysis for subsystem density functional theory. <i>Journal of Chemical Physics</i> , 2013 , 138, 094113	3.9 13
1121	N-Acyl- and N-Sulfonylformamidines from Cyanamides and Carbodiimides by Hydroalumination and Subsequent Treatment with Electrophiles. 2013 , 2013, 3356-3368	20
1120	Switching radical stability by pH-induced orbital conversion. 2013 , 5, 474-81	116
1119	Tkatchenko-Scheffler van der Waals correction method with and without self-consistent screening applied to solids. 2013 , 87,	245
1118	Nonheme Iron Oxidant Formed in the Presence of H2O2 and Acetic Acid Is the Cyclic Ferric Peracetate Complex, Not a Perferryloxo Complex. 2013 , 3, 1334-1341	85
1117	Dynamics of Ion Binding to Graphene Nanostructures. 2013 , 117, 10750-10754	11
1116	A density-functional theory-based neural network potential for water clusters including van der Waals corrections. 2013 , 117, 7356-66	128
1115	Synthesis of Cucurbit[6]uril Derivatives and Insights into Their Solubility in Water. 2013 , 2013, 3857-3865	24

1114	Cyanide detection using a triazolopyridinium salt. 2013 , 15, 2386-9	74
1113	Liquid Structure and Cluster Formation in Ionic Liquid/Water Mixtures [An Extensive ab initio Molecular Dynamics Study on 1-Ethyl-3-Methylimidazolium Acetate/Water Mixtures [Part. 2013 , 227, 177-204	36
1112	Effect of van der Waals Interactions on the Adsorption of Olympicene Radical on Cu(111): Characteristics of Weak Physisorption versus Strong Chemisorption. 2013 , 117, 2893-2902	44
1111	Stefan Grimme. 2013 , 52, 9076-9077	
1110	Coordination of 12-Electron Organometallic Fragments to the Arene Ring of Nonsymmetric Group 10 POCOP Pincer Complexes. 2013 , 32, 2661-2673	37
1109	Computational methods for contemporary carbene chemistry. 2013 , 3, 242-272	20
1108	On the role of anionic ligands in the site-selectivity of oxidative C-H functionalization reactions of arenes. 2013 , 4, 2767	81
1107	Natures of benzene-water and pyrrole-water interactions in the forms of π and π types: theoretical studies from clusters to liquid mixture. 2013 , 19, 1273-83	16
1106	Quantitative crystal structure analysis of 1,3,4-thiadiazole derivatives. 2013 , 15, 4549	40
1105	On the directionality of halogen bonding. 2013 , 15, 10350-7	117
1104	A relativistic DFT methodology for calculating the structures and NMR chemical shifts of octahedral platinum and iridium complexes. 2013 , 15, 7740-54	69
1103	Chalcogen-Nitrogen Secondary Bonding Interactions in the Gas Phase [Spectrometric Detection of Ionized Benzo-2,1,3-telluradiazole Dimers. 2013 , 2013, 2751-2756	19
1102	Immobilizing individual atoms beneath a corrugated single layer of boron nitride. 2013 , 13, 2098-103	52
1101	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugar-phosphate backbone and their comparison with modern density functional theory. 2013 , 15, 7295-310	25
1100	Facile carbon monoxide reduction at intramolecular frustrated phosphane/borane Lewis pair templates. 2013 , 52, 2243-6	132
1099	Reactivity and Regioselectivity of Methylacetylene Cyclotrimerization over the Phillips Cr/Silica Catalyst: A DFT Study. 2013 , 3, 1172-1183	20
1098	Performance of dispersion-corrected double hybrid density functional theory: a computational study of OCS-hydrocarbon van der Waals complexes. <i>Journal of Chemical Physics</i> , 2013 , 138, 164319	3.9 20
1097	Accounting for van der Waals interactions between adsorbates and surfaces in density functional theory based calculations: selected examples. 2013 , 3, 13085	120

1096	Aminolysis of phenyl N-phenylcarbamate via an isocyanate intermediate: theory and experiment. 2013 , 78, 6440-9		20
1095	The melatonin conformer space: benchmark and assessment of wave function and DFT methods for a paradigmatic biological and pharmacological molecule. 2013 , 117, 2269-77		77
1094	Interactions of platinum clusters with a graphite substrate. 2013 , 15, 11950-9		56
1093	Combinations of ethers and B(C ₆ F ₅) ₃ function as hydrogenation catalysts. 2013 , 52, 7492-5		160
1092	Methanol clusters (CH ₃ OH) _n : putative global minimum-energy structures from model potentials and dispersion-corrected density functional theory. <i>Journal of Chemical Physics</i> , 2013 , 138, 224303	3-9	38
1091	Efficient Methods for the Quantum Chemical Treatment of Protein Structures: The Effects of London-Dispersion and Basis-Set Incompleteness on Peptide and Water-Cluster Geometries. 2013 , 9, 3240-51		61
1090	Redox control of molecular motions in bipyridinium appended calixarenes. 2013 , 11, 4383-9		22
1089	Ab initio dynamics trajectory study of the heterolytic cleavage of H ₂ by a Lewis acid [B(C ₆ F ₅) ₃] and a Lewis base [P(tBu) ₃]. <i>Journal of Chemical Physics</i> , 2013 , 138, 154305	3-9	30
1088	Analytic Derivatives of Quartic-Scaling Doubly Hybrid XYGJ-OS Functional: Theory, Implementation, and Benchmark Comparison with M06-2X and MP2 Geometries for Nonbonded Complexes. 2013 , 9, 1971-1976		12
1087	Computational investigations on base-catalyzed diaryl ether formation. 2013 , 78, 5436-43		15
1086	Stoichiometric Reactions of Enamines Derived from Diphenylprolinol Silyl Ethers with Nitro Olefins and Lessons for the Corresponding Organocatalytic Conversions: A Survey. 2013 , 96, 799-852		63
1085	Structural and energetic factors controlling the enantioselectivity of dinucleotide formation under prebiotic conditions. 2013 , 15, 6235-42		1
1084	How are hydrogen bonds modified by metal binding?. 2013 , 18, 499-522		7
1083	Structural and electronic properties of a large-scale Moiré pattern of hexagonal boron nitride on Cu(111) studied with density functional theory. 2013 , 5, 5589-95		30
1082	Effect of distal interactions on O ₂ binding to heme. 2013 , 117, 3755-70		37
1081	Nature of M-C Bonds in the Metallogermylene Complexes of Chromium, Molybdenum, and Tungsten [(η -C ₅ H ₅)(CO) ₃ M{GeN(SiMe ₃)R}] and [(η -C ₅ H ₅)(CO) ₃ M{GeN(Ph)R}] (R = Ph, Mesityl (Mes)): A Theoretical Study. 2013 , 32, 3395-3403		14
1080	Free energy and electronic properties of water adsorption on the SnO ₂ (110) surface. 2013 , 29, 5487-99		38
1079	Global optimization of clusters using electronic structure methods. 2013 , 113, 2091-2109		155

1078	Complexes of 4-substituted phenolates with HF and HCN: energy decomposition and electronic structure analyses of hydrogen bonding. 2013 , 34, 696-705		8
1077	Adenosine triphosphate hydrolysis mechanism in kinesin studied by combined quantum-mechanical/molecular-mechanical metadynamics simulations. 2013 , 135, 8908-19		48
1076	Electronic structures of octahedral Ni(II) complexes with "click" derived triazole ligands: a combined structural, magnetometric, spectroscopic, and theoretical study. 2013 , 52, 6880-92		68
1075	The organozinc rich compounds [Cp*M(ZnR) ₅] (M = Fe, Ru; R = Cp*, Me, Cl, Br). 2013 , 52, 7152-60		8
1074	Monomeric Ferrocene Bis-Imidazoline Bis-Palladacycles: Variation of Pd-Pd Distances by an Interplay of Metallophilic, Dispersive, and Coulombic Interactions. 2013 , 32, 5810-5817		36
1073	Adsorption on Fe-MOF-74 for C ₁₀ H ₈ Hydrocarbon Separation. 2013 , 117, 12648-12660		94
1072	Multi-component crystals of 4-phenylpyridine: challenging the boundaries between co-crystal and organic salt formation with insight into solid-state proton transfer. 2013 , 15, 5250		22
1071	Benchmarking of London Dispersion-Accounting Density Functional Theory Methods on Very Large Molecular Complexes. 2013 , 9, 1580-91		315
1070	Application of the generalized connectivity-based hierarchy to biomonomers: enthalpies of formation of cysteine and methionine. 2013 , 117, 4973-80		20
1069	Nonlocal van der Waals functionals: the case of rare-gas dimers and solids. <i>Journal of Chemical Physics</i> , 2013 , 138, 204103	3.9	37
1068	Non-covalent interactions and thermochemistry using XDM-corrected hybrid and range-separated hybrid density functionals. <i>Journal of Chemical Physics</i> , 2013 , 138, 204109	3.9	109
1067	Synthesis of dibenzo[b,f]silepins with a benzoquinolyl ligand. 2013 , 15, 2366-9		16
1066	The intrinsic conformational features of amino acids from a protein coil library and their applications in force field development. 2013 , 15, 3413-28		49
1065	Density Functional Simulations as a Tool To Probe Molecular Interactions in Wet Supercritical CO ₂ . 2013 , 31-49		1
1064	Analysis of an alternative to the H-atom abstraction mechanism in methane C-H bond activation by nonheme iron(IV)-oxo oxidants. 2013 , 42, 10260-70		13
1063	Elucidating the breathing of the metal-organic framework MIL-53(Sc) with ab initio molecular dynamics simulations and in situ X-ray powder diffraction experiments. 2013 , 135, 15763-73		154
1062	Unraveling the reaction mechanisms governing methanol-to-olefins catalysis by theory and experiment. 2013 , 14, 1526-45		207
1061	Relative stability of different DNA guanine quadruplex stem topologies derived using large-scale quantum-chemical computations. 2013 , 135, 9785-96		94

1060	Structural and Mechanistic Basis of the Fast Metathesis Initiation by a Six-Coordinated Ruthenium Catalyst. 2013 , 32, 3625-3630	35
1059	Is There Still Room for Parameter Free Double Hybrids? Performances of PBE0-DH and B2PLYP over Extended Benchmark Sets. 2013 , 9, 3444-52	33
1058	Diaminoethane adsorption and water substitution on hydrated TiO ₂ : a thermochemical study based on first-principles calculations. 2013 , 15, 10824-34	11
1057	Highly accurate incremental CCSD(T) calculations on aqua- and amine-complexes. 2013 , 111, 1161-1172	8
1056	Use of metalloligands [CuL] (H ₂ L = salen type di-Schiff bases) in the formation of heterobimetallic copper(II)-uranyl complexes: photophysical investigations, structural variations, and theoretical calculations. 2013 , 52, 7508-23	71
1055	Creation of ternary multicomponent crystals by exploitation of charge-transfer interactions. 2013 , 19, 10663-71	30
1054	Quantum mechanical treatment of binding energy between DNA nucleobases and carbon nanotube: A DFT analysis. 2013 , 54, 65-71	18
1053	Interaction of Small Gases with the Unsaturated Metal Centers of the HKUST-1 Metal Organic Framework. 2013 , 117, 14570-14578	119
1052	Chirality affects aggregation kinetics of single-walled carbon nanotubes. 2013 , 47, 1844-52	47
1051	Sampling of Transition States for Predicting Diastereoselectivity Using Automated Search Method-Aqueous Lanthanide-Catalyzed Mukaiyama Aldol Reaction. 2013 , 9, 2882-6	43
1050	How to understand quantum chemical computations on DNA and RNA systems? A practical guide for non-specialists. 2013 , 64, 3-11	37
1049	Water nanodroplets: predictions of five model potentials. <i>Journal of Chemical Physics</i> , 2013 , 138, 194303.9	38
1048	Influence of Crystal Packing on an Organometallic Ruthenium(IV) Complex Structure: The Right Distance for the Right Reason. 2013 , 32, 3784-3787	27
1047	Development of computational methodologies for metal-organic frameworks and their application in gas separations. 2013 , 113, 8261-323	394
1046	Benzene adsorption on binary Pt ₃ M alloys and surface alloys: a DFT study. 2013 , 15, 12197-214	25
1045	Computational organic chemistry. 2013 , 109, 235	12
1044	Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences. 2013 , 113, 2110-2142	1049
1043	Enhanced vapor-phase processing in fluorinated Fe ₄ single-molecule magnets. 2013 , 52, 5897-905	24

1042	On the oxidation state of iron in iron-mediated C-C couplings. 2013 , 748, 51-55	46
1041	Differences in the sublimation energy of benzene and hexahalobenzenes are caused by dispersion energy. 2013 , 117, 4331-7	17
1040	Oxygen defects and surface chemistry of ceria: quantum chemical studies compared to experiment. 2013 , 113, 3949-85	675
1039	Aromatic Claisen Rearrangements of O-prenylated tyrosine and model prenyl aryl ethers: Computational study of the role of water on acceleration of Claisen rearrangements. 2013 , 2013, 2823	16
1038	Intermolecular interactions of formic acid with benzene: Energy decomposition analyses with ab initio MP2 and double-hybrid density functional computations. 2013 , 113, n/a-n/a	11
1037	Electronic effects of triarylphosphines in metal-free hydrogen activation: a kinetic and computational study. 2013 , 4, 2788	85
1036	Nature of closed- and open-shell interactions between noble metals and rare gas atoms. 2013 , 113, 1981-1991	16
1035	Selective CO ₂ Adsorption on Metal-Organic Frameworks Based on Trinuclear Cu ₃ -Pyrazolato Complexes: An Experimental and Computational Study. 2013 , 13, 2628-2635	17
1034	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. 2013 , 9, 2256-63	53
1033	Corrected small basis set Hartree-Fock method for large systems. 2013 , 34, 1672-85	276
1032	A novel sorbent for chromatographic separations: a silica matrix modified with non-covalently bonded tetrakis(β -cyclodextrin)-porphyrin conjugates. 2013 , 36, 2072-80	4
1031	Towards Reagents for Bimetallic Activation Reactions: Polyhydride Complexes with Ru ₂ H ₃ , Ru ₂ ZnH ₆ , and Cu ₂ Ru ₂ H ₆ Cores. 2013 , 2013, 3039-3048	11
1030	Stereochemical outcome of copper-catalyzed C-H insertion reactions. An experimental and theoretical study. 2013 , 78, 5851-7	15
1029	How is a metabolic intermediate formed in the mechanism-based inactivation of cytochrome P450 by using 1,1-dimethylhydrazine: hydrogen abstraction or nitrogen oxidation?. 2013 , 19, 7361-9	30
1028	A Drude polarizable model for liquid hydrogen sulfide. 2013 , 117, 5222-9	18
1027	Accurate metal-ligand bond energies in the D _{2h} -C ₂ H ₄ and D _{3h} -C ₆₀ complexes of Pt(PH ₃) ₂ , with application to their Bis(triphenylphosphine) analogues. 2013 , 111, 1599-1611	7
1026	Complete low-barrier side-chain route for olefin formation during methanol conversion in H-SAPO-34. 2013 , 305, 76-80	87
1025	Towards first principles calculation of electron impact mass spectra of molecules. 2013 , 52, 6306-12	115

1024	π-Stacking effects on the EPR parameters of a prototypical DNA spin label. 2013 , 15, 10466-71	2
1023	A DFT/TDDFT study on the optoelectronic properties of the amine-capped magic (CdSe) ₁₃ nanocluster. 2013 , 15, 10996-1005	53
1022	H Atom Adsorption on a Silicate Surface: The (010) Surface of Forsterite. 2013 , 117, 12612-12621	24
1021	DFT studies of structure and vibrational spectra of 4-benzylidene-1-phenyl-2-selenomorpholino-1H-imidazol-5(4H)-one and its derivatives. 2013 , 110, 333-42	6
1020	MOF-FF: A flexible first-principles derived force field for metal-organic frameworks. 2013 , 250, 1128-1141	129
1019	C ₂₀ H ₄ (C ₄ F ₈) ₃ : a fluorine-containing annulated corannulene that is a better electron acceptor than C ₆₀ . 2013 , 52, 7505-8	49
1018	Surface control of alkyl chain conformations and 2D chiral amplification. 2013 , 135, 8814-7	33
1017	CH Stretching Region: Computational Modeling of Vibrational Optical Activity. 2013 , 9, 3096-108	21
1016	Methane CH Activation by Palladium Complexes with Chelating Bis(NHC) Ligands: A DFT Study. 2013 , 32, 3469-3480	55
1015	Factors that distort the heme structure in Heme-Nitric Oxide/Oxygen-Binding (H-NOX) protein domains. A theoretical study. 2013 , 118, 28-38	3
1014	Comparative study of friction properties for hydrogen- and fluorine-modified diamond surfaces: A first-principles investigation. 2013 , 608, 74-79	24
1013	The Mechanism for the Thermally Driven Self-Assembly of Pyrazine into Ordered Lines on Si(100). 2013 , 117, 15749-15753	8
1012	Realistic energy surfaces for real-world systems: an IMOMO CCSD(T):DFT scheme for rhodium-catalyzed hydroformylation with the 6-DPPon ligand. 2013 , 19, 16272-81	24
1011	Coordination and bond activation in complexes of regioisomeric phenylpyridines with the nickel(II) chloride cation in the gas phase. 2013 , 117, 1171-80	14
1010	Water-ionomer interfacial interactions investigated by infrared spectroscopy and computational methods. 2013 , 29, 13890-7	13
1009	Single-Molecule Piezoelectric Deformation: Rational Design from First-Principles Calculations. 2013 , 117, 16783-16790	16
1008	Theoretical ⁵⁷ Fe Mössbauer spectroscopy for structure elucidation of [Fe] hydrogenase active site intermediates. 2013 , 52, 14205-15	21
1007	Decarboxylative palladium(II)-catalyzed synthesis of aryl amidines from aryl carboxylic acids: development and mechanistic investigation. 2013 , 19, 13803-10	24

1006	Simulation of Adsorption Processes at Metallic Interfaces: An Image Charge Augmented QM/MM Approach. 2013 , 9, 5086-97		56
1005	Polycationic ligands in gold catalysis: synthesis and applications of extremely acidic catalysts. 2013 , 135, 18815-23		107
1004	Properties of Weakly Bound Molecular Oxygen on the Rutile TiO ₂ (110) Surface from Density Functional Theory. 2013 , 117, 17151-17158		2
1003	Kinetic modeling of hydrogen conversion at [Fe] hydrogenase active-site models. 2013 , 117, 4806-17		22
1002	A tripodal molecule on a gold surface: orientation-dependent coupling and electronic properties of the molecular legs. 2013 , 7, 6170-80		11
1001	A fragment method for systematic improvement of anharmonic adsorbate vibrational frequencies: acetylene on Cu(001). <i>Journal of Chemical Physics</i> , 2013 , 139, 214704	3-9	4
1000	Dissecting anion-cation interaction energies in protic ionic liquids. 2013 , 52, 2368-72		90
999	Binding interactions in dimers of phenalenyl and closed-shell analogues. 2013 , 117, 3642-9		33
998	Clarification on the decarboxylation mechanism in KasA based on the protonation state of key residues in the acyl-enzyme state. 2013 , 117, 8095-104		6
997	Characterization of the Methane-Graphene Hydrophobic Interaction in Aqueous Solution from Ab Initio Simulations. 2013 , 9, 5070-5		13
996	Probing the C^{II} triplet state coupling to nuclear spins inside and out. 2013 , 371, 20120475		12
995	DFT Study on the Effect of Water on the Carbonation of Portlandite. 2013 , 52, 2168-2173		11
994	Modification and unexpected reactivity of 2-borylbenzaldimines: acylated and silylated derivatives as well as dimeric compounds. 2013 , 78, 11747-55		5
993	Dispersion corrected double high-hybrid and gradient-corrected density functional theory study of light cation-dihydrogen (M^+H_2 , where M = Li, Na, B and Al) van der Waals complexes. 2013 , 24, 549-558		13
992	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. <i>Journal of Chemical Physics</i> , 2013 , 138, 204304	3-9	17
991	Effects of electronic and nuclear interactions on the excited-state properties and structural dynamics of copper(I) diimine complexes. 2013 , 117, 1921-31		54
990	The role of different structural motifs in the ultrafast dynamics of second generation protein stains. 2013 , 117, 14951-9		13
989	Ultrafast conformational dynamics of electron transfer in ExBox4+?perylene. 2013 , 117, 12438-48		109

