

BIOVIA TURBOMOLE 関連論文リスト (1/30)

No.	First author	Title	Year	Journal name	Link
1	Julia Rienmüller	Isolation of a planar π -aromatic Bi5- ring in a cobalt-based inverse-sandwich-type complex	2025	Nature Chemistry	link
2	Yuka Yasuda	Enhanced Luminance of Pentaazaphenylene - Based Delayed Fluorescence Emitters by Breaking Forbidden Transition	2025	Angewandte Chemie International Edition	link
3	Josef Tomeček	Metal-Metal Bonding in Tri-Actinide Clusters: A DFT Study of $[\text{An}_3\text{Cl}_6]_z$ ($z=1-6$) and $[\text{An}_3\text{Cl}_6\text{Cp}_3]_z$ ($z=-2,+3$; $\text{An}=\text{Ac}, \text{Th}, \text{Pa}, \text{U}, \text{Np}, \text{Pu}$)	2025	ChemPhysChem	link
4	Yusuke Hirasawa	Yatiaric acids A-C, three novel seco-serratane triterpenoids from <i>Myrica gale</i> var. <i>tomentosa</i>	2025	Journal of Natural Medicines	link
5	Annasaheb Dhawale	Multifunctional chemosensors for the simultaneous detection of copper and mercury ions: applications in test strip fabrication, spiking studies, and logic gate ...	2025	ACS omega	link
6	Adam Šrut	Analyzing spectral distributions of charge transfer character in ensembles: a case study on the reaction center of photosystem II	2025	Physical Chemistry Physics	link
7	Olga I. Kalchenko	Stability constants and DFT calculations of anionic calixarene complexes with antiretroviral drugs Tenofovir and Emtricitabine	2025	Journal of Inclusion Phenomena and Macrocyclic Chemistry	link
8	Amin Kiani	Intermolecular interaction potential maps from energy decomposition for interpreting reactivity and intermolecular interactions	2025	Physical Chemistry Physics	link

BIOVIA TURBOMOLE 関連論文リスト (2/30)

9	Kristoffer J. M. Lundgren	The Cu B site in particulate methane monooxygenase may be used to produce hydrogen peroxide	2025	Dalton Transactions	link
10	Kavya S. Keremane	Push-pull carbazole twin dyads as efficient sensitizers/co-sensitizers for DSSC application: effect of various anchoring groups on photovoltaic performance	2025	Journal of Materials Chemistry C	link
11	Seraj A. Ansari	Exploring the complexation behaviour of NpO ₂ ²⁺ with diglycolamide in ionic liquid vs. aqueous solution	2025	Dalton Transactions	link
12	Jesús Lucia-Tamudo	First principles prediction of wavelength-dependent isomerization quantum yields of a second-generation molecular nanomotor	2025	Physical Chemistry Physics	link
13	Jindřich Fanfrlík	Heats of formation on the way from B ₂ H ₆ to B ₂₀ H ₁₆ : thermochemical consequences of multicenter bonding in ab initio and DFT methods	2025	Dalton Transactions	link
14	Anton Florian Ketzler	Benchmark of Density Functional Theory in the Prediction of ¹³ C Chemical Shielding Anisotropies for Anisotropic Nuclear Magnetic Resonance-Based Structural Elucidation	2025	Journal of Chemical Theory and Computation	link
15	Alessia Giordana	Exploring coinage bonding interactions in [Au(CN) ₄] ⁻ assemblies with silver and zinc complexes: a structural and theoretical study	2025	Physical Chemistry Physics	link
16	Hallam J. M. Greene	How a toxic pollutant avoids photodegradation: Relaxation pathways of UV-excited 2, 4-dinitrophenol in aqueous solution	2025	Proceedings of the National Academy of Sciences of the United States of America	link

BIOVIA TURBOMOLE 関連論文リスト (3/30)

17	Cedric Uhlmann		A Novel Synthetic Pathway to Lanthanide Triple - Decker Complexes: Selective Expansion of a Sandwich Complex by an Insertion Reaction	2025	Angewandte International Edition	Chemie	link
18	Dávid P. Jelenfi		Molecular conductance calculations of single-molecule junctions using projection-based density functional embedding	2025	The Journal of Chemical Physics		link
19	Bramantya Bramantya		Computational insights into two-photon absorption of centrosymmetric organoboron complexes	2025	Chemical Physics Letters		link
20	Maryam Dehabadi	Haji	Predicting Reduction Potentials of Blue Copper Proteins Using Quantum Mechanical Calculations	2025	Inorganic Chemistry		link
21	Philipp Huber		Accurate and Efficient Description of Acidic Zeolites with Plane - Wave Density Functional Theory Using Range - Separated Hybrid Functionals	2025	ChemPhysChem		link
22	Susovan Bera		Synthesis, structural characterization, and DFT investigation of a mixed-valence Co (iii)/Co (ii) complex stabilized by supramolecular interactions	2025	RSC Advances		link
23	Joan Cardona		Exploring hyperfine coupling in molecular qubits	2025	Chemical Science		link
24	Harry Ramanantoanina		Molecular - Metallic Binding Characteristics of the Intermetalloid f - /p - Block Cluster [(La@In ₂ Bi ₁₁) ₂ Bi ₂] ₆	2025	Angewandte Chemie		link
25	Maryam Sadat Kiai		Experimental and DFT calculations for C/ZnO@S cathode and prelithiation Si anode for advanced sulfur-based batteries	2025	Ionics		link

BIOVIA TURBOMOLE 関連論文リスト (4/30)

26	Andrey Sinyavskiy	Bridging the gap between variational and perturbational DFT-based methods for calculating excited states	2025	Journal of Chemical Theory and Computation	link
27	Sourav Majumdar	Mechanism of the Non - Kasha Fluorescence in Pyrene	2025	Journal of Computational Chemistry	link
28	Tejendra Banana	Exploring the effect of squaraine infusion on the two-photon absorption cross-section of a few functionalized BODIPY-like systems	2025	Physical Chemistry Chemical Physics	link
29	Tiia Jacklin	Quantum-mechanical treatment of thermal effects on the structure and ¹³ C NMR shielding of buckminsterfullerene C ₆₀	2025	Physical Chemistry Chemical Physics	link
30	Iulia-Andreea Aghion	Synthesis and coordination ability of the first phosphavinyl (selenoxo) phosphorane: an electronic story	2025	RSC Advances	link
31	Irina A. Kolesnik	$n \rightarrow \pi^*$ and chalcogen bonds in azole-substituted isoindole derivatives: a combined crystallographic and computational study	2025	CrystEngComm	link
32	Xiaoli Sun	Reproducibility of QM/MM calculations for the SARS-CoV-2 main protease	2025	Journal of Chemical Theory and Computation	link
33	Qian Wang	Magnetically Induced Current-Density Susceptibility of Circum[n]coronenes	2025	The Journal of Physical Chemistry A	link
34	Jonas Braun	Stability and Ultrafast Dynamics of Luminescent Biquinoxen-Bis- σ H-Adducts	2025	Molecules	link

BIOVIA TURBOMOLE 関連論文リスト (5/30)

35	Qing-Xia Zhang	Pnictogen-Bonding Catalysis Compared with Ion Transport in Lipid Bilayer Membranes: Entering the Goldilocks Inverted Region	2025	CCS Chemistry	link
36	S. A. Katsyuba	Revisiting Tautomerism and Rotamerism of 1,2-Dyhydro-N-(2-hydroxyethyl)-4,6-dimethyl-2-oxopyrimidine (Drug Xymedon) in Aqueous and Lipophilic Media	2025	Russian Journal of General Chemistry	link
37	Samantha E. Knoth	Surface interactions and radical generation in TCD decomposition: a DFT approach	2025	Journal of Molecular Modeling	link
38	Simon Metz	Excitonic Coupling of a TADF Assistant Dopant and a Multi - Resonance TADF Emitter	2025	Advanced Optical Materials	link
39	Kavya S. Keremane	New carbazole-based symmetric double D–A type chromophores for DSSC application: Impact of di-anchoring nature on photoelectrochemical processes	2025	Journal of Photochemistry and Photobiology A: Chemistry	link
40	Jordi Buils	Synthesis, X-ray characterization, and DFT calculations of gold–nucleobase complexes: on the importance of regium bonds and anion– π interactions	2025	CrystEngComm	link
41	Catalina Nicolau	Noncovalent binding phenomena in the adsorption of amino acids on Ag/Au surfaces: a theoretical approach	2025	Physical Chemistry Chemical Physics	link
42	Sergi Burguera	Are Noncovalent C—H... Au Bonds Comparable to C—H... π Bonds? A Theoretical Perspective	2025	Chemistry—An Asian Journal	link
43	Ali Al-Jaaidi	Ultrafast Dynamics of Diketopyrrolopyrrole Dimers	2025	Journal of Computational Chemistry	link

BIOVIA TURBOMOLE 関連論文リスト (6/30)

44	Rosa M. Gomila	Noble gas bonds facilitate anion...anion supramolecular assemblies: insights from CSD and DFT analysis	2025	CrystEngComm		link
45	Tse-Min Chiang	Two-photon absorption with spin-orbit coupling: Methodology and application to fac-Ir(ppy) ₃	2025	APL Computational Physics		link
46	Michael Hymas	Excited state deactivation in phytochemical flavonoids: astragalin and kaempferol	2025	Physical Chemistry Physics	Chemical	link
47	Edoardo Fabbrini	Automatized Platform for Bandgap Optimization in Diarylethene Derivatives via Structural Substitutions	2025	International Journal of Quantum Chemistry		link
48	Leonard Gura	Low- Temperature Transformations in Amorphous Silica Bilayers on Ru(0001) After Crystal-Glass Transition: Closer Look	2025	Chemistry-A European Journal		link
49	S. M. Gayomi K. Samarakoon	[Palladium-decabismuth(4+)]-tetrakis(tetrachloridoaluminate) Cluster Compound, [Pd@Bi ₁₀][AlCl ₄] ₄ : Synthesis, Crystal Structure, and Electronic Structure	2025	Molbank		link
50	Erik Van Dyke	Towards detection of molecular parity violation via chiral co-sensing: the 1H/31P model system	2025	Physical Chemistry Physics	Chemical	link
51	Nóra Kovács	An evaluation of local double hybrid density functionals	2025	Chemical Physics Letters		link
52	Benedikt Zerulla	Multi-Scale Modeling of Surface Second-Harmonic Generation in Centrosymmetric Molecular Crystalline Materials: How Thick is the Surface?	2024	Advanced Optical Materials		link
53	Mitchell R. Whittam	Circular dichroism of relativistically-moving chiral molecules	2024	Scientific Reports		link

BIOVIA TURBOMOLE 関連論文リスト (7/30)

54	Sergi Burguera	Unconventional C—Hlg...H—C (Hlg = Cl, Br, and I) Interactions Involving Organic Halides: A Theoretical Study	2024	Molecules	link
55	M. Gururaj Acharya	Performance of anionic dimeric surfactant on AZ31 Magnesium alloy in neutral medium unveiled through experimental and theoretical investigation	2024	Surface Science and Technology	link
56	Dang-Bao-An Tran	Continuous-wave cavity ringdown for high-sensitivity polarimetry and magnetometry measurements	2024	The Journal of Chemical Physics	link
57	Danillo Valverde	Computational investigations of the detailed mechanism of reverse intersystem crossing in inverted singlet–triplet gap molecules	2024	ACS Applied Materials & Interfaces	link
58	Xiaoze Sun	Insight of super-capacitive properties of flexible gel polymer electrolyte containing butyl imidazole ionic liquids with different anions based on PVDF-HFP	2024	Journal of Polymer Research	link
59	Qian Wang	Changing aromatic properties through stacking: the face-to-face dimer of Ni(II) bis(pentafluorophenyl)norcorrole	2024	Physical Chemistry Chemical Physics	link
60	Hao Jiang	H ₂ formation from the E ₂ –E ₄ states of nitrogenase	2024	Physical Chemistry Chemical Physics	link
61	Marc Reimann	Rydberg electron stabilizes the charge localized state of the diamine cation	2024	Nature Communications	link
62	Patricia Godermajer	Degradable bispiperidone derivative amine networks with monomer recovery	2024	Polymer Chemistry	link

BIOVIA TURBOMOLE 関連論文リスト (8/30)