988	Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer. 2013 , 9, 3848-54	2
987	Enabling forbidden processes: quantum and solvation enhancement of nitrate anion UV absorption. 2013 , 117, 12868-77	27
986	Modeling Water Adsorption on Rutile (110) Using van der Waals Density Functional and DFT+U Methods. 2013 , 117, 23638-23644	31
985	Effects of Oxide Roughness at Metal Oxide Interface: MgO on Ag(001). 2013 , 117, 5075-5083	20
984	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. 2013 , 4, 1669-75	57
983	Energetics of nonbonded ortho interactions in alkylbenzenes. 2013 , 117, 2873-8	5
982	Energetics of atmospherically implicated clusters made of sulfuric acid, ammonia, and dimethyl amine. 2013 , 117, 3819-25	91
981	Incremental CCSD(T)(F12*)/MP2: A Black Box Method To Obtain Highly Accurate Reaction Energies. 2013 , 9, 5381-94	63
980	Theoretical investigation of phosphinidene oxide polypyridine ruthenium(II) complexes: toward the design of a new class of photochromic compounds. 2013 , 117, 12821-30	14
979	A New Tabu-Search-Based Algorithm for Solvation of Proteins. 2013 , 9, 814-21	11
978	O ₂ binding to heme is strongly facilitated by near-degeneracy of electronic states. 2013 , 14, 3551-8	29
977	Hierarchical simulations of hybrid polymer/solid materials. 2013 , 9, 6696	56
976	Charge transfer through DNA/DNA duplexes and DNA/RNA hybrids: complex theoretical and experimental studies. 2013 , 180-181, 127-34	9
975	Quantitative analysis of intermolecular forces for hydrogen bond driven self-assembly of resorcinol and bis(pyridine) substituted ethylene cocrystals, before and after [2 + 2] dimerization. 2013 , 24, 1597-1605	4
974	The Performance of Density Functionals for Sulfate-Water Clusters. 2013 , 9, 1368-80	61
973	4,4'-Dithiodipyridine on Au(111): A Combined STM, STS, and DFT Study. 2013 , 117, 20060-20067	9
972	Elaboration of Hydrogen-Bonded 2D Supramolecular Assemblies on Au(111) From Solutions: Toward Naphthalene Tetracarboxylic Diimide/Melamine Nanoporous Networks. 2013 , 117, 8737-8745	19
971	Conformational heterogeneity of methyl 4-hydroxycinnamate: a gas-phase UV-IR spectroscopic study. 2013 , 117, 4798-805	15

- 970 An Enamine/HB(C₆F₅)₂ Adduct as a Dormant State in Frustrated Lewis Pair Chemistry. **2013**, 32, 6745-6752 18
- 969 Tetraedrisch, wenn flüssig. **2013**, 61, 1203-1206 1
- 968 The sulfur shift: an activation mechanism for periplasmic nitrate reductase and formate dehydrogenase. **2013**, 52, 10766-72 42
- 967 Nonplanar tertiary amides in rigid chiral tricyclic dilactams. Peptide group distortions and vibrational optical activity. **2013**, 117, 9626-42 6
- 966 Synthesis and structure of base-stabilized germanium(II) diazide IPrGe(N₃)₂. **2013**, 52, 7236-41 11
- 965 Scission of Olefins on Acidic Zeolites: A Periodic PBE-D Study in H-ZSM-5. **2013**, 117, 23609-23620 49
- 964 Separation of carbon dioxide from nitrogen or methane by supported ionic liquid membranes (SILMs): influence of the cation charge of the ionic liquid. **2013**, 117, 15131-40 51
- 963 Extension of the B3LYP dispersion-correcting potential approach to the accurate treatment of both inter- and intra-molecular interactions. **2013**, 132, 1 34
- 962 Synthesis and Reactions of a Cyclopentadienyl-Amidinate Titaniumtert-Butoxyimido Compound. **2013**, 32, 7520-7539 19
- 961 Adaptive aggregation of peptide model systems. **2013**, 117, 7050-63 14
- 960 Synthesis of ChalcogenidoimidodiphosphinatoRhI Complexes and DFT Investigation of Their Catalytic Activation in Olefin Hydroformylation. **2013**, 2013, 1170-1183 8
- 959 DFT Studies of Pristine Hexagonal Ge₁Sb₂Te₄(0001), Ge₂Sb₂Te₅(0001), and Ge₁Sb₄Te₇(0001) Surfaces. **2013**, 117, 15075-15089 27
- 958 Pair-Wise and Many-Body Dispersive Interactions Coupled to an Optimally Tuned Range-Separated Hybrid Functional. **2013**, 9, 3473-8 20
- 957 Force field-based conformational searches: efficiency and performance for peptide receptor complexes. **2013**, 111, 2489-2500 2
- 956 Analysis of van der Waals density functional components: Binding and corrugation of benzene and C₆₀ on boron nitride and graphene. **2013**, 87, 87
- 955 Das letzte Alkan mit gestreckter Grundzustandskonformation. **2013**, 125, 482-485 27
- 954 The last globally stable extended alkane. **2013**, 52, 463-6 86
- 953 Charge generationtransport in organic materials. **2013**, 219-244 1

952	Pathways and kinetics of methane and ethane C-H bond cleavage on PdO(101). <i>Journal of Chemical Physics</i> , 2013 , 139, 104702	3.9	40
951	Atypical water lattices and their possible relevance to the amorphous ices: A density functional study. 2013 , 3, 042119		5
950	Cobalt(III)-Binding of Gluconate and 2-Amino-2-Deoxy-Gluconate. 2013 , 68, 739-742		2
949	Semilocal and hybrid meta-generalized gradient approximations based on the understanding of the kinetic-energy-density dependence. <i>Journal of Chemical Physics</i> , 2013 , 138, 044113	3.9	136
948	An effective energy gradient expression for divide-and-conquer second-order Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 2013 , 138, 044102	3.9	19
947	Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. 2013 , 15, 053046		129
946	Possible mechanisms of fullerene C ₆₀ antioxidant action. 2013 , 2013, 821498		42
945	Non-additivity of polarizabilities and van der Waals C ₆ coefficients of fullerenes. <i>Journal of Chemical Physics</i> , 2013 , 138, 114107	3.9	29
944	Microbial hydrogen splitting in the presence of oxygen. 2013 , 41, 1317-24		1
943	Importance of H-abstraction in the final step of nitrosoalkane formation in the mechanism-based inactivation of cytochrome P450 by amine-containing drugs. 2013 , 14, 24692-705		19
942	Theoretical description of X-ray absorption spectroscopy of the graphene-metal interfaces. <i>Journal of Chemical Physics</i> , 2013 , 138, 154706	3.9	31
941	The Al(ORF) ₃ /H ₂ O/Phosphane [RF = C(CF ₃) ₃] System [Protonation of Phosphanes and Absolute Brønsted Acidity. 2013 , 2013, 3054-3062		13
940	Dispersion corrections in graphenic systems: a simple and effective model of binding. 2013 , 25, 445010		27
939	Solid-State Organization and Ambipolar Field-Effect Transistors of Benzothiadiazole-Cyclopentadithiophene Copolymer with Long Branched Alkyl Side Chains. 2013 , 5, 833-846		18
938	Structure, magnetism and colour in simple bis(phosphine)nickel(II) dihalide complexes: an experimental and theoretical investigation. 2013 , 69, 1437-47		5
937	Catalytic mechanism of the arylsulfatase promiscuous enzyme from <i>Pseudomonas aeruginosa</i> . 2013 , 19, 2185-92		46
936	Photochemistry of N-methylformamide: matrix isolation and nonadiabatic dynamics. 2013 , 14, 827-36		12
935	Systematic theoretical investigation of the phthalocyanine based dimer: MnPc ₂ /F16CoPc ₂ 2013 , 87,		8

934	On the fly first principles study of the classical scattering of an Ar atom from the LiF(100) surface. <i>Journal of Chemical Physics</i> , 2013 , 139, 044707	3.9	6
933	Harris-type van der Waals density functional scheme. 2013 , 88,		6
932	Nonlocal van der Waals density functional made simple and efficient. 2013 , 87,		373
931	Basis set converged weak interaction energies from conventional and explicitly correlated coupled-cluster approach. <i>Journal of Chemical Physics</i> , 2013 , 138, 154101	3.9	27
930	C ₂₀ H ₄ (C ₄ F ₈) ₃ : A Fluorine-Containing Annulated Corannulene that Is a Better Electron Acceptor Than C ₆₀ . 2013 , 125, 7653-7656		14
929	Crystal Structure of 3R-LiTiS ₂ and its Stability Compared to Other Polymorphs. 2013 , 639, 2822-2825		10
928	Inclusion of screening effects in the van der Waals corrected DFT simulation of adsorption processes on metal surfaces. 2013 , 87,		19
927	Temperature effects in the vibrational spectra of self-assembled monolayers. 2013 , 111, 086102		5
926	Quantification of finite-temperature effects on adsorption geometries of π -conjugated molecules: Azobenzene/Ag(111). 2013 , 88,		36
925	Stereochemical inversion in difunctionalised pillar[5]arenes. 2013 , 25, 596-608		22
924	Efficient basis sets for non-covalent interactions in XDM-corrected density-functional theory. <i>Journal of Chemical Physics</i> , 2013 , 139, 214109	3.9	23
923	Pressure dependent stability and structure of carbon dioxide--a density functional study including long-range corrections. <i>Journal of Chemical Physics</i> , 2013 , 139, 174501	3.9	14
922	A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules. <i>Journal of Chemical Physics</i> , 2013 , 138, 244104	3.9	176
921	C ₅₈ on Au(111): a scanning tunneling microscopy study. <i>Journal of Chemical Physics</i> , 2013 , 138, 104703	3.9	12
920	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. <i>Journal of Chemical Physics</i> , 2013 , 139, 154702	3.9	107
919	Interaction of platinum nanoparticles with graphitic carbon structures: a computational study. 2013 , 14, 2984-9		33
918	Predicting the paramagnet-enhanced NMR relaxation of H ₂ O encapsulated in endofullerene nitroxides by density-functional theory calculations. 2013 , 371, 20110634		5
917	Energetik der Anion-Kation-Wechselwirkung in protischen ionischen Flüssigkeiten. 2013 , 125, 2425-2429		17

- 916 Zu First-Principles-Berechnungen von Elektronenstoßinduzierten Massenspektren von Molekülen. **2013**, 125, 6426-6433 7
- 915 Stefan Grimme. **2013**, 125, 9246-9247
- 914 Theoretical study of the local atomic and electronic structure of dimetacyano azobenzene molecules on Bi (111) substrate. **2013**, 430, 012036 1
- 913 The family of ferrocene-stabilized silylium ions: synthesis, ²⁹Si NMR characterization, Lewis acidity, substituent scrambling, and quantum-chemical analyses. **2013**, 19, 16579-94 67
- 912 MFU-4l – a metal-organic framework for highly effective H(2)/D(2) separation. **2013**, 25, 635-9 114
- 911 Facile Carbon Monoxide Reduction at Intramolecular Frustrated Phosphane/Borane Lewis Pair Templates. **2013**, 125, 2299-2302 57
- 910 Dispersionsvermittelte Konformationsisomerie in großen Egebundenen Acen-Dimeren. **2013**, 125, 11092-11096 10
- 909 6-Trifluoromethyl-Phenanthridines through Radical Trifluoromethylation of Isonitriles. **2013**, 125, 10992-10995 77
- 908 Phosphastannirane: a phosphorus/tin(II) Lewis pair that undergoes alkyne and alkene addition. **2013**, 52, 5640-3 52
- 907 Comprehensive and accurate Ab initio energy surface of simple alanine peptides. **2013**, 14, 3284-93 8
- 906 Phosphastanniran: Ein Phosphor/Zinn(II)-Lewis-Paar, das Alkine und Alkene addiert. **2013**, 125, 5750-5754 21
- 905 Combinations of Ethers and B(C6F5)3 Function as Hydrogenation Catalysts. **2013**, 125, 7640-7643 64
- 904 Dispersion-driven conformational isomerism in Ebonded dimers of larger acenes. **2013**, 52, 10892-5 39
- 903 Preorganized anion traps for exploiting anion-πinteractions: an experimental and computational study. **2013**, 19, 16988-7000 25
- 902 Highly Strained Phenylene Bicyclophanes. **2013**, 125, 12308-12312 12
- 901 Binding of CO2 by a Mes2PCH2CH2B(C6F5)2 species: an involvement of the ground state species in a low-energy pathway. **2013**, 19, 16512-7 6
- 900 Influence of the solvent on the stability of bis(terpyridine) structures on graphite. **2013**, 4, 269-77 11
- 899 The Cyclodextrin/benzene complex and its hydrogen bonds - a theoretical study using molecular dynamics, quantum mechanics and COSMO-RS. **2013**, 9, 118-34 22

- 898 Computational study of the rate constants and free energies of intramolecular radical addition to substituted anilines. **2013**, 9, 1620-9 23
- 897 Density Functional Theory with Modified Dispersion Correction for Metals Applied to Self-Assembled Monolayers of Thiols on Au(111). **2013**, 2013, 1-9 33
- 896 A computational study of base-catalyzed reactions of cyclic 1,2-diones: cyclobutane-1,2-dione. **2013**, 9, 594-601 9
- 895 Chromatographically separable rotamers of an unhindered amide. **2014**, 10, 701-6 7
- 894 Theoretical study of the adsorption of benzene on coinage metals. **2014**, 10, 1775-84 46
- 893 Theoretical Simulations of Reactive and Nonreactive Scattering of Light Diatomic Molecules from Metal Surfaces: Past, Present, and Future. **2014**, 2014, 1-21
- 892 UHV deposition and characterization of a mononuclear iron(III) β -diketonate complex on Au(111). **2014**, 5, 2139-48 6
- 891 Terahertz Vibrations and Hydrogen-Bonded Networks in Crystals. **2014**, 4, 74-103 49
- 890 Quasi-1D physics in metal-organic frameworks: MIL-47(V) from first principles. **2014**, 5, 1738-48 20
- 889 Substitution effect and effect of axle's flexibility at (pseudo-)rotaxanes. **2014**, 10, 1299-307 4
- 888 Computer Simulations of Prebiotic Systems. **2014**, 5 5
- 887 A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+. **2014**, 2, e449 32
- 886 Local electric dipole moments for periodic systems via density functional theory embedding. *Journal of Chemical Physics*, **2014**, 141, 234110 3.9 26
- 885 B–B Bond Cleavage and Ru–B Bond Formation from a Phosphinoborane: Synthesis of a Bis-Borane Aryl-Ruthenium Complex. **2014**, 33, 7157-7163 12
- 884 Valence electronic structure of sublimated Fe₄ single-molecule magnets: an experimental and theoretical characterization. **2014**, 2, 9599-9608 21
- 883 Resolving the anomalous infrared spectrum of the MeCN-HCl molecular cluster using ab initio molecular dynamics. **2014**, 16, 24685-90 7
- 882 Theory of Gold-Mediated Reactions: From Single Metal Site to Cluster. **2014**, 1-30
- 881 Manifestation of Fermi resonance in the vibrational spectra of 5-ioduracil, and its deuterio-derivatives isolated in low-temperature Ar matrices. **2014**, 40, 1097-1103 4

880	Role of size and shape selectivity in interaction between gold nanoclusters and imidazole: a theoretical study. 2014 , 20, 2534	17
879	Symmetry-resolved surface-derived electronic structure of MoS ₂ (0 0 0 1). 2014 , 26, 455501	8
878	Catalytic Hydrocarbon Oxidation by Palladium-bis-NHC-Complexes. 2014 , 57, 1372-1376	13
877	Atropisomerization in Confined Space; Cucurbiturils as Tools to Determine the Torsional Barrier of Substituted Biphenyls. 2014 , 2014, 105-110	7
876	Nature of Sigma-Type Lithium Bonding Interaction in Nanoscale. 2014 , 04, 1441020	
875	Structural stabilities and transformations in cationized asparagine at finite temperatures: An ab initio molecular dynamics study. 2014 , 13, 1450024	
874	Assessment of theoretical procedures for a diverse set of isomerization reactions involving double-bond migration in conjugated dienes. 2014 , 441, 166-177	39
873	A computational study of hexachlorobenzene-soil organic matter-interactions. 2014 , 13, 1450009	5
872	Analysis of SnS ₂ hyperdoped with V proposed as efficient absorber material. 2014 , 26, 395501	5
871	Using Metal Vinylidene Complexes to Probe the Partnership Between Theory and Experiment. 2014 , 41-68	
870	Contribution of phenylalanine side chain intercalation to the TATA-box binding protein-DNA interaction: molecular dynamics and dispersion-corrected density functional theory studies. 2014 , 20, 2499	14
869	The relative energies of polypeptide conformers predicted by linear scaling second-order Møller-Plesset perturbation theory. 2014 , 57, 1393-1398	9
868	Shared memory multiprocessing implementation of resolution-of-the-identity second-order Møller-Plesset perturbation theory with attenuated and unattenuated results for intermolecular interactions between large molecules. 2014 , 112, 836-843	10
867	Interplay between non-covalent interactions in complexes and crystals with halogen bonds. 2014 , 83, 1181-1203	122
866	Nitrogen-rich multinuclear ferrocenophanes as multichannel chemosensor molecules for transition and heavy-metal cations. 2014 , 14, 14339-55	12
865	Rational design of a room temperature molecular spin switch. The light-driven coordination induced spin state switch (LD-CISS) approach. 2014 , 43, 17395-405	54
864	Effects of density functionals and dispersion interactions on geometries, bond energies and harmonic frequencies of EUX ₃ (E=N, P, CH; X=H, F, Cl). 2014 , 133, 846-55	3
863	d ¹⁰ -ML ₂ Complexes: Structure, Bonding, and Catalytic Activity. 2014 , 139-161	1

862	A QM/MM study of the catalytic mechanism of β -1,4-glucan lyase from the red seaweed <i>Gracilariopsis lemaneiformis</i> . 2014 , 4, 54398-54408		5
861	Machine learning estimates of natural product conformational energies. 2014 , 10, e1003400		26
860	QM/MM molecular dynamics studies of metal binding proteins. 2014 , 4, 616-45		62
859	A one-pot multistep cyclization yielding thiadiazoloimidazole derivatives. 2014 , 10, 2989-96		6
858	Multifunctional Benzothiadiazole-Based Small Molecules Displaying Solvatochromism and Sensing Properties toward Nitroarenes, Anions, and Cations. 2014 , 3, 242-9		19
857	Nonstabilised Azomethine Ylids from N-Oxides: Unravelling the Deprotonation of N-Methylmorpholine N-Oxide. 2014 , 67, 1309		6
856	Many-body exchange-overlap interactions in rare gases and water. <i>Journal of Chemical Physics</i> , 2014 , 141, 224106	3.9	23
855	Investigation of the hydrated 7-hydroxy-4-methylcoumarin dimer by combined IR/UV spectroscopy. <i>Journal of Chemical Physics</i> , 2014 , 141, 194304	3.9	5
854	Fast and efficient optimization of Molecular Dynamics force fields for microporous materials: Bonded interactions via force matching. 2014 , 197, 339-347		9
853	The thermodynamics of proton hydration and the electrochemical surface potential of water. <i>Journal of Chemical Physics</i> , 2014 , 141, 18C512	3.9	32
852	Pair-potential approach to accurate dispersion energies between group 12 (Zn, Cd, Hg) clusters. 2014 , 118, 12274-9		2
851	Validation of molecular crystal structures from powder diffraction data with dispersion-corrected density functional theory (DFT-D). 2014 , 70, 1020-32		177
850	Theoretical study of stability and charge-transport properties of coronene molecule and some of its halogenated derivatives: a path to ambipolar organic-based materials?. <i>Journal of Chemical Physics</i> , 2014 , 141, 134708	3.9	21
849	On the mechanism of the palladium bis(NHC) complex catalyzed CH functionalization of propane: experiment and DFT calculations. 2014 , 20, 14872-9		32
848	Ag[Fe(CO) ₅] ₂ (+): a bare silver complex with Fe(CO) ₅ as a ligand. 2014 , 53, 13460-2		26
847	Origin of inversion versus retention in the oxidative addition of 3-chloro-cyclopentene to Pd(0)L(n). 2014 , 79, 12136-47		14
846	Photochemistry of glycolaldehyde in cryogenic matrices. <i>Journal of Chemical Physics</i> , 2014 , 140, 224319	3.9	9
845	Low-Cost Quantum Chemical Methods for Noncovalent Interactions. 2014 , 5, 4275-84		66

844	Quantum delocalization of protons in the hydrogen-bond network of an enzyme active site. 2014 , 111, 18454-9		87
843	The 3-Acetyloxaphosphirane/1,3,2-Dioxaphosphol-4-ene Rearrangement. 2014 , 2014, 1727-1734		11
842	Helical gold nanorods as chiral recognition nanostructures: a relativistic density functional theory study. 2014 , 136, 17757-61		7
841	How important is self-consistency for the dDsC density dependent dispersion correction?. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A516	3.9	23
840	Recommending Hartree-Fock theory with London-dispersion and basis-set-superposition corrections for the optimization or quantum refinement of protein structures. 2014 , 118, 14612-26		46
839	Insights into the Relationship of Catalytic Activity and Structure: A Comparison Study of Three Carbonic Anhydrase Mimics. 2014 , 46, 683-700		14
838	Quantitative description of structural effects on the stability of gold(I) carbenes. 2014 , 20, 14270-81		41
837	Stacking-dependent energetics and electronic structure of ultrathin polymorphic V2VI3 topological insulator nanofilms. 2014 , 90,		8
836	The CHARMM-TURBOMOLE interface for efficient and accurate QM/MM molecular dynamics, free energies, and excited state properties. 2014 , 35, 2076-86		40
835	Raman spectra from ab initio molecular dynamics and its application to liquid S-methyloxirane. <i>Journal of Chemical Physics</i> , 2014 , 141, 094503	3.9	43
834	Structural, energetic, and electronic properties of La(III)-dimethyl sulfoxide clusters. 2014 , 118, 11602-11		4
833	Quasichemical analysis of the cluster-pair approximation for the thermodynamics of proton hydration. <i>Journal of Chemical Physics</i> , 2014 , 140, 224507	3.9	24
832	Non-covalent functionalization of single wall carbon nanotubes and graphene by a conjugated polymer. 2014 , 105, 013103		17
831	The individual and collective effects of exact exchange and dispersion interactions on the ab initio structure of liquid water. <i>Journal of Chemical Physics</i> , 2014 , 141, 084502	3.9	223
830	Double-hybrid density-functional theory applied to molecular crystals. <i>Journal of Chemical Physics</i> , 2014 , 141, 044105	3.9	21
829	Syntheses and Solid-State Structures of Et2SbTeEt and Et2BiTeEt. 2014 , 2014, 4858-4864		15
828	Carbon Nitride Photocatalysts for Water Splitting: A Computational Perspective. 2014 , 118, 24833-24842		88
827	A comparative synthetic, magnetic and theoretical study of functional M(II)-tubane-type Co(II) and Ni(II) complexes. 2014 , 43, 7847-59		37