63	Wei Chen	Experimental and computational analysis of the structure-activity relationship of ionic gel electrolytes based on bistrifluoromethanesulfonimide salts for supercapacitors	2024	Journal of Materiomics	link
64	Markus Nyman	A digital twin for a chiral sensing platform	2024	Laser & Photonics Reviews	link
65	Daniel Blasco	The aromatic nature of auracycles and diauracycles based on calculated ring-current strengths	2024	Dalton Transactions	link
66	Robin Grotjahn	Chemically Accurate Singlet–Triplet Gaps of Arylcarbenes from Local Hybrid Density Functionals	2024	The Journal of Physical Chemistry A	link
67	Annina Z. Lieberherr	Optimal transport distances to characterize electronic excitations	2024	Journal of Chemical Theory and Computation	link
68	Raphael I. Petrikat	A Photoswitchable Metallocycle Based on Azobenzene: Synthesis, Characterization, and Ultrafast Dynamics	2024	Chemistry – A European Journal	link
69	Ahmadreza Rajabi	A DFT perspective on organometallic lanthanide chemistry	2024	Dalton Transactions	link
70	Réka A. Horváth	Which model density is best in pair natural orbital local correlation theory?	2024	Chemical Physics Letters	link
71	Ericka Roy Miller	Ultrafast photochemistry and electron diffraction for cyclobutanone in the S2 state: Surface hopping with time-dependent density functional theory	2024	The Journal of Chemical Physics	link
72	Praveen Naik	Exploring optical, electrochemical, thermal, and theoretical aspects of simple carbazole-derived organic dyes	2024	Heliyon	link

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73	Nirvik Ghosh	Crystallographic, theoretical and conductivity studies of two new complexes [Ni (II) and Cu (II)] based on mixed ligands approach	2024	Journal of Molecular Structure	link
74	Thomas V. Papineau	Which electronic structure method to choose in trajectory surface hopping dynamics simulations? Azomethane as a case study	2024	The Journal of Physical Chemistry Letters	link
75	Matthias Zajonz	Excited state dipole moments of two dicyanobenzene isomers from thermochromic shifts and ab initio calculations	2024	Journal of Photochemistry and Photobiology A: Chemistry	link
76	Zheng-Wang Qu	Mechanism of Alkaline Earth Metal Amide Catalyzed Hydrogenation of Challenging Alkenes and Arenes	2024	ChemSusChem	link
77	Thomas Gasevic	Benchmark Study on the Calculation of ²⁰⁷ Pb NMR Chemical Shifts	2024	Inorganic Chemistry	link
78	Robert Toews	Cyclohepta[def]fluorene as a bistable molecule: first principles studies on its electronic structure and the effects of benzo-extension, substitution and solvation	2024	Physical Chemistry Chemical Physics	link
79	Sergi Burguera	Manganese mature bonds in biological systems: PDB inspection and DFT calculations	2024	Physical Chemistry Chemical Physics	link
80	Felix R. S. Purtscher	Probing the range of applicability of structure- and energy-adjusted QM/MM link bonds III: QM/MM MD simulations of solid-state systems at the example of layered carbon structures	2024	Journal of Computational Chemistry	link

BIOVIA TURBOMOLE 関連論文リスト (10/30)

81	Yuriy A. Demidov	Uncovering chemical homology of superheavy elements: a close look at astatine	2024	Physical Chemistry Chemical Physics	link
82	Tejendra Banana	Effect of meso-pentafluorophenyl group on two-photon absorption in heterocorroles and heterocorrins	2024	Physical Chemistry Chemical Physics	link
83	Max Völker	Hydrogenation Studies of Iridium Pyridine Diimine Complexes with O- and S-Donor Ligands (Hydroxido, Methoxido and Thiolato)	2024	Chemistry	link
84	Mesías Orozco-Ic	Understanding Aromaticity in [5]Helicene-Bridged Cyclophanes: A Comprehensive Study	2024	The Journal of Organic Chemistry	link
85	Štěpán Marek	Widening of the fundamental gap in cluster GW for metal–molecular interfaces	2024	Physical Chemistry Chemical Physics	link
86	Magdalena W. Duszka	Computational design of boron-free triangular molecules with inverted singlet–triplet energy gap	2024	Physical Chemistry Chemical Physics	link
87	Antonia Rabe	Unraveling the enigma of Craig-type Möbius-aromatic osmium compounds	2024	Dalton Transactions	link
88	Florian Bruder	Application of the Adiabatic Connection Random Phase Approximation to Electron–Nucleus Hyperfine Coupling Constants	2024	The Journal of Physical Chemistry A	link
89	Edmund Leary	Antiaromatic non-alternant heterocyclic compounds as molecular wires	2024	Journal of Materials Chemistry C	link
90	J. Eng	The photochemistry of Rydberg-excited cyclobutanone: Photoinduced processes and ground state dynamics	2024	The Journal of Chemical Physics	link

BIOVIA TURBOMOLE 関連論文リスト (11/30)

91	Ahmed Shaalan Alag	Ab initio investigation of excited state charge transfer pathways in differently capped bithiophene cages	2024	Journal of Computational Chemistry	link
92	Sergi Burguera	On the influence of metal nanoparticle and π -system sizes in the stability of noncovalent adducts: a theoretical study	2024	Physical Chemistry Chemical Physics	link
93	Usman Ahmed	The effect of hydrogen bonding on the π depletion and the $\pi-\pi$ stacking interaction	2024	Physical Chemistry Chemical Physics	link
94	Dominique J. Luder	Polar covalent apex - base bonding in borapyrimidanes probed by solid - state NMR and DFT calculations	2024	Chemistry – A European Journal	link
95	Matheus Máximo-Canadas	Ab initio electronic absorption spectra of para - nitroaniline in different solvents: Intramolecular charge transfer effects	2024	Journal of Computational Chemistry	link
96	Andreas J. Achazi	Development of a multi - step screening procedure for redox active molecules in organic radical polymer anodes and as redox flow anolytes	2024	Journal of Computational Chemistry	link
97	Shaoting Liu	Unexpected longer T1 lifetime of 6-sulfur guanine than 6-selenium guanine: the solvent effect of hydrogen bonds to brake the triplet decay	2024	Physical Chemistry Chemical Physics	link
98	Sergi Burguera	A novel approach for estimating the strength of argentophilic and aurophilic interactions using QTAIM parameters	2024	Physical Chemistry Chemical Physics	link
99	Guillaume Bastien	Triptycene - Based Tripodal Molecular Platforms	2024	Chemistry – A European Journal	link

BIOVIA TURBOMOLE 関連論文リスト (12/30)

100	María de las Nieves Piña	Diphenylene Iodonium as a Prominent Halogen Bond Donor: The Case of Human Monoamine Oxidase B	2024	ChemPhysChem	link
101	Ariel C. Jones	Exploring non-covalent interactions in excited states: beyond aromatic excimer models	2024	Physical Chemistry Chemical Physics	link
102	Iryna Knysh	Reference CC3 Excitation Energies for Organic Chromophores: Benchmarking TD-DFT, BSE/GW, and Wave Function Methods	2024	Journal of Chemical Theory and Computation	link
103	Vitor Angelo Fonseca Deichmann	Design and Synthesis of Red-Absorbing Fluoran Leuco Dyes Supported by Computational Screening	2024	ACS Omega	link
104	Jascha Martini	Vibronic Splitting of the Electronic Origin in Two Conformers of the 3 - Tolunitrile Dimer	2024	ChemPhysChem	link
105	Pierre-François Loos	A mountaineering strategy to excited states: Accurate vertical transition energies and benchmarks for substituted benzenes	2024	Journal of Computational Chemistry	link
106	Michał Andrzej Kochman	Nonadiabatic Molecular Dynamics Simulations Provide Evidence for Coexistence of Planar and Nonplanar Intramolecular Charge Transfer Structures in Fluorazene	2024	The Journal of Physical Chemistry A	link
107	Marko Horbatsch	Calculation of Low-Lying Electronic Excitations of Magnesium Monofluoride: How Well Do Coupled-Cluster Methods Work?	2024	Atoms	link
108	Swati Singh Rajput	Why does the orientation of azulene affect the two-photon activity of a porphyrinoid–azulene system?	2024	Physical Chemistry Chemical Physics	link

BIOVIA TURBOMOLE 関連論文リスト (13/30)

109	Christopher Sheldon	Hybrid RPA:DFT Approach for Adsorption on Transition Metal Surfaces: Methane and Ethane on Platinum (111)	2024	Journal of Chemical Theory and Computation	link
110	Mirza Wasif Baig	Relativistic two-component density functional study of ethyl 2-(2-Iodobenzylidenehydrazinyl)thiazole-4-carboxylate	2024	Computational and Theoretical Chemistry	link
111	Martin Kaupp	Toward the next generation of density functionals: Escaping the zero-sum game by using the exact-exchange energy density	2024	Accounts of Chemical Research	link
112	Hannah M. Work	HCV Antiviral Drugs Have the Potential to Adversely Perturb the Fetal-Maternal Communication Axis through Inhibition of CYP3A7 DHEA-S Oxidation	2024	Drug Metabolism and Disposition	link
113	Ryan L. Dempsey	Computational study of the interactions of tetravalent actinides (An = Th–Pu) with the α -Fe ₁₃ Keggin cluster	2024	Dalton Transactions	link
114	Hao Jiang	Putative reaction mechanism of nitrogenase with a half-dissociated S ₂ B ligand	2024	Dalton Transactions	link
115	Mesías Orozco-Ic	Core-electron contributions to the magnetic response of molecules with heavy elements and their significance in aromaticity assessments	2024	Chemical Science	link
116	Laura Galleni	The C1s core levels of polycyclic aromatic hydrocarbons and styrenic polymers: A first-principles study	2024	The Journal of Chemical Physics	link
117	Risa Amano	Optical force and torque in near-field excitation of C ₃ H ₆ : A first-principles study using RT-TDDFT	2024	The Journal of Chemical Physics	link

BIOVIA TURBOMOLE 関連論文リスト (14/30)

118	Jindřich Fanfrlík	Heats of Formation on the Way from B ₂ H ₆ to B ₂₀ H ₁₆ : Thermochemical Consequences of Multicenter Bonding in Ab initio and DFT Methods	2024	Dalton Transactions	link
119	J. T. Kohn	A semi-automated quantum-mechanical workflow for the generation of molecular monolayers and aggregates	2024	The Journal of Chemical Physics	link
120	Daisuke Nishizawa	Near-field induced local excitation dynamics of Na ₁₀ and Na ₁₀ -N ₂ from real-time TDDFT	2024	The Journal of Chemical Physics	link
121	Gregory Gate	The tautomer-specific excited state dynamics of 2,6-diaminopurine using resonance-enhanced multiphoton ionization and quantum chemical calculations	2024	Photochemistry and Photobiology	link
122	Lukas Hehn	Chelate Complexes of 3d Transition Metal Ions—A Challenge for Electronic-Structure Methods?	2024	Journal of Chemical Theory and Computation	link
123	Georgios K. Stavroglou	Tailoring ammonia capture in MOFs and COFs: A multi-scale and machine learning comprehensive investigation of functional group modification	2024	ChemPhysChem	link
124	Zheng-Wang Qu	Mechanism of Borane-Catalyzed Oligomerization of Arylallenes and Arylacetylenes	2024	European Journal of Organic Chemistry	link
125	Joanna Jankowska	Photo-oxidation of methanol in complexes with pyrido [2, 3-b] pyrazine: a nonadiabatic molecular dynamics study	2024	Physical Chemistry Chemical Physics	link
126	Zheng-Wang Qu	Reactivity of Frustrated Lewis Pair: Carbocation versus Radical Intermediates	2024	Chemistry – A European Journal	link
127	Özlem Yönder	A computational chemistry study on the evolution of oxygen functional groups during char burnout	2024	Fuel	link

BIOVIA TURBOMOLE 関連論文リスト (15/30)

128	Ismael A. Elayan	Beyond Explored Functionals: A Computational Journey of Two-Photon Absorption	2024	Journal of Chemical Theory and Computation	link
129	Rosendo Valero	Estimating Nonradiative Excited-State Lifetimes in Photoactive Semiconducting Nanostructures	2024	The Journal of Physical Chemistry C	link
130	Frédéric Célerse	Unveiling the Full Dynamical and Reactivity Profiles of Acetylcholinesterase: A Comprehensive All-Atom Investigation	2024	ACS Catalysis	link
131	Eimear Madden	The effect of particle size on the optical and electronic properties of hydrogenated silicon nanoparticles	2024	Physical Chemistry Chemical Physics	link
132	Hagen Neugebauer	Toward Benchmark-Quality Ab Initio Predictions for 3d Transition Metal Electrocatalysts: A Comparison of CCSD(T) and ph-AFQMC	2023	Journal of Chemical Theory and Computation	link
133	Yuriy Boiko	Grafting of phosphorus-containing tetrahydroxy (thia) calixarenes on silica enhances europium (III) adsorption	2023	Phosphorus, Sulfur, and Silicon and the Related Elements	link
134	Benjamin Peerless	ϕ -Aromaticity in prismatic {Bi6}-based clusters	2023	Nature Chemistry	link
135	Kevin Issler	Time-resolved photoelectron spectroscopy of 4-(dimethylamino) benzethyne—an experimental and computational study	2023	Physical Chemistry Chemical Physics	link
136	Muhammad Naeem Ahmed	Crystal engineering with 1, 3, 4-oxadiazole derivatives: on the importance of CH \cdots N and CH \cdots π interactions	2023	CrystEngComm	link
137	Pierre-François Loos	Heptazine, Cyclazine, and Related Compounds: Chemically-Accurate Estimates of the Inverted Singlet–Triplet Gap	2023	The Journal of Physical Chemistry Letters	link