826	Mosaic Texture and Double c-Axis Periodicity of β -NiOOH: Insights from First-Principles and Genetic Algorithm Calculations. 2014 , 5, 3981-5		49
825	Theoretical Study on Novel Mixed Valence, P-H Functional P-Ligands, and Their Tautomerization. 2014 , 25, 651-657		2
824	Epoxyalcohols: bioactivation and conjugation required for skin sensitization. 2014 , 27, 1860-70		10
823	Ribose-Protonated DNA Base Excision Repair: A Combined Theoretical and Experimental Study. 2014 , 126, 10208-10212		5
822	Alkane activation on crystalline metal oxide surfaces. 2014 , 43, 7536-47		107
821	Quantum fluctuations and isotope effects in ab initio descriptions of water. <i>Journal of Chemical Physics</i> , 2014 , 141, 104502	3.9	59
820	Spin-State-Dependent Properties of an Iron(III) Hydrogenase Mimic. 2014 , 2014, 3587-3599		11
819	X-ray structure of a Hg ²⁺ complex of mercuric reductase (MerA) and quantum mechanical/molecular mechanical study of Hg ²⁺ transfer between the C-terminal and buried catalytic site cysteine pairs. 2014 , 53, 7211-22		39
818	Universal tight binding model for chemical reactions in solution and at surfaces. II. Water. <i>Journal of Chemical Physics</i> , 2014 , 141, 044504	3.9	5
817	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. 2014 , 10, 5577-85		39
816	Confinement Effect of Zeolite Cavities on Methanol-to-Olefin Conversion: A Density Functional Theory Study. 2014 , 118, 24935-24940		26
815	Spectroscopic studies of the Salmonella enterica adenosyltransferase enzyme SeCobA: molecular-level insight into the mechanism of substrate Cob(II)alamin activation. 2014 , 53, 7969-82		11
814	DFT study of the reaction of a two-coordinate iron(II) dialkyl complex with molecular oxygen. 2014 , 118, 11056-61		6
813	Functional model for the [Fe] hydrogenase inspired by the frustrated Lewis pair concept. 2014 , 136, 16626-34		55
812	Activation barriers of oxygen transformation at the active site of [FeFe] hydrogenases. 2014 , 53, 11890-902		20
811	Dual character of excited charge carriers in graphene on Ni(111). 2014 , 89,		7
810	Dispersion-correcting potentials can significantly improve the bond dissociation enthalpies and noncovalent binding energies predicted by density-functional theory. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A542	3.9	20
809	Accurate and Efficient Model Energies for Exploring Intermolecular Interactions in Molecular Crystals. 2014 , 5, 4249-55		258

808	Communication: resolving the three-body contribution to the lattice energy of crystalline benzene: benchmark results from coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2014 , 140, 121104	3.9	58
807	An actinide metallacyclopropene complex: synthesis, structure, reactivity, and computational studies. 2014 , 136, 17249-61		58
806	Controlling the stereochemistry and regularity of butanethiol self-assembled monolayers on au(111). 2014 , 136, 17087-94		28
805	The effect of hydrogen bonding on torsional dynamics: a combined far-infrared jet and matrix isolation study of methanol dimer. <i>Journal of Chemical Physics</i> , 2014 , 141, 174314	3.9	30
804	Hydroalumination of a chlorotrialkynylsilane: spontaneous stepwise 1,3-dyotropic rearrangement via an intermediate silyl cation. 2014 , 20, 8771-81		25
803	Evaluating interaction energies of weakly bonded systems using the Buckingham-Hirshfeld method. <i>Journal of Chemical Physics</i> , 2014 , 140, 184105	3.9	2
802	Hydrogen physisorption on metal-organic framework linkers and metalated linkers: a computational study of the factors that control binding strength. 2014 , 136, 17827-35		62
801	Insight into the description of van der Waals forces for benzene adsorption on transition metal (111) surfaces. <i>Journal of Chemical Physics</i> , 2014 , 140, 084704	3.9	149
800	Syntheses and Structures of 10-Trimethylelement-Substituted 1,8-Dichloroanthracenes. 2014 , 2014, 941-947		6
799	Ab initio calculation of the electronic absorption spectrum of liquid water. <i>Journal of Chemical Physics</i> , 2014 , 140, 164511	3.9	6
798	Conformational equilibrium of 2-deoxyadenosine molecules isolated in inert Ar matrices. 2014 , 40, 565-568		3
797	Epitaxial hexagonal boron nitride on Ir(111): A work function template. 2014 , 89,		72
796	The Dynamic Equilibrium Between (AlOMe) _n Cages and (AlOMe) _n [(AlMe ₃) _m Nanotubes in Methylaluminoxane (MAO): A First-Principles Investigation. 2014 , 47, 8556-8569		35
795	Challenges in first-principles NPT molecular dynamics of soft porous crystals: a case study on MIL-53(Ga). <i>Journal of Chemical Physics</i> , 2014 , 141, 064703	3.9	23
794	Method of increments for the halogen molecular crystals: Cl, Br, and I. <i>Journal of Chemical Physics</i> , 2014 , 141, 124707	3.9	13
793	Understanding the Kondo resonance in the d-CoPc/Au(111) adsorption system. <i>Journal of Chemical Physics</i> , 2014 , 141, 084713	3.9	30
792	Terahertz spectroscopy and solid-state density functional theory calculation of anthracene: effect of dispersion force on the vibrational modes. <i>Journal of Chemical Physics</i> , 2014 , 140, 174509	3.9	35
791	Short-range solvation effects on chiroptical properties: a time-dependent density functional theory and ab initio molecular dynamics computational case study on austinol. 2014 , 118, 11751-7		6

790	Guest-host interaction in an aza crown analog. 2014 , 114, 708-719		5
789	To be or not to be butterfly: New mechanistic insights in the Aza-Michael asymmetric addition of lithium (R)-N-benzyl-N-(β -methylbenzyl)amide. 2014 , 35, 1846-53		3
788	Benchmarking the performance of density functional theory and point charge force fields in their description of sl methane hydrate against diffusion Monte Carlo. <i>Journal of Chemical Physics</i> , 2014 , 140, 174703	3.9	36
787	Intermolecular hydroamination of vinylarenes by iminoanilide alkaline-earth catalysts: a computational scrutiny of mechanistic pathways. 2014 , 20, 8988-9001		18
786	Anion recognition by uranyl-salophen derivatives as probed by infrared multiple photon dissociation spectroscopy and ab initio modeling. 2014 , 20, 11783-92		12
785	Density functional theory approach to gold-ligand interactions: separating true effects from artifacts. <i>Journal of Chemical Physics</i> , 2014 , 140, 244313	3.9	11
784	Trinuclear Early/Late-Transition-Metal Thiolate Complexes. 2014 , 2014, 3510-3520		4
783	The extended stability range of phosphorus allotropes. 2014 , 53, 11629-33		113
782	Multiscale simulation of pollution gases adsorption in porous organic cage CC3. 2014 , 35, 174-80		13
781	Halogen Bonding from Dispersion-Corrected Density-Functional Theory: The Role of Delocalization Error. 2014 , 10, 5436-47		88
780	On combining temperature and pressure effects on structural properties of crystals with standard ab initio techniques. <i>Journal of Chemical Physics</i> , 2014 , 141, 124115	3.9	50
779	Geometrical and optical benchmarking of copper(II) guanidine-quinoline complexes: insights from TD-DFT and many-body perturbation theory (part II). 2014 , 35, 2146-61		26
778	Copper-Assisted Hemiacetal Synthesis: A CuI Chain Obtained by a One-Step in situ Reaction of Picolinaldehyde. 2014 , 2014, 3271-3278		3
777	Gated electron sharing within dynamic naphthalene diimide-based oligorotaxanes. 2014 , 53, 4442-9		51
776	Theoretical Chemistry in Belgium. 2014 ,		1
775	FDE-vdW: A van der Waals inclusive subsystem density-functional theory. <i>Journal of Chemical Physics</i> , 2014 , 141, 044127	3.9	19
774	Matrix effect on vibrational frequencies: experiments and simulations for HCl and HNgCl (Ng = Kr and Xe). <i>Journal of Chemical Physics</i> , 2014 , 140, 094303	3.9	20
773	Density functional theory based generalized effective fragment potential method. <i>Journal of Chemical Physics</i> , 2014 , 140, 244101	3.9	3

772	Consecutive Aromatic Carbon-Fluorine Bond and Carbon-Hydrogen Bond Activations by Iridium Porphyrins. 2014 , 33, 7059-7068	13
771	Cu,Zn-superoxide dismutase without Zn is folded but catalytically inactive. 2014 , 426, 4112-4124	35
770	Dispersion corrected RPBE studies of liquid water. <i>Journal of Chemical Physics</i> , 2014 , 141, 064501	3.9 90
769	Exchange functional that tests the robustness of the plasmon description of the van der Waals density functional. 2014 , 89,	319
768	Assessments of semilocal density functionals and corrections for carbon dioxide adsorption on metal-organic frameworks. 2014 , 15, 3157-65	11
767	Predicting the Relative Solubilities of Racemic and Enantiopure Crystals by Density-Functional Theory. 2014 , 126, 8013-8016	1
766	Synthesis of Phosphonium-Substituted Vinylidene Complexes from [HC≡CCH ₂ PPh ₃] ⁺ : Exploring the Competition between Allene and Vinylidene Formation.. 2014 , 33, 7260-7269	9
765	Combined experimental and theoretical study of fast atom diffraction on the $\sqrt{2}\times\sqrt{2}$ reconstructed GaAs(001) surface. 2014 , 90,	29
764	Polarizable molecular mechanics studies of Cu(I)/Zn(II) superoxide dismutase: bimetallic binding site and structured waters. 2014 , 35, 2096-106	9
763	Ab initio investigation of the UO ₃ polymorphs: structural properties and thermodynamic stability. 2014 , 53, 12253-64	30
762	The Key Role of van der Waals Interactions in MPC/Au(111) (M = Co, Fe, H ₂) Systems Based on First-Principles Calculations. 2014 , 118, 27843-27849	14
761	Spectroscopic signatures and structural motifs in isolated and hydrated caffeine: a computational study. 2014 , 4, 58116-58126	5
760	Coupled-cluster interaction energies for 200-atom host-guest systems. 2014 , 15, 3270-81	17
759	Structure and compressibility of the high-pressure molecular phase II of carbon dioxide. 2014 , 89,	19
758	Understanding a Host-Guest Model System through ¹²⁹ Xe NMR Spectroscopic Experiments and Theoretical Studies. 2014 , 126, 9995-9998	3
757	Electron Transfer in a Supramolecular Associate of a Fullerene Fragment. 2014 , 126, 2202-2207	12
756	Semiconducting clathrates meet gas hydrates: Xe@Sn. 2014 , 20, 6693-8	12
755	Predicting adsorption enthalpies on silicalite and HZSM-5: A benchmark study on DFT strategies addressing dispersion interactions. 2014 , 35, 809-19	29

754	Ab initio molecular dynamics study of hydrogen cleavage by a Lewis base [tBu3P] and a Lewis acid [B(C6F5)3] at the mesoscopic level--dynamics in the solute-solvent molecular clusters. 2014 , 15, 3714-9		15
753	The common effects of surface and internal bonds on the electronic structure of Bi2Te3 nano-films by first-principles calculation. 2014 , 1, 025043		1
752	Trapping in water [An important prerequisite for complex reactivity in astrophysical ices: the case of acetone (CH3)2C = O and ammonia NH3. 2014 , 443, 2991-3000		19
751	A mechanophysical phase transition provides a dramatic example of colour polymorphism: the tribochromism of a substituted tri(methylene)tetrahydrofuran-2-one. 2014 , 8, 70		3
750	The Influence of Structure on Reactivity in Alkene Metathesis. 2014 , 81-188		0
749	Computational approaches to homogeneous gold catalysis. 2015 , 357, 213-83		22
748	Characteristics of a σ -Hole and the Nature of a Halogen Bond. 2015 , 359, 1-25		17
747	Accurate Structure and Bonding Description of the Transition Metal-Disulfur Monoxide Complexes [(PMe3)2M(S2O)] (M = Ni, Pd, Pt): Grimme Dispersion Corrected DFT Study. 2014 , 640, 370-379		2
746	The ground state and electronic structure of Gd@C82: a systematic theoretical investigation of first principle density functionals. <i>Journal of Chemical Physics</i> , 2014 , 141, 244306	3.9	20
745	Occupied and unoccupied electronic structure of Na doped MoS2(0001). 2014 , 105, 241602		26
744	Characterization of a multicomponent lithium lithiate from a combined x-ray diffraction, NMR spectroscopy, and computational approach. 2014 , 53, 13282-7		16
743	Mapping the force field of a hydrogen-bonded assembly. 2014 , 5, 3931		122
742	The Ring and Exchange-Ring Approximations Based on Kohn-Sham Reference States. 2014 , 97-144		3
741	Isolated neutral peptides. 2015 , 364, 225-70		35
740	On the Transferability of Three Water Models Developed by Adaptive Force Matching. 2014 , 10, 25-43		9
739	Theoretical methods for vibrational spectroscopy and collision induced dissociation in the gas phase. 2015 , 364, 99-151		20
738	Further aspects of ochratoxin A-cation interactions: complex formation with zinc ions and a novel analytical application of ochratoxin A-magnesium interaction in the HPLC-FLD system. 2014 , 6, 1295-307		6
737	Squeezing water clusters between graphene sheets: energetics, structure, and intermolecular interactions. 2014 , 16, 26004-15		10

736	A role for [Fe ₄ S ₄] clusters in tRNA recognition--a theoretical study. 2014 , 42, 5426-35	6
735	Structural and energetic basis of isopropylmalate dehydrogenase enzyme catalysis. 2014 , 281, 5063-76	14
734	Topological isomerism in a chiral handcuff catenane. 2014 , 5, 90-100	20
733	The polymerisation of oligo(ethylene glycol methyl ether) methacrylate from a multifunctional poly(ethylene imine) derived amide: a stabiliser for the synthesis and dispersion of magnetite nanoparticles. 2014 , 5, 524-534	10
732	Chiral surface networks of 3-HPLN [A molecular analog of rounded triangle assembly. 2014 , 629, 65-74	7
731	Synthesis, characterization and study of the catalytic properties of Zn(II) camphor derived complexes. 2014 , 760, 186-196	9
730	The effect of C-H...O bonding and Cl... interactions in electrocatalytic dehalogenation of C2 chlorides containing an acidic hydrogen. 2014 , 140, 497-504	6
729	Tuning magnetism by electric field in MnPS ₃ /Sc ₂ CO ₂ van der Waals heterostructure. 2023 , 122, 082902	0
728	Synthesizability of transition-metal dichalcogenides: a systematic first-principles evaluation. 2023 , 2, 015001	0
727	Charge Density Evolution Governing Interfacial Friction. 2023 , 145, 5536-5544	0
726	Molecular Basis of the Electron Bifurcation Mechanism in the [FeFe]-Hydrogenase Complex HydABC. 2023 , 145, 5696-5709	0
725	Oxygenated Boron Species Generated In Situ by Protonolysis Enables Precision Synthesis of Alternating Polyesters. 2023 , 56, 1907-1920	1
724	Ti ³⁺ defects bridge a Cu-N _x structure to improve electron transport for photocatalytic nitrogen fixation. 2023 , 462, 142039	0
723	Allosteric regulation of reaction stage I in tryptophan synthase upon the ligand binding. 2023 , 158, 115101	0
722	Paradox of thiourea: A false-positive and promoter for electrochemical nitrogen reduction on nickel sulfide catalysts. 2023 , 328, 122485	0
721	Semicrystalline IrO _x with Abundant Boundaries for Overall Water Splitting. 2023 , 62, 4011-4019	0
720	Orthogonal luminescence lifetime encoding by intermetallic energy transfer in heterometallic rare-earth MOFs. 2023 , 14,	0
719	Theoretical Study on the Catalytic CO ₂ Hydrogenation over the MOF-808-Encapsulated Single-Atom Metal Catalysts. 2023 , 127, 4051-4062	0

- 718 Effect of Diffusion Constraints and ZnOx Speciation on Nonoxidative Dehydrogenation of Propane and Isobutane over ZnO-Containing Catalysts. **2023**, 13, 3356-3369 1
- 717 Site of the Hydroxyl Group Determines the Surface Behavior of Bipolar Chain-Oxidized Cholesterol Derivatives-Langmuir Monolayer Studies Supplemented with Theoretical Calculations. **2023**, 127, 2011-2021 0
- 716 Models for boronic acid receptors II: a computational structural, bonding, and thermochemical investigation of the $\text{RB}(\text{OH})_2\text{H}_2\text{O}\text{NH}_3$ and $\text{RB}(\text{OCH}_2\text{CH}_2\text{O})\text{NH}_3\text{H}_2\text{O}$ potential energy surfaces (R = H, methyl, phenyl, and ortho-methyl-phenyl). 0
- 715 How Doping Affects the Activity of the Aluminum Oxide Support. 0
- 714 Fluorinated Multi-Walled Carbon Nanotubes Coated Separator Mitigates Polysulfide Shuttle in Lithium-Sulfur Batteries. **2023**, 16, 1804 0
- 713 2D carbon nitride as a support with single Cu, Ag, and Au atoms for carbon dioxide reduction reaction. **2023**, 25, 8574-8582 1
- 712 Substituent Effect on Ligand-Centered Electrocatalytic Hydrogen Evolution of Phosphorus Corroles. 0
- 711 Synthesis of ONO-Ligated Tetrylenes Based on 2,6-bis(2-Hydroxyphenyl)pyridines: Influence of Ligand Sterics on the Structure of the Products. **2023**, 26, 0
- 710 Mechanism and Selectivity of Copper-Catalyzed Bromination of Distal $\text{C}(\text{sp}^3)\text{H}$ Bonds. 0
- 709 Stride Strategy to Enable a Quasi-ergodic Search of Reaction Pathways Demonstrated by Ring-opening Polymerization of Cyclic Esters. 0
- 708 Nuclear quantum effects on zeolite proton hopping kinetics explored with machine learning potentials and path integral molecular dynamics. **2023**, 14, 0
- 707 The Role of Ligands in Oxidative Addition Chemistry of Low-Valent Main Group Derivatives: Not Only Stabilization but Also Activation. 0
- 706 Impact of the electrode conductivity on the electrolyte interfacial structuring and its implications to the $\text{NaO}/+$ electrochemical performance. 0
- 705 Temperature-induced transformation between layered herringbone polymorphs in molecular bilayer organic semiconductors. **2023**, 7, 0
- 704 Achieving high Li^+ diffusion in reduced graphene oxide/ $\text{NaTi}_2(\text{PO}_4)_3$ heterostructures for enhanced lithium ions storage. **2023**, 58, 4541-4551 0
- 703 Unconventional Dual Donor-Acceptor Topologies of Aromatic Rings in Amine-Based Polymeric Tetrahedral $\text{Zn}(\text{II})$ Compounds Involving Unusual Non-Covalent Contacts: Antiproliferative Evaluation and Theoretical Studies. **2023**, 13, 382 0
- 702 Nanoscale and Real-Time Nuclear-Electronic Dynamics Simulation Study of Charge Transfer at the Donor-Acceptor Interface in Organic Photovoltaics. **2023**, 14, 2292-2300 0
- 701 Rapid Interlayer Charge Separation and Extended Carrier Lifetimes due to Spontaneous Symmetry Breaking in Organic and Mixed Organic-Inorganic Dion-Jacobson Perovskites. **2023**, 145, 5297-5309 0

- 700 The Role of the Transient Atropisomerism and Chirality of Flurbiprofen Unveiled by Laser-Ablation Rotational Spectroscopy. ○
- 699 Quasi-one-dimensional Mn₆Bi₅ and its electronic structure. **2023**, 122, 083102 ○
- 698 Carbon Dioxide Reduction on Transition Metal Dichalcogenides with Ni and Cu Edge Doping: A Density-Functional Theory Study. ○
- 697 On the Reactivity of Mes*P(PMe₃)₃ towards Aluminum(I) Compounds: Evidence for the Intermediate Formation of Phosphaaluminenes. ○
- 696 Self-Circulating Adsorption/Desorption Structure of Non-Noble High-Entropy Alloy Electrocatalyst Facilitates Efficient Water Splitting. **2023**, 11, 5055-5064 ○
- 695 Biosorption of lead ions (Pb²⁺) from water samples using dried Lemna minor biomass: experimental and density functional theory studies. ○
- 694 Drastic Gas Sensing Selectivity in 2-Dimensional MoS₂ Nanoflakes by Noble Metal Decoration. **2023**, 17, 4404-4413 ○
- 693 Machine Learning-Boosted Design of Ionic Liquids for CO₂ Absorption and Experimental Verification. **2023**, 127, 2022-2027 ○
- 692 Isolation, Structure Elucidation, and First Total Synthesis of Quinomycins K and L, Two New Octadepsipeptides from the Maowei Sea Mangrove-Derived Streptomyces sp. B475. **2023**, 21, 143 ○
- 691 Diamane-like Films Based on Twisted G/BN Bilayers: DFT Modelling of Atomic Structures and Electronic Properties. **2023**, 13, 841 ○
- 690 Anionic S-doping of a ZnMn₂O₄/CNTs cathode material enhances its Zn²⁺ storage performance in aqueous zinc-ion batteries. **2023**, 564, 232863 ○
- 689 High thermoelectric performance of layered LaAgXO₃ (X=Se,Te) from electrical and thermal transport calculations. **2023**, 7, ○
- 688 Physical Insights on the Phonon Dispersion of TiS₂. 2200821 ○
- 687 Hirshfeld and AIM Analysis of the Methylone Hydrochloride Crystal Structure and Its Impact on the IR Spectrum Combined with DFT Study. **2023**, 13, 383 1
- 686 Theoretical investigation of the MXene precursors Mo_xV_{4-x}AlC₃ (0 ≤ x ≤ 4). **2023**, 13, ○
- 685 The pivotal role of Ag species on porous nanosheets in the significant reduction of soot ignition temperature. **2023**, 461, 142107 ○
- 684 GAFF-AIC: reoptimisation of the GAFF force field for realistic densities and viscosities in aromatic isocyanates. **2023**, 49, 576-588 ○
- 683 Significantly Stabilizing Hydrogen Evolution Reaction Induced by Nb-Doping Pt/Co(OH)₂ Nanosheets. 2207569 ○

- 682 Histidine oxidation in lytic polysaccharide monooxygenase. **2023**, 28, 317-328 ○
- 681 Impedimetric sensor for iron (III) detection based on small molecule (E)-2-((phenylimino)methyl) phenol-modified platinum electrode. ○
- 680 Machine learning assisted screening of MXenes pseudocapacitive materials. **2023**, 564, 232834 ○
- 679 Bifunctional catalyst of CuMn-HZSM-5 for selective catalytic reduction of NO and CO oxidation under oxygen atmosphere. **2023**, 462, 142113 ○
- 678 Nickel foam supported hierarchical NiCo₂S₄@NiFe LDH heterostructures as highly efficient electrode for long cycling stability supercapacitor. **2023**, 446, 142098 ○
- 677 High-rate lithium storage performance of TiNb₂O₇ anode due to single-crystal structure coupling with Cr³⁺-doping. **2023**, 564, 232672 ○
- 676 A quantum chemical computation and model investigation for autoignition kinetic of a long chain oxygenate: Tri-propylene glycol methyl ether. **2023**, 343, 127933 ○
- 675 Copolymerization of α -Alkenyltrimethylsilane/Propylene with Heterogeneous Ziegler-Natta Catalyst: How Dose Alkenyl Length Affect Comonomer Incorporation?. 2300004 ○
- 674 Enhanced Ultra-Long Room Temperature Phosphorescence by Intermolecular Donor-Acceptor Interaction in Polymer Network. 2202915 ○
- 673 Not antiaromaticity gain, but increased asynchronicity enhances the Diels-Alder reactivity of tropone. **2023**, 59, 3703-3706 ○
- 672 Fabrication of stable multi-level resistance states in a Nb-doped Ge₂Sb₂Te₅ device. **2023**, 11, 3770-3777 ○
- 671 Synthesizing Cr-Based Two-Dimensional Conjugated Metal-Organic Framework Through On-Surface Substitution Reaction. 2207877 ○
- 670 Revealing Internal Rotation and ¹⁴N Nuclear Quadrupole Coupling in the Atmospheric Pollutant 4-Methyl-2-nitrophenol: Interplay of Microwave Spectroscopy and Quantum Chemical Calculations. **2023**, 28, 2153 ○
- 669 Effect of terminations on the hydrogen evolution reaction mechanism on Ti₃C₂ MXene. **2023**, 11, 6886-6900 ○
- 668 Ultrahigh-Voltage LiCoO₂ at 4.7V by Interface Stabilization and Band Structure Modification. ○
- 667 Machine Learning Models for Predicting Molecular UV-Vis Spectra with Quantum Mechanical Properties. **2023**, 63, 1462-1471 ○
- 666 Design of Olefin-Phobic Zeolites for Efficient Ethane and Ethylene Separation. **2023**, 35, 2078-2087 ○
- 665 DFT and ONIOM Simulation of 1,3-Butadiene Polymerization Catalyzed by Neodymium-Based Ziegler-Natta System. **2023**, 15, 1166 ○

- 664 A High-pressure Filled Ice in the H₂O-CO₂-H₄ System, with Possible Consequences for the CO₂-H₄ Biosignature Pair. **2023**, 944, 209 ○
- 663 Redox Switching Behavior in Resistive Memory Device Designed Using a Solution-Processable Phenalenyl-Based Co(II) Complex: Experimental and DFT Studies. **2023**, 62, 4170-4180 ○
- 662 Anisotropic van der Waals dispersion forces in polymers: Structural symmetry breaking leads to enhanced conformational search. **2023**, 5, ○
- 661 The Atomistic Understanding of the Ice Recrystallization Inhibition Activity of Antifreeze Glycoproteins. **2023**, 13, 405 ○
- 660 Templated Synthesis of Exfoliated Porous Carbon with Dominant Graphitic Nitrogen. ○
- 659 Dipole Cooperativity and Polarization Frustration Determine the Secondary Structure Distribution of Short Alanine Peptides in Water. **2023**, 127, 3126-3138 ○
- 658 Investigations on Novel 1,3-Diazetidene Based Four-Membered N-Heterocyclic Carbenes. ○
- 657 Room-temperature photosynthesis of propane from CO₂ with Cu single atoms on vacancy-rich TiO₂. **2023**, 14, ○
- 656 Exceptional Photocatalytic Hydrogen Peroxide Production from Sandwich-Structured Graphene Interlayered Phenolic Resins Nanosheets with Mesoporous Channels. 2213173 ○
- 655 Hole doping dependent electronic instability and electron-phonon coupling in infinite-layer nickelates. **2023**, 107, ○
- 654 Catalytic CO Oxidation by Single Atom Catalysts of Transition Metal-doped β-Borophene: A First Principles Study. **2023**, 52, 249-253 ○
- 653 Comprehensive Mechanism for CO Electroreduction on Dual-Atom-Catalyst-Anchored N-Doped Graphene. ○
- 652 Rational Cofomer Selection in the Development of 6-Propyl-2-thiouracil Pharmaceutical Cocrystals. **2023**, 16, 370 ○
- 651 Creating and Stabilizing an Oxidized Pd Surface under Reductive Conditions for Photocatalytic Hydrogenation of Aromatic Carbonyls. **2023**, 145, 5353-5362 1
- 650 BiOCl Nanoflowers with High Levels of Oxygen Vacancy for Photocatalytic CO₂ Reduction. **2023**, 6, 3608-3617 ○
- 649 First principles study on stacking-dependent electronic structure of CrI₃/h-In₂Se₃ heterostructures. **2023**, 133, 085703 ○
- 648 Tunable Donor-Acceptor Linear Conjugated Polymers Involving Cyanostyrylthiophene Linkages for Visible-Light-Driven Hydrogen Production. **2023**, 28, 2203 ○
- 647 Electronic Structure and Geometry of the Lowest 2LMCT State of Fe(III) Potential Fluorescent Emitters. **2023**, 62, 4284-4290 ○

- 646 Ferromagnetic GdX (X = Cl, Br) Monolayers with Large Perpendicular Magnetic Anisotropy and High Curie Temperature. **2023**, 127, 4643-4650 ○
- 645 Protonic conductivity in metalloprotein nanowires. **2023**, 11, 3626-3633 ○
- 644 Two-dimensional rectangular bismuth bilayer: A novel dual topological insulator. **2023**, 18, ○
- 643 The single-atom catalytic activity of the hydrogen evolution reaction of the experimentally synthesized boridene 2D material: a density functional theory study. **2023**, 29, ○
- 642 Comparisons of bpy and phen Ligand Backbones in Cr-Mediated (Co-)Electrocatalytic CO₂ Reduction. ○
- 641 An exotic 3-center/4-electron carbon-carbon pi long-bond: Is it tangible?. **2023**, 142, ○
- 640 Disorder-tuned conductivity in amorphous monolayer carbon. **2023**, 615, 56-61 ○
- 639 Heterogeneous metal trimer catalysts on Mo₂TiC₂O₂ MXene for highly active N₂ conversion to NH₃. **2023**, 539, 113036 ○
- 638 Excited state processes of dinuclear Pt(II) complexes bridged by 8-hydroxyquinoline. **2023**, 52, 4008-4016 ○
- 637 Theoretical investigations on the structures and electronic and optical properties of neutral and anionic M₂-doped B₂₄ clusters (M = Li, Na, and K). **2023**, 47, 6612-6620 ○
- 636 Catalysis of surface dispersed Cu²⁺ species on t-ZrO₂: square-planar Cu catalyzed cross-coupling of arylboronic acid and imidazole. **2023**, 13, 2247-2254 ○
- 635 Electrically Tunable Topological Phase Transition in van der Waals Heterostructures. **2023**, 23, 2173-2178 ○
- 634 Revisiting the Storage Capacity Limit of Graphite Battery Anodes: Spontaneous Lithium Overintercalation at Ambient Pressure. **2023**, 2, ○
- 633 QM Calculations Revealed that Outer-Sphere Electron Transfer Boosted O-O Bond Cleavage in the Multiheme-Dependent Cytochrome bd Oxygen Reductase. **2023**, 62, 4066-4075 ○
- 632 A DFT study of Ni-catalyzed (3 + 3)-annulation between donor-acceptor cyclopropanes and diaziridines. **2023**, 10, 1948-1958 ○
- 631 Effect of intermolecular interaction of the charge-transfer complex between molecular tweezers and C60/C70 on second-order nonlinear optical properties. **2023**, 25, 8799-8808 ○
- 630 Spin-crossing in heterogeneous ethane dehydrogenation by atomically dispersed Co/SiO₂. **2023**, 3, 100534 ○
- 629 The transition metal doped B cluster (TM₄B₁₈) as catalysis for nitrogen fixation. **2023**, 539, 113031 ○

- 628 Mechanism for the synthesis of medium-chain 1-alkenes from fatty acids catalyzed by binuclear iron UndA decarboxylase. **2023**, 420, 123-133 ○
- 627 Aggregation Triggers Red/Near-Infrared Light Hydrogen Production of Organic Dyes with High Efficiency. **2023**, 13, 3723-3734 ○
- 626 Assessment of the performance of six indices in predicating the aromaticity of planar porphyrinoids. **2023**, 29, ○
- 625 Oxygen Vacancy Promoted Generation of Monatomic Oxygen Anion over Ni²⁺-Doped MgO for Efficient Glycolysis of Waste PET**. ○
- 624 Dehydrogenation reaction of triethylamine by an electrophilic terminal phosphinidene complex. **2023**, 52, 3275-3278 ○
- 623 Insights into the regioselectivity and diastereoselectivity of the Nazarov cyclization of 3-alkenyl-2-indolylmethanol with tryptophol. **2023**, 10, 1721-1730 ○
- 622 Reactivity and Selectivity of the Diels-Alder Reaction of Anthracene in [Pd₆L₄]¹²⁺ Supramolecular Cages: A Computational Study. **2023**, 62, 4330-4340 ○
- 621 Unexpected Piezoresistive Effect, Room-Temperature Ferromagnetism, and Thermal Stability of 2D Cu₂S Crystals in Reduced Graphene Oxide Membrane. 2201241 ○
- 620 Extension of the TraPPE Force Field for Battery Electrolyte Solvents. **2023**, 127, 2224-2236 ○
- 619 Inductive Effect Alone Cannot Explain Lewis Adduct Formation and Dissociation at Electrode Interfaces. **2023**, 145, 5759-5768 ○
- 618 The structure of pathogenic huntingtin exon 1 defines the bases of its aggregation propensity. **2023**, 30, 309-320 ○
- 617 Chlorine-induced mixed valence of CuO_x/C to promote the electroreduction of carbon dioxide to ethylene. ○
- 616 Computation Study on Copper-Catalyzed Aerobic Intramolecular Aminooxygenative C-C Bond Cleavage to Imides: Different Roles of Mononuclear and Dinuclear Copper Complexes. **2023**, 13, 3815-3829 ○
- 615 Designing Donor-Acceptor Cyclopropane for the Thermal Synthesis of Carbocyclic Eight-Membered Rings. **2023**, 365, 1002-1011 ○
- 614 Directing and Understanding the Translation of a Single Molecule Dipole. **2023**, 14, 2487-2492 ○
- 613 A comprehensive investigation of the plasmonic-photocatalytic properties of gold nanoparticles for CO₂ conversion to chemicals. **2023**, 15, 7051-7067 ○
- 612 A new look at the structure of the neutral Au₁₈ cluster: hollow versus filled golden cage. **2023**, 25, 9036-9042 ○
- 611 A computational study of the reaction mechanism and stereospecificity of dihydropyrimidinase. **2023**, 25, 8767-8778 ○

- 610 Cobalt-catalyzed radical-mediated carbon-carbon scission via a radical-type migratory insertion. **2023**, 14, 3352-3362 ○
- 609 Lineares und gewickeltes Cp* 2 Si: Reversibler Phasendurchgang eines Schlüsselmoleküls. ○
- 608 Effect of TiO₂-Al₂O₃ support surface properties on active phase structure and hydrodenitrogenation performances of the corresponding NiWS supported catalysts. **2023**, 343, 127922 ○
- 607 Two-Dimensional AMgB (A = Na, K; B = P, As, Sb, Bi) with Promising Optoelectronic and Thermoelectric Performances. **2023**, 5, 1405-1419 ○
- 606 Molybdenum based 2D conductive Metal-Organic frameworks as efficient single-atom electrocatalysts for N₂ reduction: A density functional theory study. **2023**, ○
- 605 Atmospheric chemical behaviors of (CF₃)₂CFCN by density-functional theory method: The relationship between electronic structure and atmosphere lifetime. ○
- 604 Activation of metal-involved halogen bonds and classical halogen bonds in gold(i) catalysis. **2023**, 52, 4517-4525 ○
- 603 Dual Behavior Regulation: Tether-Free Deep-Brain Stimulation by Photothermal and Upconversion Hybrid Nanoparticles. ○
- 602 First principles calculation study of single transition metal atom grafted Au₂₅ as efficient electrocatalysts for OER and ORR. **2023**, 540, 113030 ○
- 601 Isostructural coordination polymers of the tethering naphthalene anchored bis(2-methylpyridinecarboxamide) ligand: single crystal, XPS, EDS and theoretical studies. **2023**, 47, 5477-5487 ○
- 600 Electron heat transport in low-rank lignite: combining experimental and computational methods. ○
- 599 Upcycling natural Limestone waste for thermochemical energy storage by utilising tailored CaZrO₃ nanoadditives. ○
- 598 From M₆ to M₁₂, M₁₉ and M₃₈ molecular alloy Pt_nNi carbonyl nanoclusters: selective growth of atomically precise heterometallic nanoclusters. **2023**, 52, 3623-3642 ○
- 597 Surface-Dependent Electrocatalytic Activity of CoSe₂ for Lithium Sulfur Battery. **2023**, 10, ○
- 596 Influence of Group 15 elements on the [3 + 2] cycloaddition reactivity of G₁₅ = G₁₅-based 1,3-dipoles with cyclooctyne. **2023**, 52, 4796-4807 ○
- 595 Pt overlayer for direct oxidation of CH₄ to CH₃OH. **2023**, 108292 ○
- 594 Synthesis, X-ray characterization and DFT calculations of a series of 3-substituted 4,5-dichloroisothiazoles. **2023**, 25, 1976-1985 ○
- 593 Topology Hierarchy of Transition Metal Dichalcogenides Built from Quantum Spin Hall Layers. ○

- 592 Crystal Structures and Physicochemical Properties of Be₂N and Mg₂N. **2023**, 19, ○
- 591 Near-infrared absorbing acceptor with suppressed triplet exciton generation enabling high performance tandem organic solar cells. **2023**, 14, ○
- 590 Structural Phase Transition of Quinone-Containing PAH Derivatives on Au(111) at High Coverage. **2023**, 127, 5039-5043 ○
- 589 An investigation to understand the correlation between the experimental and density functional theory calculations of noscapine. ○
- 588 Theoretical investigations of Ti₄C₃ and Ti₄C₃T₂ (T = F, O and OH) monolayers as anode materials for Li-ion batteries. **2023**, 38, 100491 ○
- 587 Alloying of Cu with Ru Enabling the Relay Catalysis for Reduction of Nitrate to Ammonia. ○
- 586 Revealing the mechanisms of lithium-ion transport and conduction in composite solid polymer electrolytes. **2023**, 4, 101321 ○
- 585 Crotonaldehyde Adsorption on Cu-Pt Surface Alloys: A Quantum Mechanics Study. **2023**, 5, 463-478 ○
- 584 Mechanistic Insights into Enantioselective C(sp³)–H Acylation to Construct β -Amino Ketones via Photoredox and Ni(II) Dual Catalysis: A DFT Study. **2023**, 18, ○
- 583 The Pattern of Hydroxyphenyl-Substitution Influences CO₂ Reduction More Strongly than the Number of Hydroxyphenyl Groups in Iron-Porphyrin Electrocatalysts. **2023**, 13, 3902-3912 1
- 582 Efficient degradation of organic contaminants via a novel iron-based poly(ionic liquid)/polydopamine composite as the heterogeneous Fenton catalyst. ○
- 581 3-D molecular stars with covalent axial bonding. ○
- 580 Crystal and electronic structure of thiazolium pentaiodide: an experimental and theoretical study of covalent and non-covalent bonds. ○
- 579 In Situ Neutron Scattering Study of the Structure Dynamics of the Ru/Ca₂N:e⁻Catalyst in Ammonia Synthesis. **2023**, 35, 2456-2462 ○
- 578 Virtual Screening, Structural Analysis, and Formation Thermodynamics of Carbamazepine Cocrystals. **2023**, 15, 836 1
- 577 The Role of Surface Hydroxyls in the Mobility of Carboxylates on Surfaces: Dynamics of Acetate on Anatase TiO₂(101). **2023**, 14, 2542-2550 ○
- 576 Performance of Density Functionals and Semiempirical 3c Methods for Small Gold–Thiolate Clusters. **2023**, 127, 2242-2257 ○
- 575 Exploration and investigation of various solid forms of an anti-glaucoma drug β -dichlorphenamide. **2023**, 25, 1874-1883 ○

- 574 Unravelling the Mechanism and Governing Factors in Lewis Acid and Non-Covalent Diels-Alder Catalysis: Different Perspectives. **2023**, 24, 4938 ○
- 573 Semimetallic and semiconducting graphene- hBN multilayers with parallel or reverse stacking. **2023**, 107, ○
- 572 Rectangular Transition Metal-rTCNQ Organic Frameworks Enabling Polysulfide Anchoring and Fast Electrocatalytic Activity in Li-Sulfur Batteries: A Density Functional Theory Perspective. **2023**, 28, 2389 ○
- 571 Probing the n -π carbonyl-carbonyl interactions in the formaldehyde-trifluoroacetone dimer by rotational spectroscopy. **2023**, 158, 124304 ○
- 570 Interfacial contact barrier and charge carrier transport of MoS₂/metal(001) heterostructures. **2023**, 25, 9548-9558 ○
- 569 Ambipolar Electrochemistry of Pre-Intercalated Ti₃C₂T_x MXene in Ionic Liquid Electrolyte. ○
- 568 A computational investigation of the decomposition of acetic acid in H-SSZ-13 and its role in the initiation of the MTO process. **2023**, 13, 1905-1917 ○
- 567 Photocatalytic Properties of PbMoO₄ Nanocrystals against Cationic and Anionic Dyes in Several Experimental Conditions. **2023**, 2, 111-134 ○
- 566 The Raman Spectra of Co-, Fe-, and Mn-doped Bi₂Se₃ Single Crystals. **2023**, 13, 456 ○
- 565 Functional group corrections to the GFN2-xTB and PM6 semiempirical methods for noncovalent interactions in alkanes and alkenes. **2023**, 158, 124105 ○
- 564 Twisted Crystalline Organic Semiconductor Photodetectors. 2212531 ○
- 563 Mechanism and origins of ligand-controlled regioselectivity of copper-catalyzed borocarbonylation of imines with B₂pin₂ and alkyl iodides: a computational study. **2023**, 10, 2024-2032 ○
- 562 Study on the Half-Auxetic Behavior of Layered Nitrogen-Doped Graphdiyne. **2023**, 12, 1-8 ○
- 561 Dual Routes toward Observation of a trans-H₂/Hydride Complex in an Iridium Pincer System and Hydrogenation Catalytic Activity. **2023**, 42, 441-456 ○
- 560 Plurality of excitons in Ruddlesden-Popper metal halides and the role of the B-site metal cation. **2023**, 4, 1720-1730 ○
- 559 Study on Removal Mechanism for Copper Cyanide Complex Ions in Water: Ion Species Differences and Evolution Process. **2023**, 24, 5066 ○
- 558 Modeling Catalyzed Reactions on Metal-Doped Amorphous Silicates: The Case of Niobium-Catalyzed Ethylene Epoxidation. **2023**, 127, 4984-4997 ○
- 557 Selective and effective oxidation of 5-hydroxymethylfurfural by tuning the intermediates adsorption on Co-Cu-CN_x. ○