BIOVIA TURBOMOLE 関連論文リスト (16/30)

138	Markus Nyman	A digital twin for a chiral sensing platform	2023	Laser & Photonics Reviews	link
139	Julia Kohn	Computational study of ground-state properties of μ -2-bridged group 14 porphyrinic sandwich complexes	2023	Journal of Computational Chemistry	link
140	Dóra Vörös	Excited states of ortho-nitrobenzaldehyde as a challenging case for single- and multi-reference electronic structure theory	2023	Journal of Computational Chemistry	link
141	David Yubero Valdivielso	IR spectra and structures of saturated ruthenium cluster carbonyl cations $\text{Ru}_n(\text{CO})_m^+$ ($n = 1-6$)	2023	Dalton Transactions	link
142	Ali Ghiami-Shomami	Performance of the COSMO solvation model for photoacidity and basicity in water	2023	Journal of Computational Chemistry	link
143	Probal Nag	Understanding the photodynamics of 3-hydroxypyran-4-one using surface hopping simulations	2023	Journal of Photochemistry and Photobiology A: Chemistry	link
144	Tim Schrader	Performance of common density functionals for excited states of tetraphenyldibenzoperiflanthene	2023	The Journal of Physical Chemistry A	link
145	Maite Nößler	Electrochemistry and Spin-Crossover Behavior of Fluorinated Terpyridine-Based Co(II) and Fe(II) Complexes	2023	European Journal of Inorganic Chemistry	link
146	Sonia Jafari	Two local minima for structures of [4Fe-4S] clusters obtained with density functional theory methods	2023	Scientific Reports	link
147	Christoph Schissler	Marriage of an N-Fused and a Regular Porphyrin in a Cofacial Ligand System	2023	Organometallics	link
148	Zohreh Hashemi	Mapping charge-transfer excitations in Bacteriochlorophyll dimers from first principles	2023	Electronic Structure	link

BIOVIA TURBOMOLE 関連論文リスト (17/30)

149	Sergi Burguera	Materie Bonds in Technetium Compounds: CSD Survey and Theoretical Considerations	2023	Crystals	link
150	Moritz Bensberg	Corresponding active orbital spaces along chemical reaction paths	2023	The Journal of Physical Chemistry Letters	link
151	Erik Andris	Can Copper (I) and Silver (I) be Hydrogen Bond Acceptors?	2023	Chemistry – A European Journal	link
152	Adam Šrut	The Marcus dimension: identifying the nuclear coordinate for electron transfer from ab initio calculations	2023	Chemical Science	link
153	Sergi Burguera	Hg(II) · d8[M] Interactions: Are they Metallophilic Interactions or Spodium Bonds?	2023	ChemPhysChem	link
154	Iryna Knysh	Exploring Bethe–Salpeter Excited-State Dipoles: The Challenging Case of Increasingly Long Push–Pull Oligomers	2023	The Journal of Physical Chemistry Letters	link
155	O.I. Kalchenko	Complexation of water-soluble phosphorylated calixarenes with uracils. Stability constants and DFT study of the supramolecular complexes	2023	Journal of Inclusion Phenomena and Macrocyclic Chemistry	link
156	Sudip Bhunia	An insight to the role of perchlorate counter ions and different non-covalent interactions in the solid state structures of mono-anionic malonic acid bridged trinuclear mixed valence cationic complexes of cobalt with tetradentate N2O2 donor ligands	2023	Inorganica Chimica Acta	link
157	Anthony Ferté	ESIPT in the pyrrol pyridine molecule: mechanism, timescale and yield revealed using dynamics simulations	2023	Physical Chemistry Chemical Physics	link

BIOVIA TURBOMOLE 関連論文リスト (18/30)

158	Sergi Burguera	Biological noncovalent N/O... V interactions: insights from theory and protein data bank analyses	2023	Physical Chemistry Chemical Physics	link
159	Ritam Mansour	Temperature effects on the internal conversion of excited adenine and adenosine	2023	Physical Chemistry Chemical Physics	link
160	Paul De Bonfils	Synthesis and Photophysical Characterizations of Pyrroloquinolone Photosensitizers for Singlet Oxygen Production	2023	Photochemistry and Photobiology	link
161	Snehasish Thakur	A combined experimental and theoretical study of covalent vs noncovalent dimer formation in vanadium (V) complexes with Schiff base ligands	2023	Polyhedron	link
162	Henry C. Fitzhugh	Comparative Density Functional Theory Study of Magnetic Exchange Couplings in Dinuclear Transition-Metal Complexes	2023	Journal of Chemical Theory and Computation	link
163	Iryna Knysh	Excited state potential energy surfaces of N-phenylpyrrole upon twisting: reference values and comparison between BSE/GW and TD-DFT	2023	Physical Chemistry Chemical Physics	link
164	Gloria Tobajas-Curiel	Solvation rules: aromatic interactions outcompete cation- π interactions in synthetic host-guest complexes in water	2023	Chemical Communications	link
165	Jessica Groß	Computational Study on a Transfer Hydrogenation Catalysed by a Ru (II) Bis - Pyrazolyl Pyridine Complex	2023	Israel Journal of Chemistry	link
166	Hao Jiang	N ₂ binding to the E ₀ -E ₄ states of nitrogenase	2023	Dalton Transactions	link

BIOVIA TURBOMOLE 関連論文リスト (19/30)