- 556 Correlation of Experimental and Calculated Reaction Enthalpies with Ligand Donor Strengths. ○
- 555 Cold Oxidative Demetalation of Aryl Organometallics: A Novel Route to Demetalate Ullmann Intermediates without Heating. **2023**, 8, ○
- 554 Rational design of MoS₂-supported Cu single-atom catalysts by machine learning potential for enhanced peroxidase-like activity. **2023**, 15, 6686-6695 ○
- 553 Thickness-dependent catalytic activity of hydrogen evolution based on single atomic catalyst of Pt above MXene. **2023**, 35, 204001 ○
- 552 Theoretical prediction of the electronic structure, optical properties and photocatalytic performance of type-I SiS/GeC and type-II SiS/ZnO heterostructures. **2023**, 13, 7436-7442 ○
- 551 Bis(perfluoroaryl)chalcogenes ArF₂Ch (Ch = S, Se, Te) as π-Hole Donors for Supramolecular Applications Based on Noncovalent Bonding. **2023**, 23, 2593-2601 ○
- 550 Electrically tunable Gilbert damping in van der Waals heterostructures of two-dimensional ferromagnetic metals and ferroelectrics. **2023**, 122, 102402 ○
- 549 Development of Deep Potentials of Molten MgCl₂/NaCl and MgCl₂/KCl Salts Driven by Machine Learning. ○
- 548 The versatile characteristics of ArS/SGaInS van der Waals heterostructures. ○
- 547 Quantum-mechanics-based molecular dynamics simulations of the structure and performance of sulfur-enriched Li₃PS₄ cathodes. **2023**, 4, 101326 ○
- 546 Efficient Synthesis of 1H-Benzo[4,5]imidazo[1,2-c][1,3]oxazin-1-one Derivatives Using Ag₂CO₃/TFA-Catalyzed 6-endo-dig Cyclization: Reaction Scope and Mechanistic Study. **2023**, 28, 2403 ○
- 545 Elaborating and regulating ESIPT associated with solvent polarity for the novel 2-(benzo[d]thiazol-2-yl)-4-(9H-diphenylamino-9-yl)phenol fluorophore. **2023**, 121, ○
- 544 Multifunctional Triggering by Solid-Phase Molecular Motion: Relaxor Ferroelectricity, Modulation of Magnetic Exchange Interactions, and Enhancement of Negative Thermal Expansion. **2023**, 35, 2421-2428 ○
- 543 CO-Preserving Photoinduced Transfer of Cymantrenyl Moiety: a Tandem Experimental and Computational Investigation. ○
- 542 Cocrystallization of Antifungal Compounds Mediated by Halogen Bonding. **2023**, 23, 2932-2940 ○
- 541 Light-Induced Subnanometric Modulation of a Single-Molecule Electron Source. **2023**, 130, ○
- 540 DFT Studies on Ligand Controlled Highly Selective Copper-Catalyzed Borylations of Allenes. ○
- 539 New insights into the alkoxy effects on auxiliary adsorption and inhibiting charge recombination in dye-sensitized solar cells with high open circuit voltage: a theoretical investigation. **2023**, 25, 8532-8543 ○

- 538 Quantum Informed Machine-Learning Potentials for Molecular Dynamics Simulations of CO₂ Chemisorption and Diffusion in Mg-MOF-74. **2023**, 17, 5579-5587 ○
- 537 Phase-Controllable Growth of Air-Stable SnS Nanostructures for High-Performance Photodetectors with Ultralow Dark Current. ○
- 536 Unraveling the Nature and Strength of Non-Covalent Interactions on the Surface of Fullerenes. **2023**, 88, ○
- 535 Electro-Oxidation of Polyols on Bi-Modified Pt in Acidic Media (HClO₄). Understanding Activity and Selectivity Trends. ○
- 534 An automated reaction route mapping for the reaction of NO and active species on Ag₄ clusters in zeolites. **2023**, 25, 8524-8531 ○
- 533 Hydration at Highly Crowded Interfaces. **2023**, 130, ○
- 532 Photo-response of water intercalated Ti₃C₂O₂ MXene. **2023**, 25, 9522-9531 ○
- 531 Stability of a Silica-Supported Second Generation Hoveyda-Grubbs Catalyst Under Atmospheric Conditions: Experimental and Computational Studies. ○
- 530 Novel cubic silicane nanosheet as an adsorbing medium for dimethylbutane and methylhexane molecules: a first-principles study. **2023**, 121, ○
- 529 STRUCTURE AND THERMODYNAMIC CHARACTERISTICS OF INTERMEDIATE CATALYTIC ADDUCTS IN CUMENE OXIDATION IN THE PRESENCE OF 2-ETHYLHEXANOATES OF GROUP 2 METALS. **2023**, 64, 227-239 ○
- 528 Synthesis, Structure, and Electrochemical Properties of 2,3,4,5-Tetraphenyl-1-Monophosphaferrocene Derivatives. **2023**, 28, 2481 ○
- 527 Evaluating performance of the approximate 3D-RISM-KH molecular solvation theory for solvation free energies in alkanes and alkane-water partition coefficients. **2023**, 378, 121597 ○
- 526 Relativistic Effects on Rate and Product Formation in the Gas-Phase Methane Chemistry of Late Atomic Transition Metal Cations. ○
- 525 Concentration-Flux-Steered Mechanism Exploration with an Organocatalysis Application. ○
- 524 Understanding the mechanism and origins of stereoconvergence in nickel-catalyzed hydroarylation of 1,3-dienes with aryl boronates. **2023**, 52, 4849-4855 ○
- 523 Nanoscale Hydrophobicity and Electrochemical Mapping Provides Insights into Facet Dependent Silver Nanoparticle Dissolution. **2023**, 14, 2665-2673 ○
- 522 Reactions of Zinc Hydride with Silylenes: From Oxidative Addition to Ligand Exchange Reactions. **2023**, 42, 457-464 ○
- 521 Pyrazine-Functionalized Donor-Acceptor Covalent Organic Frameworks for Enhanced Photocatalytic H₂ Evolution with High Proton Transport. 2207421 ○

- 520 Insights into the Origin of High Activity of Ni₅P₄(0001) for Hydrogen Evolution Reaction. **2023**, 127, 5385-5394
- 519 Understanding the solvation structures of glyme-based electrolytes by machine learning molecular dynamics. **2023**, 100061
- 518 Identification of a Ubiquinone-Ubiquinol Quinhydrone Complex in Bacterial Photosynthetic Membranes and Isolated Reaction Centers by Time-Resolved Infrared Spectroscopy. **2023**, 24, 5233
- 517 Is DFT Accurate Enough to Calculate Regioselectivity? The Case of 1,3-Dipolar Cycloaddition of Azide to Alkynes and Alkenes.
- 516 Molybdenum disulfide under extreme conditions: An ab initio study on its melting. **2023**, 133, 105102
- 515 An investigation of Solid-State Emission of Halogenated Diphenyl Phosphanyl Anthracenes. 2202753
- 514 Engineering the catalytic properties of CeO₂ catalyst in HCl-assisted propane dehydrogenation by effective doping: A first-principles-based microkinetic simulation. 11,
- 513 First-Principles Study of Hg₀ Immobilization on a Defective Pyrite Surface. **2023**, 37, 5378-5387
- 512 Hydrothiolation of alkynes with thiol-atechol derivatives catalysed by CuNPs/TiO₂: exploring the reaction mechanism by DFT calculations. **2023**, 13, 8025-8033
- 511 Disturbance of intermolecular forces: eutectics as a new tool for the preparation of vapor-phase deposition precursors. **2023**, 25, 8336-8340
- 510 Self-Assembled Encapsulation of Cu₂X₂ (X = Br, Cl) in a Gold Phosphine Box-like Cavity with Metallophilic Au-Au Interactions. **2023**, 62, 4467-4475
- 509 The RuO₂/NiRu heterogeneous interface optimizes the d-band center of the NiRu catalyst for high-performance alkaline hydrogen evolution reaction.
- 508 Halogen-Bonded Mono-, Di-, and Tritopic N-Alkyl-3-iodopyridinium Salts. **2023**, 23, 2361-2374
- 507 Bottom-Up Synthesis of Metalated Carbyne Ribbons via Elimination Reactions. **2023**, 145, 6203-6209
- 506 Synthesis of Sulfilimines Enabled by Copper-Catalyzed S-Arylation of Sulfenamides. **2023**, 145, 6310-6318
- 505 Ultra-long-life and ultrathin quasi-solid electrolytes fabricated by solvent-free technology for safe lithium metal batteries. **2023**, 58, 132-141
- 504 Acetylene-Mediated Borophosphene Dirac Materials as Efficient Anode Materials for Lithium-Ion Batteries.
- 503 Stereochemical Properties of Two Schiff-Base Transition Metal Complexes and Their Ligand by Using Multiple Chiroptical Spectroscopic Tools and DFT Calculations. **2023**, 28, 2571

- 502 Solvation Shell Structures of Ammonia in Reline and Ethaline Deep Eutectic Solvents. **2023**, 127, 2499-2510 ○
- 501 **EE**Catalysis Made Asymmetric**Enantiomerization** Catalysis Mediated by the Chiral **E**System of a Perylene Bisimide Cyclophane. ○
- 500 Assessments of DFT-based energy decomposition analysis methods for intermolecular interactions. **2023**, 158, 124116 ○
- 499 Neural network potentials for accelerated metadynamics of oxygen reduction kinetics at Au/water interfaces. **2023**, 14, 3913-3922 ○
- 498 Divalent organic cations as a novel protective layer for perovskite materials. ○
- 497 Synergistic Catalysis in Heterobimetallic Complexes for Homogeneous Carbon Dioxide Hydrogenation. **2023**, 28, 2574 ○
- 496 PromoterPoison Partnership Protects Platinum Performance in Coked Cluster Catalysts. **2023**, 127, 5376-5384 ○
- 495 Mechanisms of adsorbing hydrogen gas on metal decorated graphene. **2023**, 7, ○
- 494 Enantiospecific Affinities of Chiral Cu Films for Both d-Ribose and l-Amino Acids. **2023**, 35, 2402-2407 ○
- 493 Constructing imine groups on the surface of Cu₁/Pd(111) as a novel strategy for CO₂ hydrogenation to methanol. **2023**, 15, 6999-7005 ○
- 492 Computational Modelling of Pyrrolic MN₄ Motifs Embedded in Graphene for Catalyst Design. **2023**, 13, 566 ○
- 491 Importance of Adatom on Pure Iron Catalyst Towards Electrocatalytic N₂ Reduction Reaction. ○
- 490 Stable Mo/1T-MoS₂ Monolith Catalyst with a Metallic Interface for Large Current Water Splitting. ○
- 489 Theoretical study on hydrogen evolution reaction in transition metal borides. ○
- 488 Two-dimensional layered DionJacobson phase organic/inorganic tin iodide perovskite field-effect transistors. **2023**, 11, 7767-7779 ○
- 487 Subsurface Li Monolayer on Cu(111) Surfaces for Upgrading Ethanol to n-Butanol: A Computational Study. ○
- 486 Theoretical study on the mechanism of water oxidation catalyzed by a mononuclear copper complex: important roles of a redox non-innocent ligand and HPO₄²⁻ anion. **2023**, 13, 8352-8359 ○
- 485 Structure and stability of the sH binary hydrate cavity and host-guest versus guest-guest interactions therein: A DFT approach. ○

- 484 Effect of the Position of Amine Groups on the CO₂, CH₄, and H₂ Adsorption Performance of Graphene Nanoflakes. **2023**, 62, 5230-5240 ○
- 483 DFT insights into competing mechanisms of guaiacol hydrodeoxygenation on a platinum cluster. **2023**, 25, 10460-10471 ○
- 482 A density functional theory study of van der Waals interaction in carbon nanotubes. **2023**, 70, 759-769 ○
- 481 Electrocatalytic activity of MoSi₂N₄ monolayers decorated with single transition metal atoms: a computational study. **2023**, 34, 245705 ○
- 480 Cobalt-catalysed nucleophilic fluorination in organic carbonates. **2023**, 52, 4585-4594 ○
- 479 Understanding the activity of single atom catalysts for CO₂ reduction to C₂ products: A high throughput computational screening. **2023**, 47, 7225-7231 ○
- 478 Effect of formic acid on O₂ + OH \rightleftharpoons HOH -HCOOH + HO₂ reaction under tropospheric condition: kinetics of cis and trans isomers. **2023**, 25, 9965-9978 ○
- 477 Strain-Modulated Photocatalytic Performance of Janus WSSe/g-GaN Heterostructures. **2023**, 127, 5544-5551 ○
- 476 A Comprehensive Ab Initio Study of Halogenated A π U and G π C Base Pair Geometries and Energies. **2023**, 24, 5530 ○
- 475 Interconversion of the Eigen/Zundel Cations on Metal Surfaces. **2023**, 73-106 ○
- 474 Quantifying the Contribution of London Dispersion Interaction and Adjacent Chain Packing on the Polymer Stiffness: A DFT Study. **2023**, 23, 2971-2979 ○
- 473 Graphene Capping of Cu Back-End-of-Line Interconnects Reduces Resistance and Improves Electromigration Lifetime. **2023**, 6, 4170-4177 ○
- 472 Sustainable methane utilization technology via photocatalytic halogenation with alkali halides. **2023**, 14, ○
- 471 Computational Design and Theoretical Properties of WC₃N₆, an H-Free Melaminite and Potential Multifunctional Material. **2023**, 145, 6986-6993 ○
- 470 Wide-Humidity Range Applicable, Anti-Freezing, and Healable Zwitterionic Hydrogels for Ion-Leakage-Free Iontronic Sensors. ○
- 469 Computational Investigation of Precursor Blocking during Area-Selective Atomic Layer Deposition Using Aniline as a Small-Molecule Inhibitor. **2023**, 39, 4265-4273 ○
- 468 Improvement of carbon dioxide electroreduction by crystal surface modification of ZIF-8. ○
- 467 Emergent second-harmonic generation in van der Waals heterostructure of bilayer MoS₂ and monolayer graphene. **2023**, 9, ○

- 466 Having Your Cake and Eating It Too: Electrode Processing Approach Improves Safety and Electrochemical Performance of Lithium-Ion Batteries. **2023**, 15, 15561-15573 ○
- 465 An effective strategy for CO₂ reduction to C₁ products using Cu-embedded MoS₂ electrocatalyst: DFT study. **2023**, 47, 6932-6942 ○
- 464 Insights into How NH₄⁺ Ions Enhance the Activity of Dimeric G-Quadruplex/Hemin DNAzyme. **2023**, 13, 4330-4338 ○
- 463 Healing double vacancy defects on graphene: reconstruction by C₂ adsorption. **2023**, 25, 10759-10768 ○
- 462 Solid-State ¹⁹F NMR Chemical Shift in Square-Planar Nickel(II) Fluoride Complexes Linked by Halogen Bonds. **2023**, 62, 4835-4846 ○
- 461 Methanol Synthesis on Copper-Doped F Centers. **2023**, 127, 5321-5333 ○
- 460 Design of a Four-Atom Cluster Embedded in Carbon Nitride for Electrocatalytic Generation of Multi-Carbon Products. **2023**, 145, 7030-7039 ○
- 459 Brønsted acid-catalyzed asymmetric dearomatization for synthesis of chiral fused polycyclic enone and indoline scaffolds. **2023**, 9, ○
- 458 Unveiling the Mechanistic Singularities of Caspases: A Computational Analysis of the Reaction Mechanism in Human Caspase-1. **2023**, 13, 4348-4361 ○
- 457 Achieving Thermodynamic Stability of Single-Crystal Co-Free Ni-Rich Cathode Material for High Voltage Lithium-Ion Batteries. 2300081 ○
- 456 Room-Temperature Cu-Catalyzed Amination of Aryl Bromides Enabled by DFT-Guided Ligand Design. **2023**, 145, 6966-6975 ○
- 455 Tunable growth of one-dimensional graphitic materials: graphene nanoribbons, carbon nanotubes, and nanoribbon/nanotube junctions. **2023**, 13, ○
- 454 Cd implantation in HfMoO₃: An atomic scale study. **2023**, 7, ○
- 453 Comparative DFT study of methanol decomposition on Mo 2 C(001) and Mo 2 C(101) surfaces. ○
- 452 Intercalation of p-Aminopyridine and p-Ethylenediamine Molecules into Orthorhombic In_{1.2}Ga_{0.8}S₃ Single Crystals. **2023**, 16, 2368 ○
- 451 Excited-State Intramolecular Proton Transfer in Salicylidene-β-Hydroxy Carboxylate Derivatives: Direct Detection of the Triplet Excited State of the cis-Keto Tautomer. **2023**, 127, 2765-2778 ○
- 450 WS₂ and WS₂-ZnO Chemiresistive Gas Sensors: The Role of Analyte Charge Asymmetry and Molecular Size. ○
- 449 Decomposing Chemical Space: Applications to the Machine Learning of Atomic Energies. **2023**, 19, 2029-2038 ○

- 448 On the inverse correlation between the hydrogen bond strength and chalcogen bond strength in the cyclic supramolecular heterosynthons $[SeN]_n[HOOC]_n$. **2023**, 25, 2159-2164 ○
- 447 $NaAl_4X_4$ (X = S, Se, Te): Clusters with a planar tetracoordinate nitrogen and significantly improved stability. **2023**, 158, 144301 ○
- 446 Facile Tailoring of Surface Terminations of MXenes by Doping Nb Element: Toward Extraordinary Pseudocapacitance Performance. **2023**, 15, 15367-15376 ○
- 445 Tunable Electronic Properties of Graphene Quantum Dots Guide the CO₂-to-Formate Conversion Efficiency on SnO₂ Nanosheet. **2023**, 62, 4940-4946 ○
- 444 Theoretical Assessment of Carbon Dioxide Reactivity in Methylpiperidines: A Conformational Investigation. **2023**, 127, 3123-3132 ○
- 443 Sustainable upcycling of spent LiCoO₂ to an ultra-stable battery cathode at high voltage. ○
- 442 The Origin of Anion Autocatalysis. ○
- 441 Density functional theory and experimental study of multi-step lithiation in SnS₂ anode. **2023**, 29, 1751-1763 ○
- 440 The neglected autoxidation pathways for the formation of highly oxygenated organic molecules (HOMs) and the nucleation of the HOMs generated by limonene. **2023**, 304, 119727 ○
- 439 Spin-Resolved Band Structure of Hoffman Clathrate $[Fe(pz)_2Pt(CN)_4]$ as an Essential Tool to Predict Optical Spectra of Metal-Organic Frameworks. **2023**, 15, 15848-15862 ○
- 438 Resolving Interface Barrier Deviation from the Schottky-Mott Rule: A Mitigation Strategy via Engineering MoS₂-Metal van der Waals Contact. **2023**, 14, 2940-2949 ○
- 437 Quantitative Evaluation of the Carrier Separation Performance of Heterojunction Photocatalysts: The Case of g-C₃N₄/SrTiO₃. **2023**, 14, 2927-2932 ○
- 436 ReDD-COFFEE: a ready-to-use database of covalent organic framework structures and accurate force fields to enable high-throughput screenings. **2023**, 11, 7468-7487 ○
- 435 Solvent Polarity Governs Ultrafast Structural Dynamics: A Case Study of 4-Dimethylamino-4'-carbomethoxydiphenylacetylene. **2023**, 127, 5855-5865 ○
- 434 Water adsorption on lead dioxide from ab initio molecular dynamics simulations. **2023**, 158, 134718 ○
- 433 Defects in WS₂ monolayer calculated with a nonlocal functional: any difference from GGA?. **2023**, 5, 024001 ○
- 432 Anisotropic Strain Boosted Hydrogen Evolution Reaction Activity of F-NiCoMo LDH for Overall Water Splitting. **2023**, 170, 036509 ○
- 431 Phosphorus Optimized Metastable Hexagonal-Close-Packed Phase Nickel for Efficient Hydrogen Peroxide Production in Neutral Media. 2300636 ○

- 430 Performance of Copper Corrosion Inhibitors on Pipecoridithiocarbamic Acid in 3 wt% NaCl Solution. **2023**, ○
- 429 Pd/Xu-Phos-catalyzed asymmetric elimination of fully substituted enol triflates into axially chiral trisubstituted allenes. **2023**, 9, ○
- 428 Semimetal contacts to monolayer semiconductor: weak metalization as an effective mechanism to Schottky barrier lowering. **2023**, 56, 234001 ○
- 427 Computational Discovery of Active and Selective Metal-Nitrogen-Graphene Catalysts for Electrooxidation of Water to H₂O₂. ○
- 426 Tunable Electronic Properties of Substitutionally Doped CSb Monolayer. ○
- 425 Multi-site reaction dynamics through multi-fragment density matrix embedding. **2023**, 158, 134105 ○
- 424 Revealing the impact of organic spacers and cavity cations on quasi-2D perovskites via computational simulations. **2023**, 13, ○
- 423 5-fluorouracil-caffeic acid cocrystal delivery agent with long-term and synergistic high-performance antitumor effects. **2022**, 17, 2215-2229 ○
- 422 Unraveling Binding Mechanism and Stability of Urease Inhibitors: A QM/MM MD Study. **2023**, 28, 2697 ○
- 421 A Li₄Ti₅O₁₂ Composite Anode for Reducing Interfacial Resistance of Solid-State Batteries. 2200374 ○
- 420 2D MoSi₂N₄ as electrode material of Li-air battery [A DFT study. **2023**, 25, ○
- 419 Revealing the Pore Size-Dependent Sorption Mechanism of Toluene and Cetane in Porous Carbon by Nuclear Magnetic Resonance. **2023**, 57, 5003-5012 ○
- 418 Stereochemistry of the Reactions between Palladacycle Complexes and Primary Alkyl Iodides. **2023**, 42, 606-614 ○
- 417 Pure Silica with Ordered Silanols for Propylene/Propane Adsorptive Separation Unraveled by Three-Dimensional Electron Diffraction. **2023**, 145, 6853-6860 ○
- 416 The Electronic Nature of Cationic Group 10 Ylidyne Complexes. **2023**, 11, 129 1
- 415 Cooperative Ternary Assemblies Involving Anion-π-Anion Assemblies and Unconventional Cl⁻/Cl Interactions in Cu(II) Coordination Compounds: Experimental and Theoretical Studies. **2023**, 13, 517 ○
- 414 Solution Structures of Europium Terpyridyl Complexes with Nitrate and Triflate Counterions in Acetonitrile. **2023**, 62, 5207-5218 ○
- 413 Stereoretentive Formation of Cyclobutanes from Pyrrolidines: Lessons Learned from DFT Studies of the Reaction Mechanism. **2023**, 88, 4619-4626 ○

- 412 Stereospecific Nickel-Catalyzed Cross-Electrophile Coupling Reaction of Alkyl Mesylates and Allylic Difluorides to Access Enantioenriched Vinyl Fluoride-Substituted Cyclopropanes. **2023**, 13, 4488-4499 ○
- 411 Catalyst-Substrate Helical Character Matching Determines the Enantioselectivity in the Ishihara-Type Iodoarenes Catalyzed Asymmetric Kita-Deaeromative Spirolactonization. **2023**, 145, 7301-7312 ○
- 410 Gold(i)-containing light-emitting molecules with an inverted singlet-triplet gap. **2023**, 14, 3873-3880 ○
- 409 Engineering Catalytically Active Sites by Sculpting Artificial Edges on MoS₂ Basal Plane for Dinitrogen Reduction at a Low Overpotential. 2206357 ○
- 408 Tuning anticancer properties and DNA-binding of Pt(II) complexes via alteration of nitrogen softness/basicity of tridentate ligands. **2023**, 13, 9333-9346 ○
- 407 Engineering of a P450-based Kemp eliminase with a new mechanism. **2023**, 47, 191-199 ○
- 406 Revealing the evolution of doping anions and their impact on K-Ion storage: A case study of Se-doped In₂S₃. **2023**, 58, 165-175 ○
- 405 A DFT Study of Ruthenium fcc Nano-Dots: Size-Dependent Induced Magnetic Moments. **2023**, 13, 1118 ○
- 404 Activating photocatalytic hydrogen evolution by constructing Ni-based organic layers and tailoring its crystal facets. ○
- 403 The Ability of CO₂ Capture on Transition Metal-modified 1T'-MoS₂ Monolayers Controlled by an Electric Field. ○
- 402 First-principles study of square chalcogen bond interactions and its adsorption behavior on silver surface. **2023**, 25, 10836-10844 ○
- 401 Computational Study of the Adsorption of Small Gas Molecules on Pillar[5]arenes. **2023**, 8, ○
- 400 Study of the Reaction Mechanism of Triazines and Associated Species for H₂S Scavenging. **2023**, 8, 12165-12172 ○
- 399 Ab Initio Study of the Electronic Structure and Lattice Dynamics of Scheelite Type AgTcO₄. ○
- 398 Water Splitting on a Pt₁/C₃N₄ Single Atom Catalyst: A Modeling Approach. ○
- 397 Ti₃C₂T_x MXene van der Waals Gate Contact for GaN High Electron Mobility Transistors. ○
- 396 Stable Sulfuric Vapor Transport and Liquid Sulfur Growth on Transition Metal Dichalcogenides. **2023**, 23, 2287-2294 ○
- 395 Relationship between the Surface Reconstruction of Nickel Phosphides and Their Activity toward the Hydrogen Evolution Reaction. **2023**, 13, 4611-4621 ○

- 394 Phosphorous/Fluorine Co-doped Biomass-derived Carbon for Enhanced Sodium-ion and Lithium-ion Storage. ○
- 393 How the Conformational Movement of the Substrate Drives the Regioselective C-N Bond Formation in P450 TleB: Insights from Molecular Dynamics Simulations and Quantum Mechanical/Molecular Mechanical Calculations. **2023**, 145, 7252-7267 ○
- 392 Theoretical insights into the epitaxial growth of black arsenene enabled on GeS(001). **2023**, 35, 244001 ○
- 391 Crystal structures of two phases of Pigment Yellow 110 from X-ray powder diffraction data. **2023**, ○
- 390 New Insights into the Nature of Ti(II) and Ti(III) Active Sites in the Heterogeneous Ziegler-Natta Catalyst. **2023**, 127, 5720-5730 ○
- 389 Effect of Linker Structure and Functionalization on Secondary Gas Formation in Metal-Organic Frameworks. **2023**, 127, 2881-2888 ○
- 388 Molten salt induced formation of chitosan based carbon nanosheets decorated with CoNx for boosting rechargeable Zn-air batteries. **2023**, 641, 842-852 ○
- 387 Magnetic optimization and regulation mechanism of La₂CoMnO₆ double-perovskite ceramics by Ti-doping at Mn-site. **2023**, ○
- 386 Computational Study on Ni-Al Bimetal-Catalyzed Twofold C-H Annulation Reaction: Mechanism, Origin of Selectivity, and Role of SPO Ligand. ○
- 385 Precise electronic structure modulation on MXene-based single atom catalysts for high-performance electrocatalytic CO₂ reduction reaction: A first-principle study. **2023**, 642, 273-282 ○
- 384 Single crystal synthesis and low-lying electronic structure of V₃S₄. **2023**, 949, 169776 ○
- 383 A bipolar porphyrin molecule for stable dual-ion symmetric batteries with high potential. **2023**, 59, 4962-4965 ○
- 382 Ab Initio Dynamics of Graphene and Graphyne Electrodes in Vacuum and in the Presence of Electrolytes. **2023**, 127, 6515-6523 ○
- 381 Selective Self-Assembly and Modification of Herringbone Reconstructions at a Solid-Liquid Interface of Au(111). **2023**, 14, 3057-3062 ○
- 380 Synthesis of an aqueous, air-stable, superconducting 1T'-WS₂ monolayer ink. **2023**, 9, ○
- 379 Towards high-performance polyurethanes: a mechanism of amine catalyzed aromatic imide formation from the reaction of isocyanates with anhydrides. **2023**, 14, 1773-1780 ○
- 378 Van Der Waals Metal Contacts for Electronic and Optoelectronic Devices. ○
- 377 A Buckycatcher in Solution: A Computational Perspective. **2023**, 28, 2841 ○

- 376 Low-temperature crystal structures of the solvent dimethyl carbonate. 1-12 ○
- 375 Ru-Catalyzed Hydrogenolysis of Methanol: A Computational and Kinetics Study. ○
- 374 Understanding Primary Charge Separation in the Heliobacterial Reaction Center. **2023**, 14, 3092-3102 ○
- 373 Selective Ethylene Glycol Oxidation to Formate on Nickel Selenide with Simultaneous Evolution of Hydrogen. 2300841 ○
- 372 Structure, Properties, and Reactivity of Polyoxocationic Zirconium and Hafnium Clusters: A Computational Investigation. **2023**, 62, 5081-5087 ○
- 371 Growth of single-crystal black phosphorus and its alloy films through sustained feedstock release. ○
- 370 Evaluation of DFT+U and HSE Frameworks for Strongly Correlated Iron Oxide. **2023**, 8, ○
- 369 Tuning the odd-even effect on two-dimensional assemblies of curcumin derivatives by alkyl chain substitution: a scanning tunnelling microscopy study. **2023**, 25, 10917-10924 ○
- 368 Enhanced Solid-State Fluorescence of Flavin Derivatives by Incorporation in the Metal-Organic Frameworks MIL-53(Al) and MOF-5. **2023**, 28, 2877 ○
- 367 Phase Transition Kinetics of MAPbI₃ for Tetragonal-to-Orthorhombic Evolution. ○
- 366 Heteronuclear Trimetallic MFe₂ and M₂Fe (M=V, Nb, and Ta) Clusters for Dinitrogen Activation. ○
- 365 Layer-by-layer disentanglement of Bloch states. ○
- 364 Benzothieniodolium Cations Doubly Bonded to Anions via Halogen-Chalcogen and Halogen-Hydrogen Supramolecular Synthons. **2023**, 23, 2661-2674 ○
- 363 Self-assembly of s-indacene-tetrone on Cu(111): molecular trapping and patterning of Cu adatoms. **2023**, 25, 10591-10598 ○
- 362 Chemical Adsorption of HF, HCl, and H₂O onto YF₃ and Isostructural HoF₃ Surfaces by First Principles. **2023**, 13, 555 ○
- 361 MOF-Derived Highly Active Co-N-C Hybrid Arrays for Efficient Hydrogen Evolution Reaction. ○
- 360 The critical role of ultra-low-energy vibrations in the relaxation dynamics of molecular qubits. **2023**, 14, ○
- 359 Insights into the Three-Component Coupling Reactions of Aldehydes, Alkynes, and Amines Catalyzed by N-heterocyclic Carbene Silver: A DFT Study. **2023**, 13, 646 ○

- 358 Electric-field induced entropic effects in liquid water. ○
- 357 Role of Non-Covalent Interactions in Carbonic Anhydrase III Topiramate Complex Based on QM/MM Approach. **2023**, 16, 479 ○
- 356 Valleytronics Candidate with Spontaneous Valley Polarization in A-Type Antiferromagnetic MoSi₂N₄/MnPS₃ Heterostructure. ○
- 355 Superconductivity and charge density wave in transition metal chalcogenides: A first principle study. **2023**, 151, 115714 ○
- 354 In situ composition of Thienothiophene-based covalent organic framework on carbon nanotube as a host for high performance Li-S batteries. **2023**, ○
- 353 A novel phthalocyanine based discotic liquid crystal for efficient corrosion inhibition of mild steel. 1-9 ○
- 352 Metal Atoms Participate in the Self-Assembly and On-Surface Reaction Behaviors of 1,4-DBN on Ag(111) Surface. ○
- 351 Diazene Chemistry: Metal-Free Models of N₂ Reduction Intermediates. **2023**, 145, 7101-7106 ○
- 350 Molecular insight into the GaP(110)Water interface using machine learning accelerated molecular dynamics. **2023**, ○
- 349 Tuning the Dual Active Sites of Functionalized UiO-66 for Selective Adsorption of Yb(III). **2023**, 15, 17233-17244 ○
- 348 Structure and thermodynamic properties of adducts based on cucurbit[6]uril and Fe(III)/Fe(II) aqua complexes: A DFT examination. ○
- 347 Unraveling the Role of Orbital Interaction in the Electrochemical HER of the Trimetallic AgAuCu Nanobowl Catalyst. **2023**, 14, 3146-3151 ○
- 346 Passivating Oxygen Evolution Activity of NiFe-LDH through Heterostructure Engineering to Realize High-Efficiency Electrocatalytic Formate and Hydrogen Co-Production. ○
- 345 Modulation of oxygen-etching for generating nickel single atoms for efficient electroreduction of CO₂ to syngas (CO/H₂). **2023**, 421, 332-341 ○
- 344 Turn Waste Into Wealth: MoO₂@coal Gangue Electrocatalyst with Amorphous/Crystalline Heterostructure for Efficient Li⁺ Batteries. ○
- 343 First-principles study on the optoelectronic properties of the quasi-one-dimensional flexible semiconductor K₂PdPS₄I. **2023**, 47, 106396 ○
- 342 Role of molecular modelling in the development of metal-organic framework for gas adsorption applications. **2023**, 135, ○
- 341 Triplet Separation after the Fastest Intramolecular Singlet Fission in the Smallest Chromophore. **2023**, 19, 2092-2101 ○

- 340 The importance of the image forces and dielectric environment in modeling contacts to two-dimensional materials. **2023**, 7, ○
- 339 High-throughput manufacturing of epitaxial membranes from a single wafer by 2D materials-based layer transfer process. ○
- 338 Comprehensive exploration of graphically defined reaction spaces. **2023**, 10, ○
- 337 Single Selenium Atomic Vacancy Enabled Efficient Visible-Light-Response Photocatalytic NO Reduction to NH₃ on Janus WSSe Monolayer. **2023**, 28, 2959 ○
- 336 High-Activity Fe₃C as pH-Universal Electrocatalyst for Boosting Oxygen Reduction Reaction and Zinc-Air Battery. ○
- 335 Competitive Trapping of Single Atoms onto a Metal Carbide Surface. **2023**, 17, 6955-6965 ○
- 334 Defect-Engineered 3D Nanostructured MoS₂ for Detection of Ammonia Gas at Room Temperature. **2023**, 6, 5284-5297 ○
- 333 Bright Asymmetric Shielding Strategy-Based NIR-II Probes for Angiography and Localized Photothermal Therapy. **2023**, 6, 1639-1649 ○
- 332 Approach of Electronic Structure Calculations to Crystal. **2023**, 209-255 ○
- 331 Molecular engineering of naphthalene spacers in low-dimensional perovskites. **2023**, 11, 5024-5031 ○
- 330 Structural Sampling and Solvation Models for the Simulation of Electronic Spectra: Pyrazine as a Case Study. ○
- 329 Polarization Modulation on Charge Transfer and Band Structures of GaN/MoS₂ Polar Heterojunctions. **2023**, 13, 563 ○
- 328 Signatures of Electric Field and Layer Separation Effects on the Spin-Valley Physics of MoSe₂/WSe₂ Heterobilayers: From Energy Bands to Dipolar Excitons. **2023**, 13, 1187 ○
- 327 CO and CO₂ adsorption mechanism in Fe(pz)[Pt(CN)₄] probed by neutron scattering and density-functional theory calculations. ○
- 326 Mechanistic Insights Into the Rhodium-Catalyzed C₆₀ Alkenylation/Directing Group Migration and [3+2] Annulation: A DFT Study. **2023**, 88, 4494-4503 ○
- 325 Electrolyte Solvation Structure Manipulation and Synthetic Optimization for Enhanced Potassium Storage of Tin Phosphide/Carbon Alloy-Based Electrode. **2023**, 13, 658 ○
- 324 Step-guided epitaxial growth of blue phosphorene on vicinal Ag(111). **2023**, 7, ○
- 323 Ligand Control in Co-Catalyzed Regio- and Enantioselective Hydroboration: Homoallyl Secondary Boronates via Uncommon 4,3-Hydroboration of 1,3-Dienes. **2023**, 145, 7462-7481 ○

- 322 Thermochemistry and Kinetics of the OH- and Cl-Initiated Degradation Pathways of the HCFC-132b Atmospheric Pollutant. **2023**, 7, 892-900 ○
- 321 Integrating surface and interface engineering to improve optoelectronic performance and environmental stability of MXene-based heterojunction towards broadband photodetection. ○
- 320 Diserinol Isophthalamide: A Novel Reagent for Complexation with Biomolecular Anions in Electro spray Ionization Mass Spectrometry. **2023**, 34, 745-753 ○
- 319 Stimulating the Intrinsic Activities of the MoS₂ Nanosheet Coated on S,N-Graphene for Efficient Membrane Electrofiltration. ○
- 318 Screening Efficient Tandem Organic Solar Cells with Machine Learning and Genetic Algorithms. **2023**, 127, 6179-6191 ○
- 317 Two-dimensional C₆X (X = P₂, N₂, NP) with ultra-wide bandgap and high carrier mobility. **2023**, 10, 045602 ○
- 316 Planar Four-Membered Diboron Actinide Compound with Double M \bar{B} ius Aromaticity. **2023**, 145, 8107-8113 ○
- 315 Zr₃C₂O₂ MXene as promising candidate for NH₃ sensor with high sensitivity and selectivity at room temperature. **2023**, 624, 157125 ○
- 314 The Quantum Chemical Cluster Approach in Biocatalysis. **2023**, 56, 938-947 ○
- 313 First-principles investigation of a type-II BP/Sc₂CF₂ van der Waals heterostructure for photovoltaic solar cells. ○
- 312 Roles of the Zinc Ion and Water Molecule in the Active Site of the Copper-Zinc SOD Catalyst. **2023**, 55-59 ○
- 311 Exploration of Photocatalytic Overall Water Splitting Mechanisms in the Z-Scheme SnS₂/As Heterostructure. **2023**, 127, 6347-6355 ○
- 310 Preferential Crystallization of tert-Butyl-calix[6]arene Chlorobenzene Solvate from a Solvent Mixture. ○
- 309 Improved Elastic Image Pair Method for Finding Transition States. ○
- 308 Analysis of intermolecular interactions of n-perfluoroalkanes with circumcoronene using dispersion-corrected DFT calculations: comparison with those of n-alkanes. ○
- 307 Infrared action spectroscopy of the deprotonated formic acid trimer, trapped in helium nanodroplets. **2023**, 25, 10907-10916 ○
- 306 A combined BET and IQABEG study of the activation energy of non-polar zw-type [3+2] cycloaddition reactions. **2023**, 25, 10853-10865 ○
- 305 Cu₂C(O) Interfaces Deliver Remarkable Selectivity and Stability for CO₂ Reduction to C₂₊ Products at Industrial Current Density of 500 mA cm⁻². ○

- 304 Diverse Biological Activity of Benzofuroxan/Sterically Hindered Phenols Hybrids. **2023**, 16, 499 ○
- 303 Aluminum-based metal-organic framework support metal(II)-hydride as catalyst for the hydrogenation of carbon dioxide to formic acid: A computational study. **2023**, 541, 113116 ○
- 302 A density functional theory insight into the extraction mechanism of lithium recovery from alkaline brine by diketones. ○
- 301 Fractional Charge Density Functional Theory and Its Application to the Electro-inductive Effect. **2023**, 14, 3329-3334 ○
- 300 Enantioselective electrochemical cobalt-catalyzed aryl C-H activation reactions. **2023**, 379, 1036-1042 ○
- 299 Controlling the Binding Efficiency of Surface Confined Antibodies through the Design of Mixed Self-Assembled Monolayers. ○
- 298 Toward a Combined Molecular Dynamics and Quantum Mechanical Approach to Understanding Solvent Effects on Chemical Processes in the Pharmaceutical Industry: The Case of a Lewis Acid-Mediated S_NAr Reaction. **2023**, 27, 742-754 ○
- 297 Ammonia free catalytic reduction of nitric oxide on Ni-embedded graphene nanostructure: A density functional theory investigation. **2023**, 541, 113119 ○
- 296 Vertical Stress Induced Anomalous Spectral Shift of 13.17° Moiré Superlattice in Twist Bilayer Graphene. **2023**, 28, 3015 ○
- 295 Tuning the magnetic interactions in van der Waals Fe₃GeTe₂ heterostructures: A comparative study of ab initio methods. **2023**, 107, ○
- 294 The effects of the lattice modulation on the intermolecular motions of the MA cations of the tetragonal MAPbI₃ phase. ○
- 293 Two-dimensional rare-earth Janus 2H_{1-x}Y_x(X,Y=Cl,Br,I). **2023**, 107, ○
- 292 Pressure-Induced Structural Phase Transition and Enhanced Interlayer Coupling in Two-Dimensional Ferromagnet CrSiTe₃. **2023**, 14, 3320-3328 ○
- 291 Computational investigation of dimethoate and cyclodextrin inclusion complex: molecular structures, intermolecular interactions, and electronic analysis. ○
- 290 Defective PrOx for Efficient Electrochemical NO₂ to NH₃ in a Wide Potential Range. **2023**, 5, 753-761 ○
- 289 Transition metal (X = Mn, Fe, Co, Ni, Cu, Zn)-doped graphene as gas sensor for CO₂ and NO₂ detection: a molecular modeling framework by DFT perspective. **2023**, 29, ○
- 288 Understanding the Electronic Structure Basis for N₂ Binding to FeMoco: A Systematic Quantum Mechanics/Molecular Mechanics Investigation. **2023**, 62, 5357-5375 ○
- 287 Formation mechanism of trench defects in green InGaN/GaN multiple quantum wells. **2023**, 133, 123103 ○