167	Sulafa Abdalmageed Saadaldeen Mohammed	Experimental and computational evaluation of 1, 2, 4-triazolium-based ionic liquids for carbon dioxide capture	2023	Separations	link
168	Praveen Naik	Synthesis, optical, electrochemical, and computational investigation of new cyanopyridine-centered organic dyads	2023	Optical Materials	link
169	Nenad Jovanović	Fractal nature of benzene stacking interactions	2023	Journal of Molecular Modeling	link
170	Chengcheng Tang	One Molecule Suffices: Spectroscopy of Yariv Reagents	2023	ChemistrySelect	link
171	Tim Schrader	Koopmans' theorem for acidic protons	2023	Chemical Communications	link
172	Victor P. Vysotskiy	Assessment of DFT functionals for a minimal nitrogenase [Fe(SH) ₄ H] – model employing state-of-the-art ab initio methods	2023	The Journal of Chemical Physics	link
173	Gloria Tobajas-Curiel	Aromatic interactions with heterocycles in water	2023	Chemical Science	link
174	Kumar Sumit	Curcumin as a potential multiple-target inhibitor against SARS-CoV-2 Infection: A detailed interaction study using quantum chemical calculations	2023	Journal of the Serbian Chemical Society	link
175	Jindřich Fanfrlík	B–H⋯ π and C–H⋯ π interactions in protein–ligand complexes: carbonic anhydrase II inhibition by carborane sulfonamides	2023	Physical Chemistry Chemical Physics	link
176	Daniel Blasco	Gold (I)-containing light-emitting molecules with an inverted singlet–triplet gap	2023	Chemical Science	link
177	Georgyi Koidan	Straightforward Synthesis of Halopyridine Aldehydes via Diaminomethylation	2023	Chemistry – A European Journal	link

BIOVIA TURBOMOLE 関連論文リスト (20/30)

178	Javad Shirazi	Catalytic Reaction Mechanism of Glyoxalase II: A Quantum Mechanics/Molecular Mechanics Study	2023	The Journal of Physical Chemistry B	link
179	Maria de las Nieves Piña	Capturing volatile organic compounds using Ag and Au nanoparticles: regium- π and C-H... Ag/Au interactions at work	2023	Journal of Materials Chemistry A	link
180	Qian Wang	The magnetically induced current density of the [12] infinitene dianion	2023	Physical Chemistry Chemical Physics	link
181	Atif Mahmood	Current-Density Calculations on Zn-Porphyrin ₄₀ Nanorings	2023	The Journal of Physical Chemistry A	link
182	Amy C. Hancock	Noncovalently bound excited-state dimers: a perspective on current time-dependent density functional theory approaches applied to aromatic excimer models	2023	RSC advances	link
183	Gloria Tobajas-Curiel	Solvation rules: aromatic interactions outcompete cation- π interactions in synthetic host-guest complexes in water	2023	Chemical Communications	link
184	Łukasz Wolański	Quadripartite bond length rule applied to two prototypical aromatic and antiaromatic molecules	2023	Journal of Molecular Modeling	link
185	Gloria Tobajas-Curiel	Substituent effects on aromatic interactions in water	2023	Chemical Science	link
186	Praveen Naik	A computational approach for screening carbazole based organic dyes as potential photosensitizers for DSSCs application	2023	Results in Chemistry	link
187	Weiwei Li	Resonance effect in Brunel harmonic generation in thin film organic semiconductors	2023	Advanced Optical Materials	link

BIOVIA TURBOMOLE 関連論文リスト (21/30)

188	Jessica Groß	Computational Study on a Transfer Hydrogenation Catalysed by a Ru (II) Bis-Pyrazolyl Pyridine Complex	2023	Israel Journal of Chemistry	link
189	Ritam Mansour	Pre-Dewar structure modulates protonated azaindole photodynamics	2022	Physical Chemistry Chemical Physics	link
190	Raphael J. F. Berger	Integration of global ring currents using the Ampère–Maxwell law	2022	Physical Chemistry Chemical Physics	link
191	Lewis Hutton	Photodynamics of Gas-Phase Pyruvic Acid Following Light Absorption in the Actinic Region	2022	ChemPhotoChem	link
192	Keisuke Hirata	Excited state dynamics of protonated dopamine: hydration and conformation effects	2022	Physical Chemistry Chemical Physics	link
193	Martin Kaupp	Unusually Large Effects of Charge-assisted C-H...F Hydrogen Bonds to Anionic Fluorine in Organic Solvents: Computational Study of ¹⁹ F NMR Shifts versus Thermochemistry	2022	ChemistryOpen	link
194	Markus Bursch	Theoretical study on conformational energies of transition metal complexes	2021	Physical Chemistry Chemical Physics	link
195	Arjeta Rushiti	Activation of Molecular O ₂ on CoFe ₂ O ₄ (001) Surfaces: An Embedded Cluster Study	2021	Chemistry–A European Journal	link
196	Lin Yang	High coordination number actinide-noble gas complexes; a computational study	2021	Physical Chemistry Chemical Physics	link
197	Dickson D. Babu	A simple DA- π -A configured carbazole based dye as an active photo-sensitizer: A comparative investigation on different parameters of cell	2020	Journal of Molecular Liquids	link

BIOVIA TURBOMOLE 関連論文リスト (22/30)

198	Xiaoyan Cao	Density Functional Studies of Coenzyme NADPH and Its Oxidized Form NADP+: Structures, UV-Vis Spectra, and the Oxidation Mechanism of NADPH	2020	Journal of Computational Chemistry	link
199	Naveenchandra Pilicode	New cyanopyridine based conjugated polymers carrying auxiliary electron donors: from molecular design to blue emissive PLEDs	2020	Dyes and Pigments	link
200	Martin Sebastian Zöllner	Influence of electronic structure modeling and junction structure on first-principles chiral induced spin selectivity	2020	Journal of Chemical Theory and Computation	link
201	Rama Mohana Rao Dumpala	Aquatic interaction of uranium with two naturally ubiquitous pyrazine compounds: Speciation studies by experiment and theory	2020	Chemosphere	link
202	S. A. Khan	Palladium (II) complexes based on N, S-donor ligands: synthesis and molecular structures	2019	Journal of Structural Chemistry	link
203	Emily R. Draper	Insight into the self-assembly of water-soluble perylene bisimide derivatives through a combined computational and experimental approach	2019	Nanoscale	link
204	Matthias Stein	Intermolecular interactions in molecular organic crystals upon relaxation of lattice parameters	2019	Crystals	link
205	Lili Cao	Extremely large differences in DFT energies for nitrogenase models	2019	Physical Chemistry Chemical Physics	link
206	Octav Caldararu	Mechanism of hydrogen peroxide formation by lytic polysaccharide monooxygenase	2019	Chemical Science	link