- 286 Synthesis of imidazolium-based pentacoordinated organofluorosilicate and germanate salts. ○
- 285 The Interplay of Weakly Coordinating Anions and the Mechanical Bond: A Systematic Study of the Explicit Influence of Counterions on the Properties of (Pseudo)rotaxanes. **2023**, 28, 3077 ○
- 284 Controlled Vertical Transfer of Individual Au Atoms Using a Surface Supported Carbon Radical for Atomically Precise Manufacturing. ○
- 283 Role of Chemical Etching in the Nucleation of Nanopores in 2D MoS₂: Insights from First-Principles Calculations. **2023**, 127, 6873-6883 ○
- 282 Correlation of the spin state and catalytic property of M^{IV} single-atom catalysts in oxygen reduction reactions. ○
- 281 Noble gas (He, Ne, and Ar) solubilities in high-pressure silicate melts calculated based on deep-potential modeling. **2023**, 350, 57-68 ○
- 280 Unraveling the Molecular Mechanism of S-Nitrosation Mediated by N-Acetylmicroperoxidase-11. **2023**, 62, 5630-5643 ○
- 279 Adsorption of CO₂ on Amorphous and Crystalline Zirconia: A DFT and Experimental Study. **2023**, 127, 6998-7008 ○
- 278 Hydrophobicity Tailoring of Ferric Covalent Organic Framework/MXene Nanosheets for High-Efficiency Nitrogen Electroreduction to Ammonia. ○
- 277 Single-bonded nitrogen chain and porous nitrogen layer via Ce^{IV} compounds. ○
- 276 Metavalent Bonding in Layered Phase-Change Memory Materials. ○
- 275 Diastereoselective Synthesis of cis-2,6-Disubstituted Dihydropyran Derivatives through a Competitive Silyl-Prins Cyclization versus Alternative Reaction Pathways. **2023**, 28, 3080 ○
- 274 Rhodium-catalyzed double hydroboration of pyridine: the origin of the chemo- and regioselectivities. ○
- 273 Understanding the Effect of Single Atom Cationic Defect Sites in an Al₂O₃ (012) Surface on Altering Selenate and Sulfate Adsorption: An Ab Initio Study. **2023**, 127, 6925-6937 ○
- 272 Covalent Triazine Framework Encapsulated Ultrafine PdAu Alloy Nanoclusters as Additive-Free Catalysts for Efficient Hydrogen Production from Formic Acid. **2023**, 13, 5135-5146 ○
- 271 Controlling Hydricity of Adsorbed Catalysts with Applied Electric Fields. **2023**, 127, 6733-6743 ○
- 270 Microstructure and Thermophysical Property Prediction for Chloride Composite Phase Change Materials: A Deep Potential Molecular Dynamics Study. **2023**, 127, 6852-6860 ○
- 269 Theory of sigma bond resonance in flat boron materials. **2023**, 14, ○

- 268 Crystal growth, characterization and electronic band structure of TiSeS. **2023**, 7, ○
- 267 Bibliography. **2023**, 431-464 ○
- 266 A neural network potential with rigorous treatment of long-range dispersion. ○
- 265 Vanadium-Containing Planar Heterostructures Based on Topological Insulators. **2023**, 117, 228-233 ○
- 264 Size-Dependent Electrochemistry of Oxygenated Ti₃C₂T_x MXenes. ○
- 263 A Density Functional Study on Ethylene Trimerization and Tetramerization Using Real Sasol Cr-PNP Catalysts. **2023**, 28, 3101 ○
- 262 Efficient seawater desalination in lamellar nanochannel-based boridene filtration membrane. ○
- 261 Acceleration of Stepwise Carbon-Polygold Bonding Cleavage in Hypercoordinated Carbon-Centered Gold(I) Clusters. **2023**, 62, 6147-6154 ○
- 260 Substrate effects on spin relaxation in two-dimensional Dirac materials with strong spin-orbit coupling. **2023**, 9, ○
- 259 Copper(II)-TEMPO Interaction. ○
- 258 Noncovalent Chelation by Halogen Bonding in the Design of Metal-Containing Arrays: Assembly of Double π-Hole Donating Halolium with CuI-Containing O,O-Donors. **2023**, 62, 6128-6137 ○
- 257 Subtle hydrogen bond preference and dual Franck-Condon activity in the interesting pairing of 2-naphthol with anisole. **2023**, 25, 10427-10439 ○
- 256 Second-harmonic-generation of [(Se,Te)Cl₃]⁺[GaCl₄]⁻ with aligned ionic tetrahedra. ○
- 255 In situ engineering 3D conductive core-shell nano-networks and electronic structure of bismuth alloy nanosheets for efficient electrocatalytic CO₂ reduction. ○
- 254 A density functional theory study of Ni_x (x = 4-6) cluster impregnation effects in multi-metal (Ce, Ti) UiO-66 metal-organic frameworks. ○
- 253 First-Principles Investigation on Electronic Properties and Surface Reactions of NaTaO₃ Adsorbed with Single-Metal Atoms. **2023**, 127, 6702-6713 ○
- 252 C-P/C=O bonds assisted desolvation effect in ultra-micropores carbon for boosting Zn-ion storage capability. **2023**, 58, 332-343 ○
- 251 Interfacial assembly of binary atomic metal-N_x sites for high-performance energy devices. **2023**, 14, ○

- 250 Inhibitor and Activator: Dual Role of Subsurface Sulfide Enables Selective and Efficient Electro-Oxidation of Methanol to Formate on CuS@CuO Core-Shell Nanosheet Arrays. ○
- 249 First principles terahertz spectroscopy of molecular crystals: the crucial role of periodic boundary conditions benchmarked with experimental L-ascorbic acid spectra. ○
- 248 Importance of Dispersion in the Molecular Geometries of Mn(III) Spin-Crossover Complexes. **2023**, 127, 3072-3081 ○
- 247 Selective synthesis of butane from carbon monoxide using cascade electrolysis and thermocatalysis at ambient conditions. ○
- 246 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, ○
- 245 Enhanced adsorption capacity of tetracycline on porous graphitic biochar with an ultra-large surface area. **2023**, 13, 10397-10407 ○
- 244 Solvation Environments in Porous Ionic Liquids Determine Selectivity in CO₂ Conversion to Cyclic Carbonates. **2023**, 127, 3266-3277 ○
- 243 Molecular insights into the hydration of zwitterionic polymers. ○
- 242 A metal Lewis base activation model for Pd-catalyzed hydroamination of amines and 1,3-dienes. ○
- 241 Energy level alignments between organic and inorganic layers in 2D layered perovskites: conjugation vs. substituent. ○
- 240 Heavy atom effect through chalcogen substitution in Red Nile dye: a theoretical investigation. ○
- 239 Sulphur- and Selenium-for-Oxygen Replacement as a Strategy to Obtain Dual Type I/Type II Photosensitizers for Photodynamic Therapy. **2023**, 28, 3153 ○
- 238 Spontaneous spin and valley polarizations in a two-dimensional Cr₂S₃ monolayer. **2023**, 133, 134301 ○
- 237 Beyond steric selectivity of ions using µgstrm-scale capillaries. ○
- 236 Iminium substituent directs cyanide and hydride additions to triiron vinyliminium complexes. ○
- 235 Genuine quadruple bonds between two main-group atoms. Chemical bonding in AeF₄ (Ae = BeBa) and isoelectronic EF (E = BAl) and the particular role of d orbitals in covalent interactions of heavier alkaline-earth atoms. ○
- 234 Tailoring On-Surface Molecular Reactions and Assembly through Hydrogen-Modified Synthesis: From Triarylamine Monomer to 2D Covalent Organic Framework. ○
- 233 Promotion Effect of Well-Defined Deposited Water Layer on Carbon Monoxide Oxidation Catalyzed by Single-Atom Alloys. **2023**, 14, 3498-3505 ○

- 232 Unravelling the impact of oily alkane molecules on the optical properties of the calcite(10.4) surface. ○
- 231 Atomistic modeling of the mechanical properties: the rise of machine learning interatomic potentials. ○
- 230 Two Carbon Dioxide Molecules Consecutively Reduced by Metal-Free B₂O₂ Anions. **2023**, 127, 3082-3087 ○
- 229 Selective sorption of oxygen and nitrous oxide by an electron donor-incorporated flexible coordination network. **2023**, 6, ○
- 228 Adsorption of NO_x (x = 1, 2) Molecules on the CoFeMnSi(001) Surface: First-Principles Insights. **2023**, 8, 14005-14012 1
- 227 Influence of defects on the valley polarization properties of monolayer MoS₂ grown by chemical vapor deposition. **2023**, 107, ○
- 226 Efficient solar fuel production enabled by an iodide oxidation reaction on atomic layer deposited MoS₂. ○
- 225 Characterization of Hole States at the Zn-Doped Hematite/Water Interface from Ab Initio Simulations. **2023**, 13, 5298-5306 ○
- 224 A unique case of polymorphism in polyiodide networks resulting from the reaction of the drug methimazole and I₂. ○
- 223 Methoxy Functionalization of Phenethylammonium Ligand for Efficient Perovskite Light-Emitting Diodes. ○
- 222 Computational Protocol for the Identification of Candidates for Radioastronomical Detection and Its Application to the C₃H₃NO Family of Isomers. **2023**, 28, 3226 ○
- 221 Broad Electronic Modulation of Two-Dimensional Metal-Organic Frameworks over Four Distinct Redox States. ○
- 220 Mechanism Research on Excited-State Photoinduced Electron Transfer in a Pyrazine Derivative under an External Electric Field. **2023**, 127, 3356-3361 ○
- 219 Insights into the Fluxional Processes of Monomethylcyclohexenyl Manganese Tricarbonyl. **2023**, 28, 3232 ○
- 218 Hydrogen sharing between two nitroxyl radicals in the gas phase and other microsolvation effects on the infrared spectrum of a bulky hydroxylamine. ○
- 217 Proton Transport in Perfluorinated Ionomer Simulated by Machine-Learned Interatomic Potential. **2023**, 14, 3581-3588 ○
- 216 Novel Strategy of Machine Learning for Predicting Henry's Law Constants of CO₂ in Ionic Liquids. **2023**, 11, 6090-6099 ○
- 215 Pressure-Induced Stability of Methane Hydrate from Machine Learning Force Field Simulations. **2023**, 127, 7071-7077 ○

- 214 Chirality Effects and Semiconductor versus Metallic Nature in Halide Nanotubes. **2023**, 127, 7162-7171 ○
- 213 Selective methane oxidation by molecular iron catalysts in aqueous medium. **2023**, 616, 476-481 ○
- 212 Additivity of Diene Substituent Gibbs Free Energy Contributions for Diels-Alder Reactions between Me₂C=CMe₂ and Substituted Cyclopentadienes. **2023**, 8, 14160-14170 ○
- 211 Diiron Aminocarbonyl Complexes with NCE Ligands (E = O, S, Se). **2023**, 28, 3251 ○
- 210 Luminescent Zirconocene Complexes with Pendant Phosphine Chalcogenide Donor Groups. ○
- 209 Diffusion of O Atoms on a CO-Covered Ru(0001) Surface-A Combined High-Speed Scanning Tunneling Microscopy and Density Functional Theory Study at an Enhanced CO Coverage. **2023**, 127, 7197-7210 ○
- 208 Chemically circular, mechanically tough, and melt-processable polyhydroxyalkanoates. **2023**, 380, 64-69 1
- 207 Calculation of Excited State Internal Conversion Rate Constant Using the One-Effective Mode Marcus-Jortner-Levich Theory. ○
- 206 Insight into the effects of S-vacancy and O-doping in monolayer VS₂ as lithium-ion battery anodes from first-principles calculations. **2023**, 38, 102851 ○
- 205 Electrocatalytic reduction of CO₂ on size-selected nanoclusters of first-row transition metal nanoclusters: a comprehensive mechanistic investigation. ○
- 204 Probing Anisotropic Deformation and Near-Infrared Emission Tuning in Thin-Layered InSe Crystal under High Pressure. ○
- 203 Oxidation State Dependent Conjugation Controls Electrocatalytic Activity in a Two-Dimensional Di-Copper Metal-Organic Framework. **2023**, 127, 7299-7307 ○
- 202 Role of Non-covalent Interaction toward Conductivity in a One-Dimensional Tube-like Silver-Thiolate Structure. ○
- 201 Formation of active sites on transition metals through reaction-driven migration of surface atoms. **2023**, 380, 70-76 ○
- 200 Two-dimensional half-metallicity in transition metal atoms decorated Cr₂Ge₂Te₆. 11, ○
- 199 Separation of phenolic compounds from water by using monoterpenoid and fatty acid based hydrophobic deep eutectic solvents. **2023**, 381, 121806 ○
- 198 A Nickel-Catalyzed Cross-Electrophile Coupling Reaction of 1,3-Dimesylates for Alkylcyclopropane Synthesis: Investigation of Stereochemical Outcomes and Radical Lifetimes. **2023**, 13, 5472-5481 ○
- 197 Synergistic effect of phosphorus doping and MoS₂ co-catalysts on g-C₃N₄ photocatalysts for enhanced solar water splitting. **2023**, 158, 171-179 ○

- 196 Ultrafine Fe₂C Iron Carbide Nanoclusters Trapped in Topological Carbon Defects for Efficient Electroreduction of Carbon Dioxide. ○
- 195 Oxygen Vacancy Boosts the V₂O₅ Performance for the Electrochemical H₂O₂ Product. ○
- 194 Constructing ion diffusion highway in strongly coupled WSe₂-carbon hybrids enables superior energy storage performance. **2023**, ○
- 193 Interstitial Hydrogen Atom to Boost Intrinsic Catalytic Activity of Tungsten Oxide for Hydrogen Evolution Reaction. ○
- 192 Unconventional Self-Reconstructed Trimer-like Metal Zigzag Edge of 1T-Phase Transition Metal Dichalcogenides. **2023**, 14, 3651-3657 ○
- 191 First principles investigation of cobalt-phthalocyanine active site tuning via atomic linker immobilization for CO₂ electroreduction. **2023**, 422, 43-55 ○
- 190 DFT Study on the Mechanisms of Iron-Catalyzed Ortho C-H Homoallylation of Aromatic Ketones with Methylenecyclopropanes. ○
- 189 High Strength Titanium with Fibrous Grain for Advanced Bone Regeneration. ○
- 188 Design of a minimal di-nickel hydrogenase peptide. **2023**, 9, ○
- 187 Insertion of MXene-Based Materials into CuPd 3D Aerogels for Electroreduction of CO₂ to Formate. ○
- 186 A customized MOF-polymer composite for rapid gold extraction from water matrices. **2023**, 9, ○
- 185 Performance of Common Density Functionals for Excited States of Tetraphenyldibenzoperiflanthene. **2023**, 127, 3265-3273 ○
- 184 High-Performance Quasi-Solid-State Lithium-Sulfur Battery with a Controllably Solidified Cathode/Electrolyte Interface. **2023**, 15, 19066-19074 ○
- 183 Active site recovery and N-N bond breakage during hydrazine oxidation boosting the electrochemical hydrogen production. **2023**, 14, ○
- 182 Modulating the Proton-Conducting Lanes in Spinel ZnMn₂O₄ through Off-Stoichiometry. ○
- 181 The Potential Role of Lewis Acid/Base Adducts in Enhancing Stereoselectivity in Ziegler-Natta Catalysts: A DFT Study. **2023**, 127, 7220-7229 ○
- 180 SF₆ Degradation in a γ-Al₂O₃ Packed DBD System: Effects of Hydration, Reactive Gases and Plasma-Induced Surface Charges. **2023**, 43, 635-656 ○
- 179 Nucleobases adsorption studies on chair graphane nanosheets: A DFT outlook. **2023**, 152, 110683 ○

- 178 Reversible hydrogen storage tendency of light-metal (Li/Na/K) decorated carbon nitride (C₉N₄) monolayer. **2023**, ○
- 177 First-principles study on the electronic structure and photocatalytic property of a novel two-dimensional ZrS₂/InSe heterojunction. **2023**, 13, 11150-11159 ○
- 176 An investigation for H₂/N₂ adsorptive separation in SIFSIX-2-Cu-i. **2023**, ○
- 175 Competing excitation paths in luminescent heterobimetallic Ln-Al complexes: Unraveling interactions via experimental and theoretical investigations. **2023**, 26, 106614 ○
- 174 Defect engineering mediated molecules coordination activation for one-pot synthesis of secondary amine over Bi₂MoO₆ hierarchical microspheres. **2023**, 275, 118747 ○
- 173 Elucidating the Role of Contact-Induced Gap States and Passivation Molecules at Perovskite/Metal Contacts. ○
- 172 Ammonia versus Water Elimination in the Reaction of Diols with Urea under Metal Oxide Catalysis. **2023**, 13, 5643-5655 ○
- 171 MOF-derived Co/Fe@NPC-500 with large amounts of low-valent metals as an electro-Fenton cathode for efficient degradation of ceftazidime. **2023**, 333, 122755 ○
- 170 Polaron-assisted nonadiabatic dynamics in protonated TiO₂ with surface water molecule. **2023**, ○
- 169 Structure and Reactivity of the Ionic Liquid [C₁C₁Im][Tf₂N] on Cu(111). ○
- 168 Iron(II) Complexes with Porphyrin and Tetrabenzoporphyrin: CASSCF/MCQDPT2 Study of the Electronic Structures and UV-Vis Spectra by sTD-DFT. **2023**, 24, 7070 ○
- 167 Type-II MoSi₂N₄/MoS₂ van der Waals Heterostructure with Excellent Optoelectronic Performance and Tunable Electronic Properties. ○
- 166 First-principles study of electronic and optical properties of novel 2D TiOS monolayer and bilayer. Dimensionality reduction opens up a band gap in TiOS. **2023**, 48, 106438 ○
- 165 Insights into the excited state hydrogen bond and proton transfer behaviors associated with solvent polarity for NHBQ fluorophore: a theoretical study. **2023**, 142, ○
- 164 Tunable hydrogen evolution activity of black antimony phosphorus monolayers via strain engineering: a first-principles calculation. **2023**, 129, ○
- 163 First-principles calculations of SnCo as potential anode materials for high-performance lithium-ion batteries and beyond. **2023**, 142, ○
- 162 Anharmonic Correction to Free Energy Barriers from DFT-Based Molecular Dynamics Using Constrained Thermodynamic Integration. ○
- 161 Dehydration of a crystal hydrate at subglacial temperatures. **2023**, 616, 288-292 ○

- 160 Reactivity Factors in Catalytic Methanogenesis and Their Tuning upon Coenzyme F430 Biosynthesis. ○
- 159 Surface Control Behavior toward Crystal Regulation and Anticorrosion Capacity for Zinc Metal Anodes. ○
- 158 Exploring the Charge Density Wave Phase of $1T\bar{1}TaSe_2$: Mott or Charge-Transfer Gap?. **2023**, 130, ○
- 157 Understanding Li interaction in TiO_2 /graphene composites for high-performance Li-ion battery anodes: A first principles study. **2023**, 660, 414878 ○
- 156 Active learning strategies for atomic cluster expansion models. **2023**, 7, ○
- 155 Conjugation of a Silver-Based Coordination Polymer with Curcumin: A New Case of an Inorganic Polymeric Co-crystal. ○
- 154 A conserved hymenopteran-specific family of cytochrome P450s protects bee pollinators from toxic nectar alkaloids. **2023**, 9, ○
- 153 Understanding the kinetics and atmospheric degradation mechanism of Chlorotrifluoroethylene ($CF_2=CFCl$) initiated by OH radicals. ○
- 152 An Expedited Route to Optical and Electronic Properties at Finite Temperature via Unsupervised Learning. **2023**, 28, 3411 ○
- 151 Stacks of Equidistant 5,6-Dichloro-2,3-dicyanosemiquinone (DDQ) Radicals under Variable-Temperature and High-Pressure Conditions. ○
- 150 Theoretical investigation on NO reduction electro-catalyzed by transition-metal-anchored SnOSe nanotubes. ○
- 149 Accurate Structures and Spectroscopic Parameters of Phenylalanine and Tyrosine in the Gas Phase: A Joint Venture of DFT and Composite Wave-Function Methods. ○
- 148 Impact of organic/inorganic wavefunction delocalization on the electronic and optical properties of one-dimensional hybrid perovskites. ○
- 147 Ultrafast formation of exciplex species in dicyanoanthracene ZSM-5 revealed by transient emission and vibrational spectroscopy. ○
- 146 Spectroscopic Investigation of the Metal Coordination of the Aromatic Amino Acids with Zinc and Cadmium. ○
- 145 The Microwave Rotational Electric Resonance (RER) Spectrum of Benzothiazole. **2023**, 28, 3419 ○
- 144 Peripheral Coordination-Dependent Descriptor for Selective Interactions between Near-Frontier Molecular Orbitals and Single-Atom Catalysts. ○
- 143 Condensation and asymmetric amplification of chirality in achiral molecules adsorbed on an achiral surface. **2023**, 14, ○

- 142 Peroxo-Diiron(III/III) as the Reactive Intermediate for N-Hydroxylation Reactions in the Multidomain Metalloenzyme SznF: Evidence from Molecular Dynamics and Quantum Mechanical/Molecular Mechanical Calculations. 5808-5818 ○
- 141 Dielectric Saturation in Water from a Long-Range Machine Learning Model. ○
- 140 COSMO-RS Exploration of Highly CO₂-Selective Hydrogen-Bonded Binary Liquid Absorbents under Humid Conditions: Role of Trace Ionic Species. ○
- 139 Tc doping in V₂O₅ as an Li-ion battery cathode to enhance the electrochemical performance: A first-principles study. ○
- 138 Theoretical Study on the Interaction between Cis-2 Bis(benzofuro) [60]fullerene Derivative and NO Dominated Double Gas Molecule. **2023**, ○
- 137 Theoretical Study on Origin of CVD Growth Direction Difference in Graphene/hBN Heterostructures. **2023**, ○
- 136 Spectroscopical and Molecular Studies of Four Manganese(I) PhotoCORMs with Bioinspired Ligands Containing Non-Coordinated Phenol Groups. **2023**, 28, 3439 ○
- 135 Mechanism of metalated pyrrole-singlet oxygen chemiluminescent reaction. **2023**, 238, 116421 ○
- 134 Rhenium(V) Tris(pyrazolyl)borate Complexes as Ligands in Square Planar Palladium and Platinum Complexes. **2023**, 49, 33-40 ○
- 133 MIL-101(Fe) MetalOrganic Framework Nanoparticles Functionalized with Amino Groups for Cr(VI) Capture. ○
- 132 Ethylene Hydrogenation Molecular Mechanism on MoCy Nanoparticles. ○
- 131 On the coexistence of ferroelectric and antiferroelectric polymorphs in NaNbO₃ fibers at room temperature. ○
- 130 Ferroelectric order in hybrid organic-inorganic perovskite NH₄PbI₃ with non-polar molecules and small tolerance factor. **2023**, 9, ○
- 129 Designing dithiolene and bis(iminothiolato)-based 1D metal-organic-frameworks for electrocatalytic hydrogen evolution reaction. **2023**, 142, ○
- 128 Non-covalent interactions in polymorphs of urea under pressure. **2023**, 142, ○
- 127 Steric Effects on the Chelation of Mn²⁺ and Zn²⁺ by Hexadentate Polyimidazole Ligands: Modeling Metal Binding by Calprotectin Site 2. ○
- 126 Cobalt and Iron Phthalocyanine Derivatives: Effect of Substituents on the Structure of Thin Films and Their Sensor Response to Nitric Oxide. **2023**, 13, 484 ○
- 125 On the Dynamic Behavior of Pacman Phosphanes-A Case of Cooperativity and Redox Isomerism. ○

- 124 Adjustment of the single atom/nanoparticle ratio in Pd/CNT catalysts for phenylacetylene selective hydrogenation. ○
- 123 Promising M₂CO₂/MoX₂ (M = Hf, Zr; X = S, Se, Te) Heterostructures for Multifunctional Solar Energy Applications. **2023**, 28, 3525 ○
- 122 Clay-supported acidic ionic liquid as an efficient catalyst for conversion of carbohydrates to 5-hydroxymethylfurfural. **2023**, 121847 ○
- 121 The Impact of the Solvent Dielectric Constant on A⁻-NH₃ Dative Bond Depends on the Nature of the Lewis Electron-Pair Systems. ○
- 120 Halide Perovskite glues activate two-dimensional covalent organic framework crystallites for selective NO₂ sensing. **2023**, 14, ○
- 119 Snapshots of sequential polyphosphide rearrangement upon metallatetrylene addition. ○
- 118 Nanosecond Laser Confined Bismuth Moiety with Tunable Structures on Graphene for Carbon Dioxide Reduction. ○
- 117 Enantiodivergent Photochemical Rearrangements Due to Different Coordination Modes at an Oxazaborolidine Lewis Acid Catalyst. 5896-5905 ○
- 116 Catalytic production of ammonia from dinitrogen employing molybdenum complexes bearing N-heterocyclic carbene-based PCP-type pincer ligands. ○
- 115 Synergy of Small Antiviral Molecules on a Black-Phosphorus Nanocarrier: Machine Learning and Quantum Chemical Simulation Insights. **2023**, 28, 3521 ○
- 114 Enhanced Photoassisted Li-O₂ Battery with Ce-UiO-66 Metal-Organic Framework Based Photocathodes. ○
- 113 A molecular understanding of citrate adsorption on calcium oxalate polyhydrates. ○
- 112 Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins. **2023**, 28, 3487 ○
- 111 Does a Machine-Learned Potential Perform Better Than an Optimally Tuned Traditional Force Field? A Case Study on Fluorohydrins. ○
- 110 Highly Selective Electrochemical Reduction of CO₂ into Methane on Nanotwinned Cu. ○
- 109 A DFT Study on the Conformation, Properties of the Excited States, and Excimer's Formation of Tetraphenylcyclotetrasiloxane. **2023**, 8, ○
- 108 A Deep Neural Network Potential to Study the Thermal Conductivity of MnBi₂Te₄ and Bi₂Te₃/MnBi₂Te₄ Superlattice. ○
- 107 Superior hydrogen storage capacity of Vanadium decorated biphenylene (Bi+V): A DFT study. **2023**, ○

- 106 Spin-Forbidden Addition of Molecular Oxygen to Stable Enol Intermediates
Decarboxylation of 2-Methyl-1-tetralone-2-carboxylic Acid. **2023**, 24, 7424 ○
- 105 Oxygen vacancies-enriched Fe-Cu bimetallic minerals-based magnetic biochar activated peroxydisulfate for durable sulfonamides degradation: pH-dependence adsorption and singlet oxygen evolution mechanism. **2023**, 317, 123866 ○
- 104 Janus structures of the C_{2h} polymorph of gallium monochalcogenides: first-principles examination of Ga₂XY (X/Y = S, Se, Te) monolayers. **2023**, 13, 12153-12160 ○
- 103 Drastic influence of substituent position on orientation of 2D layers enables efficient and stable 3D/2D perovskite solar cells. **2023**, 101380 ○
- 102 Multifunctional solvent molecule design enables high-voltage Li-ion batteries. **2023**, 14, ○
- 101 Spectroscopic visualization and phase manipulation of chiral charge density waves in 1T-TaS₂. **2023**, 14, ○
- 100 Reactivity of frustrated Lewis pairs with BOC protected diazocarboxylates: FLP capture of diazene. ○
- 99 Metallocene-Naphthalimide Derivatives: The Effect of Geometry, DFT Methodology, and Transition Metals on Absorption Spectra. **2023**, 28, 3565 ○
- 98 Enabling Molecular-Level Computational Description of Redox and Proton-Coupled Electron Transfer Reactions of Samarium Diiodide. ○
- 97 Copper lattice tension boosts full-cell CO electrolysis to multi-carbon olefins and oxygenates. **2023**, ○
- 96 Adsorption, activation, and conversion of carbon dioxide on small copper-tin nanoclusters. ○
- 95 Thermochemistry of the Smallest Hyperbolic Paraboloid Hydrocarbon: A High-Level Quantum Chemical Perspective. **2023**, 9, 41 ○
- 94 Dichotomy of Delocalization/Localization and Charge-Shift Bonding in Germanazene and Its Heavier Group 14 Analogues: A Valence Bond Study. ○
- 93 Rational Control of Near-Infrared Colloidal Thick-Shell Eco-Friendly Quantum Dots for Solar Energy Conversion. ○
- 92 In-Plane Anomalous Hall Effect in PT -Symmetric Antiferromagnetic Materials. **2023**, 130, ○
- 91 Computational Study on a Transfer Hydrogenation Catalysed by a Ru(II) Bis-Pyrazolyl Pyridine Complex. ○
- 90 Concerted Proton-Coupled Electron Transfer to a Graphite Adsorbed Metalloporphyrin Occurs by Band to Bond Electron Redistribution. ○
- 89 Synergetic C-H bond activation and C-D formation on CuO_x facilitates facile conversion of methane to methanol. **2023**, 627, 157283 ○

- 88 Highly efficient hydrogen production from methanol by single nickel atoms anchored on defective boron nitride nanosheet. ○
- 87 Strategies for the Design of PEDOT Analogues Unraveled: the Use of Chalcogen Bonds and π Holes. ○
- 86 Base-Triggered Oxidative Addition to Gold. ○
- 85 Tunable Schottky contacts in graphene/XAu₄Y (X, Y = Se, Te) heterostructures. ○
- 84 Halogen bonding: a designer strategy for graphyne-like two-dimensional architectures. **2023**, 142, ○
- 83 Structure phase engineering strategy through acetic acid coupling to boost hydrogen evolution reaction performance of 2H phase MoS₂ at wide pH range. **2023**, 347, 128428 ○
- 82 New organotin(IV) complexes derived from 1-adamantanethiol: synthesis, crystal structure, DFT calculation, and in vitro antifungal activity and cytotoxicity. ○
- 81 Ruthenium-doped boron nitride nanotubes as promising electrocatalysts for carbon dioxide reduction to methane. **2023**, 109942 ○
- 80 Catalytic Dehydrogenative (3 + 2) Cycloaddition of Alkylbenzenes via π Coordination. ○
- 79 L-Histidine-based computation devices. **2023**, 97, ○
- 78 Regiodivergent Nucleophilic Fluorination under Hydrogen Bonding Catalysis: A Computational and Experimental Study. ○
- 77 Theoretical predication of two-dimensional ferroelectric metal X₂Y₃ monolayer and Van der Waals heterostructures. **2023**, 115739 ○
- 76 One Molecule Suffices: Spectroscopy of Yariv Reagents. **2023**, 8, ○
- 75 Adsorption characteristics of sulfonamide antibiotic molecules on carbon nanotube and the effects of environment. **2023**, 29, ○
- 74 Mechanism of Stoichiometrically Governed Titanium Oxide Brownian Tree Formation on Stepped Au(111). ○
- 73 Exploring the Interaction of Pyridine-Based Chalcones with Trinuclear Silver(I) Pyrazolate Complex. **2023**, 11, 175 ○
- 72 Sensitized Singlet Fission in Rigidly Linked Axial and Peripheral Pentacene-Subphthalocyanine Conjugates. ○
- 71 Electronic signatures of Lorentzian dynamics and charge fluctuations in lithiated graphite structures. **2023**, 14, ○

- 70 Regium Bonds Involving Nucleobases: Theoretical Study and Biological Implications. ○
- 69 Analysis of the First Ion Coordination Sphere: A Toolkit to Analyze the Coordination Sphere of Ions. ○
- 68 DFT studies of the adsorption and decomposition of dimethyl ether on copper surface. **2023**, 157310 ○
- 67 Sustainable Microplastic Remediation with Record Capacity Unleashed via Surface Engineering of Natural Fungal Mycelium Framework. ○
- 66 Tuning the reactivity of carbon surfaces with oxygen-containing functional groups. **2023**, 14, ○
- 65 Graphdiyne Supported Single-cluster Catalysts Catalyzed Electrochemical Nitrogen Reduction Reaction: A First-Principles Investigation. **2023**, 100507 ○
- 64 Construction of the Fast Potassiation Path in $Sb_x Bi_{1-x}$ @NC Anode with Ultrahigh Cycling Stability for Potassium-Ion Batteries. ○
- 63 Insights into atomic-electronegativity-controlled excited state intramolecular proton transfer behavior for the novel ONIP compound: A TDDFT study. ○
- 62 The first chrysin-based receptor for anions recognition: Experimental investigations, DFT studies and its in vitro antitumor activity. **2023**, 135637 ○
- 61 New detail insight into Halloysite structure: mechanism behind nanotubular morphology described by density functional theory and molecular dynamics supported by experiments. **2023**, 135639 ○
- 60 Theoretical study of local S coordination environment on Fe single atoms for peroxymonosulfate-based advanced oxidation processes. **2023**, 131469 ○
- 59 Activation persulfate for efficient tetrabromobisphenol A degradation via carbon-based materials: synergistic mechanism of doped N and Fe. **2023**, 131471 ○
- 58 Green β -cyclodextrin nanosponges for the efficient adsorption of light rare earth elements: cerium and lanthanum. **2023**, 143108 ○
- 57 The geometry of calix[3]pyrrole and the formation of the calix[3]pyrrole-Fluorine complex in solution. **2023**, 142, ○
- 56 The Relevance of Lithium Salt Solvate Crystals in Superconcentrated Electrolytes in Lithium Batteries. **2023**, 16, 3700 ○
- 55 Excitonic absorption signatures of twisted bilayer WSe₂ by electron energy-loss spectroscopy. **2023**, 107, ○
- 54 Fabrication of MoS₂/Bi₂S₃ heterostructure for photocatalytic degradation of Metronidazole and Cefalexin and antibacterial applications under NIR light: experimental and theoretical approach. **2023**, 129, ○
- 53 In Situ 1D Carbon Chain-Mail Catalyst Assembly for Stable Lithium-Sulfur Full Batteries. ○

- 52 Linear BeNCO and OBeNC: kinetically stable neutral Be-bearing free molecules. ○
- 51 Understanding the Hydrocracking of Polycyclic Aromatic Hydrocarbons within FAU Zeolites: Hydrogen Splitting Catalyzed by the Frustrated Lewis Pair. **2023**, 127, 8083-8095 ○
- 50 Revealing the two-dimensional electronic structure and anisotropic superconductivity in a natural van der Waals superlattice (PbSe) 1.14NbSe₂. **2023**, 7, ○
- 49 Tunable electronic and optical properties of MoTe₂/InSe heterostructure via external electric field and strain engineering. **2023**, 35, 315501 ○
- 48 Spontaneous Hybrid Nano-Domain Behavior of the Organic-Inorganic Hybrid Perovskites. ○
- 47 Room Temperature Surface Bio-Sulfurisation via Natural Sativum Annilin and Bioengineering of Nanostructured CuS/Cu₂S. **2023**, 2, ○
- 46 Multi-scale modeling of natural organic matter-heavy metal cations interactions: Aggregation and stabilization mechanisms. **2023**, 238, 120007 ○
- 45 Unveiling Root Cause of Defect Assisted Filamentation and Implication on Resistive Switching in MoS₂ Atomristor. **2023**, ○
- 44 Static and Dynamical Quantum Studies of CX₃-AlX₂ and CSiX₃-BX₂ (X = F, Cl, Br) Complexes with Hydrocyanic Acid: Unusual Behavior of Strong π -Hole at Tritel Center. **2023**, 24, 7881 ○
- 43 Physical Mechanism of Nonlinear Spectra in Triangene. **2023**, 28, 3744 ○
- 42 Combined Structural and Computational Study of the mRubyFT Fluorescent Timer Locked in Its Blue Form. **2023**, 24, 7906 ○
- 41 Pyrene-Based Polyimide Covalent Organic Framework with Temperature-Dependent Fluorescence. ○
- 40 Electrochemically stable frustrated Lewis pairs on dual-metal hydroxides for electrocatalytic CO₂ reduction. ○
- 39 ??????????AIMD ??????????. **2023**, 30, 707-720 ○
- 38 On-Surface Synthesis of a Carbon Nanoribbon Composed of 4-8-Membered Rings. **2023**, 17, 8717-8722 ○
- 37 2-Propanol interacting with Co₃O₄(001): A combined vSFS and AIMD study. **2023**, 158, ○
- 36 Computational Study of the Fe(II) and π -Ketoglutarate-Dependent Aryloxyalkanoate Dioxygenase (AAD-1) in the Degradation of the Herbicide 2,4-Dichlorophenoxyacetic Acid. **2023**, 63, 2759-2768 ○
- 35 A Rational Design of Metal-Organic Framework Nanozyme with High-Performance Copper Active Centers for Alleviating Chemical Corneal Burns. **2023**, 15, ○

- 34 Sparse tensor based nuclear gradients for periodic Hartree-Fock and low-scaling correlated wave function methods in the CP2K software package: A massively parallel and GPU accelerated implementation. **2023**, 158, ○
- 33 Bet-PyTorch: A GPU-supported implementation for machine learning atomic potentials training. **2023**, 158, ○
- 32 Bismuth Nanoplatelets: Universal Synthetic Strategy and Emerging Application for PEC-Type Photodetectors. **2023**, 100349 ○
- 31 Thermodynamics and molecular insights into anionic structural effects on toluene absorption with ionic liquids. **2023**, 276, 118817 ○
- 30 Bi3O4Br/Ti3C2 Schottky junction with enhanced active species generation for boosting visible-light photodegradation bisphenol A activity. **2023**, 318, 124001 ○
- 29 High-Throughput Screening of Heterogeneous Transition Metal Dual-Atom Catalysts by Synergistic Effect for Nitrate Reduction to Ammonia. ○
- 28 Interplay between copper redox and transfer and support acidity and topology in low temperature NH3-SCR. **2023**, 14, ○
- 27 Exploring the structure of halomethanes with xenon: An NMR and MD investigation. **2023**, 382, 122011 ○
- 26 Synergistic dual atomic sites with localized electronic modulation enable high-performance lithium-oxygen batteries. **2023**, 466, 143351 ○
- 25 Mono-nuclear ruthenium catalyst for hydrogen evolution. **2023**, ○
- 24 Infrared light utilization based on pyroelectric effect to improve the efficiency and stability of BaTiO3 for photocatalytic NO removal. **2023**, 443, 114826 ○
- 23 High-performance precious metal-free direct ammonia fuel cells endowed by Co-doped Ni4Cu1 anode catalysts. **2023**, 334, 122856 ○
- 22 Optical properties of in-plane chemically ordered i-MAX structures. **2023**, 25, 13665-13672 ○
- 21 Evolutionary adaptation from hydrolytic to oxygenolytic catalysis. ○
- 20 Role of anharmonicity in phonon-mediated superconductivity of quasi-van der Waals layered XP2 (X=As, Sb, Bi) structures: Insight from first-principles calculations. **2023**, 959, 170440 ○
- 19 Fundamental understanding of C2H4 production from C2H6 oxidation on stoichiometric IrO2(1 1 0) surface. **2023**, 631, 157456 ○
- 18 Application of T4,4,4-graphyne for anode of Na-ion battery: first principle theoretical study. 1-7 ○
- 17 Elucidation of the electrocatalytic activity origin of Fe3C species and application in the NOx full conversion to valuable ammonia. **2023**, 467, 143371 ○

- 16 Tuning electronic structures and optical properties of Ti₂CO₂ MXenes by applying stress. **2023**, 661, 414940
- 15 Cineole \square Decanoic Acid Hydrophobic Natural Deep Eutectic Solvent for Toluene Absorption. **2023**, 122036
- 14 Defect-induced atomic-level intimate interface of a hollow Ov-CeO₂/CdS photocatalyst with a Z-scheme to boost hydrogen evolution. **2023**, 646, 209-218
- 13 A rapid aroma quantification method: Colorimetric sensor-coupled multidimensional spectroscopy applied to black tea aroma. **2023**, 124622
- 12 Reconfigurable band alignment of SWSe/h-BP heterostructures for photoelectric applications.
- 11 A supramolecular self-assembly of peptide-derived compounds via 1,5-disubstituted tetrazole-based supramolecular synthons: An experimental and computational study. **2023**, 1288, 135732
- 10 Acetylene Semi-Hydrogenation on Intermetallic Ni₃In Catalysts: Ni Ensemble and Acetylene Coverage Effects from a Theoretical Analysis. 7358-7370
- 9 Insights into the carbonization mechanism of PAN-derived carbon precursor fibers and establishment of a kinetics-driven accelerated reaction template for atomistic simulation.
- 8 The mechanical, electronic and photocatalytic properties of two novel BCN monolayer.
- 7 Catalytic Reaction Mechanism of Glyoxalase II: A Quantum Mechanics/Molecular Mechanics Study.
- 6 Mechanistic Insights of Copper Catalyzed Trifluoromethyl Aziridine Opening: Regioselective and Stereospecific Aryl Grignard Addition.
- 5 A highly selective C-rhamnosyltransferase from *Viola tricolor* and insights into its mechanisms. **2023**,
- 4 Structure-Engineered Low-Cost Carbon Microbelt Hosts for Highly Robust Potassium Metal Anode.
- 3 First-principles study of SiC and GeC monolayers with adsorbed non-metal atoms. **2023**, 13, 14879-14886
- 2 A Computational Investigation into the Hydrogenation of NO on Water Ice Surfaces to Rationalize the NO:HNO:NOH Disparity in Space.
- 1 High-temperature reactivity of vanadium oxide clusters in methane activation: Vibrational degrees of freedom matter. **2023**, 158,