BIOVIA TURBOMOLE 関連論文リスト (23/30)

207	Hannes Konrad Buchholz	Accurate lattice energies of organic molecular crystals from periodic turbomole calculations	2018	Journal of Computational Chemistry	link
208	Samuel Bouvron	Charge transport in a single molecule transistor probed by scanning tunneling microscopy	2018	Nanoscale	link
209	Mirko Matthias Lindic	Excited state dipole moments of anisole in gas phase and solution	2018	Journal of Photochemistry and Photobiology A: Chemistry	link
210	Praveen Naik	Investigation of new carbazole based metal-free dyes as active photo-sensitizers/co-sensitizers for DSSCs	2018	Dyes and Pigments	link
211	Gang Feng	Hydrogen Spillover to Copper Clusters on Hydroxylated γ -Al ₂ O ₃	2018	The Journal of Physical Chemistry C	link
212	Praveen Naik	Molecular Engineering of a New Organic Chromophore with D- π -A Architecture for Dye-Sensitized Solar Cells	2018	Materials Today: Proceedings	link
213	Rashid R. Valiev	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34] octaphyrins	2018	Physical Chemistry Chemical Physics	link
214	Praveen Naik	Synthesis, characterization and performance studies of a new metal-free organic sensitizer for DSSC application	2018	Materials Today: Proceedings	link
215	Mohd. Athar	Investigation of structural and conformational equilibrium of Oxacalix [4] arene: A density functional theory approach	2017	Journal of Molecular Liquids	link
216	Praveen Naik	Molecular design and theoretical investigation of new metal-free heteroaromatic dyes with D- π -A architecture as photosensitizers for DSSC application	2017	Journal of Photochemistry and Photobiology A: Chemistry	link

BIOVIA TURBOMOLE 関連論文リスト (24/30)

217	Praveen Naik	Structurally simple D-A-type organic sensitizers for dye-sensitized solar cells: effect of anchoring moieties on the cell performance	2017	Journal of the Iranian Chemical Society	link
218	Praveen Naik	New carbazole based metal-free organic dyes with D- π -A- π -A architecture for DSSCs: Synthesis, theoretical and cell performance studies	2017	Solar Energy	link
219	Yannick J. Franzke	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays	2017	Physical Chemistry Chemical Physics	link
220	Shailja Jain	The Unusual Role of Aromatic Solvent in Single - Site Aluminum Chemistry: Insights from Theory	2017	Chemistry—A European Journal	link
221	Shuming Bai	On the decay of the triplet state of thionucleobases	2017	Physical Chemistry Chemical Physics	link
222	Michael Dommett	Excited state proton transfer in 2'-hydroxychalcone derivatives	2017	Physical Chemistry Chemical Physics	link
223	Antonio Prlj	Rationalizing fluorescence quenching in meso-BODIPY dyes	2016	Physical Chemistry Chemical Physics	link
224	Dage Sundholm	Analysis of the magnetically induced current density of molecules consisting of annelated aromatic and antiaromatic hydrocarbon rings	2016	Physical Chemistry Chemical Physics	link
225	Kasper P. Kepp	Theoretical study of spin crossover in 30 iron complexes	2016	Inorganic Chemistry	link
226	Petr Štěpánek	Magnetic circular dichroism of chlorofullerenes: Experimental and computational study	2016	Chemical Physics Letters	link

BIOVIA TURBOMOLE 関連論文リスト (25/30)

227	Raviraj M. Kulkarni	Experimental and theoretical studies on the oxidation of lomefloxacin by alkaline permanganate	2016	Desalination and Water Treatment	link
228	Vincent Baijot	Effect of temperature and O2 pressure on the gaseous species produced during combustion of aluminum	2016	Chemical Physics Letters	link
229	Florian H. Hodel	What Influences the Water Oxidation Activity of a Bioinspired Molecular Coll4O4 Cubane? An In-Depth Exploration of Catalytic Pathways	2016	Acs Catalysis	link
230	Andreas J. Achazi	Theoretical and experimental investigation of crown/ammonium complexes in solution	2016	Journal of Computational Chemistry	link
231	Dickson D. Babu	Molecular engineering and theoretical investigation of metal-free organic Chromophores for dye-sensitized solar cells	2016	Advanced Science Letters	link
232	Mario Barbatti	Effects of different initial condition samplings on photodynamics and spectrum of pyrrole	2016	International Journal of Quantum Chemistry	link
233	Antonio Prlj	Low-lying $\pi \pi^*$ states of heteroaromatic molecules: a challenge for excited state methods	2016	Journal of Chemical Theory and Computation	link
234	Isaac Benkyi	New insights into aromatic pathways of carbachlorins and carbaporphyrins based on calculations of magnetically induced current densities	2016	Physical Chemistry Chemical Physics	link
235	Joseph P.W. Wellington	Should environmental effects be included when performing QTAIM calculations on actinide systems? A comparison of QTAIM metrics for Cs2UO2Cl4,	2016	Polyhedron	link

BIOVIA TURBOMOLE 関連論文リスト (26/30)

		U(Se ₂ PPh ₂) ₄ and Np(Se ₂ PPh ₂) ₄ in gas phase, COSMO and PEECM			
236	Junais Habeeb Mokkath	Tunable optical absorption in silicene molecules	2016	Journal of Materials Chemistry C	link
237	Rashid R. Valiev	Predicting the degree of aromaticity of novel carbaporphyrinoids	2015	Physical Chemistry Chemical Physics	link
238	Christoph Bannwarth	The Association of Two “Frustrated” Lewis Pairs by State-of-the-Art Quantum Chemical Methods	2015	Israel Journal of Chemistry	link
239	Hongmei Wu	Novel dengue virus NS2B/NS3 protease inhibitors	2015	Antimicrobial Agents and Chemotherapy	link
240	Kasper P. Kepp	Halide binding and inhibition of laccase copper clusters: the role of reorganization energy	2015	Inorganic Chemistry	link
241	Carina F. Pupim	Spurious phosphorus pyramidalization induced by some DFT functionals	2015	Journal of the Brazilian Chemical Society	link
242	Antonio Prlj	Excited state dynamics of thiophene and bithiophene: new insights into theoretically challenging systems	2015	Physical Chemistry Chemical Physics	link
243	Cina Foroutan-Nejad	Unwilling U-U bonding in U ₂ @C ₈₀ : cage-driven metal-metal bonds in di-uranium fullerenes	2015	Physical Chemistry Chemical Physics	link
244	Mario Barbatti	Why water makes 2-aminopurine fluorescent?	2015	Physical Chemistry Chemical Physics	link
245	Vangelis Daskalakis	Structure and properties of the catalytic site of nitric oxide reductase at ambient temperature	2015	Biochimica et Biophysica Acta (BBA) - Bioenergetics	link

BIOVIA TURBOMOLE 関連論文リスト (27/30)

246	Simon Lobsiger	Intersystem crossing rates of S1 state keto-amino cytosine at low excess energy	2015	The Journal of Chemical Physics	link
247	Rachel Crespo-Otero	Stepwise double excited-state proton transfer is not possible in 7-azaindole dimer	2015	Chemical Science	link
248	Boris M. Polyak	Modeling processes of non-radiative relaxation of electronically excited states of fluorescent probe 4-dimethylaminochalcone and its complexes with water using non-adiabatic molecular dynamics	2014	Journal of Photochemistry and Photobiology A: Chemistry	link
249	Celesztina Domonkos	Role of the conformational flexibility of evodiamine in its binding to protein hosts: a comparative spectroscopic and molecular modeling evaluation with rutaecarpine	2014	Physical Chemistry Chemical Physics	link
250	R. R.Valiev	The computational and experimental investigations of photophysical and spectroscopic properties of BF ₂ dipyrromethene complexes	2014	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	link
251	Adélia A. J. Aquino	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbon-tetracyanoethylene complexes	2014	Physical Chemistry Chemical Physics	link
252	Gangotri Dey	Copper (I) carbene hydride complexes acting both as reducing agent and precursor for Cu ALD: a study through density functional theory	2014	Theoretical Chemistry Accounts	link
253	Dhananjay Dey	Quantitative Evaluation of C-H...O and C-H... π Intermolecular Interactions in Ethyl-3-benzyl-1-methyl-2-oxindoline-3-carboxylate and 3-Methyl-but-2-en-1-yl-	2014	Journal of Chemical Crystallography	link

BIOVIA TURBOMOLE 関連論文リスト (28/30)

		1,3-dimethyl-2-oxoindoline-3-carboxylate: Insights from PIXEL and Hirshfeld Analysis			
254	Heike Fliegl	Coupled-cluster calculations of the lowest 0-0 bands of the electronic excitation spectrum of naphthalene	2014	Physical Chemistry Chemical Physics	link
255	Gangotri Dey	Copper reduction and atomic layer deposition by oxidative decomposition of formate by hydrazine	2014	RSC advances	link
256	Rahul Shukla	Experimental and theoretical analysis of $\text{lp} \cdots \pi$ intermolecular interactions in derivatives of 1,2,4-triazoles	2014	CrystEngComm	link
257	Dhananjay Dey	Quantitative Insights into the Crystal Structures of Nitro Derivatives of Ethyl (2E)-2-cyano-3-phenylprop-2-enoate: Inputs from X-Ray Diffraction, DFT Calculations and Hirshfeld Surface Analysis	2014	Journal of Chemical Crystallography	link
258	Jianwen Liu	Selective oxidation of propene by vanadium oxide monomers supported on silica	2014	Journal of catalysis	link
259	Mats Linder	On the method-dependence of transition state asynchronicity in Diels-Alder reactions	2013	Physical Chemistry Chemical Physics	link
260	Marc Steinmetz	Benchmark study of the performance of density functional theory for bond activations with (Ni, Pd) - based transition - metal catalysts	2013	ChemistryOpen	link
261	Thomas J. L. Mustard	Mechanism and the origins of stereospecificity in copper-catalyzed ring expansion of vinyl oxiranes: a traceless dual transition-metal-mediated process	2013	Journal of the American Chemical Society	link

BIOVIA TURBOMOLE 関連論文リスト (29/30)

262	LiHong Hu	Accurate reaction energies in proteins obtained by combining QM/MM and large QM calculations	2013	Journal of Chemical Theory and Computation	link
263	Arnošt Mládek	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	Physical Chemistry Chemical Physics	link
264	Raphael J. F. Berger	Relativistic effects in triphenylbismuth and their influence on molecular structure and spectroscopic properties	2012	Physical Chemistry Chemical Physics	link
265	Mario Barbatti	Critical appraisal of excited state nonadiabatic dynamics simulations of 9H-adenine	2012	The Journal of Chemical Physics	link
266	Mikko Kaipio	Effect of fluorine substitution on the aromaticity of polycyclic hydrocarbons	2012	The Journal of Physical Chemistry A	link
267	Raphael J. F. Berger	Prediction of a cyclic helical oligoacetylene showing anapolar ring currents in the magnetic field	2012	Zeitschrift für Naturforschung B	link
268	Patxi García-Novo	Interaction between anions and substituted molecular bowls	2012	Physical Chemistry Chemical Physics	link
269	J.-M. Ducéré	Tail effect on trihydroxysilanes dimerization: A dispersion-corrected density functional theory study	2012	Surface science	link
270	Andreas Glöß	The MP2 binding energy of the ethene dimer and its dependence on the auxiliary basis sets: a benchmark study using a newly developed infrastructure for the processing of quantum chemical data	2012	Molecular Physics	link

BIOVIA TURBOMOLE 関連論文リスト (30/30)

271	Jean-Marie Ducéré	A computational chemist approach to gas sensors: Modeling the response of SnO ₂ to CO, O ₂ , and H ₂ O Gases	2012	Journal of Computational Chemistry	link
272	P. Kozyra	On the nature of spin- and orbital-resolved Cu ⁺ -NO charge transfer in the gas phase and at Cu(I) sites in zeolites	2012	Structural Chemistry	link
273	Christian Brand	Ground and Electronically Excited Singlet - State Structures of 5-Fluoroindole Deduced from Rotationally Resolved Electronic Spectroscopy and ab Initio Theory	2012	ChemPhysChem	link
274	D. Rama Mohana Rao	Thermodynamic study of Eu (III) complexation by pyridine monocarboxylates	2012	The Journal of Chemical Thermodynamics	link
275	Manuel Renz	Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS	2012	Journal of Chemical Theory and Computation	link