BIOVIA TURBOMOLE 関連論文リスト（1/12）

No.	First author	Title	Year	Journal name	Link
1	Eimear Madden	The effect of particle size on the optical and electronic properties of hydrogenated silicon nanoparticles	2024	Physical Chemistry Chemical Physics	link
2	Hao Jiang	H2 formation from the E2–E4 states of nitrogenase	2024	Physical Chemistry Chemical Physics	link
3	Dang-Bao-An Tran	Continuous-wave cavity ringdown for high-sensitivity polarimetry and magnetometry measurements	2024	The Journal of Chemical Physics	link
4	Marc Reimann	Rydberg electron stabilizes the charge localized state of the diamine cation	2024	Nature Communications	link
5	Štěpán Marek	Widening of the fundamental gap in cluster GW for metal–molecular interfaces	2024	Physical Chemistry Chemical Physics	link
6	Praveen Naik	Exploring optical, electrochemical, thermal, and theoretical aspects of simple carbazole-derived organic dyes	2024	Heliyon	link
7	Ryan L. Dempsey	Computational Study of the Interactions of Tetravalent Actinides (An=Th-Pu) with the α-Fe13 Keggin Cluster	2024	Dalton Transactions	link
8	Ahmed Shaalan Alag	Ab initio investigation of excited state charge transfer pathways in differently capped bithiophene cages	2024	Journal of Computational Chemistry	link
9	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

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10	Qian Wang	The magnetically induced current density of the [12] infinitene dianion	2023	Physical Chemistry Chemical Physics	link
11	Atif Mahmood	Current-Density Calculations on Zn-Porphyrin40 Nanorings	2023	The Journal of Physical Chemistry A	link
12	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
13	Gloria Tobajas-Curiel	Solvation rules: aromatic interactions outcompete cation-π interactions in synthetic host–guest complexes in water	2023	Chemical Communications	link
14	Łukasz Wolański	Quadripartite bond length rule applied to two prototypical aromatic and antiaromatic molecules	2023	Journal of Molecular Modeling	link
15	Gloria Tobajas-Curiel	Substituent effects on aromatic interactions in water	2023	Chemical Science	link
16	Praveen Naik	A computational approach for screening carbazole based organic dyes as potential photosensitizers for DSSCs application	2023	Results in Chemistry	link
17	Weiwei Li	Resonance effect in Brunel harmonic generation in thin film organic semiconductors	2023	Advanced Optical Materials	link
18	Jessica Groß	Computational Study on a Transfer Hydrogenation Catalysed by a Ru (II) Bis-Pyrazolyl Pyridine Complex	2023	Israel Journal of Chemistry	link
19	Ritam Mansour	Pre-Dewar structure modulates protonated azaindole photodynamics	2022	Physical Chemistry Chemical Physics	link

20	Raphael J. F. Berger	Integration of global ring currents using the Ampère–Maxwell law	2022	Physical Chemistry Chemical Physics	link
21	Lewis Hutton	Photodynamics of Gas-Phase Pyruvic Acid Following Light Absorption in the Actinic Region	2022	ChemPhotoChem	link
22	Keisuke Hirata	Excited state dynamics of protonated dopamine: hydration and conformation effects	2022	Physical Chemistry Chemical Physics	link
23	Martin Kaupp	Unusually Large Effects of Charge-assisted C-H···F Hydrogen Bonds to Anionic Fluorine in Organic Solvents: Computational Study of 19F NMR Shifts versus Thermochemistry	2022	ChemistryOpen	link
24	Markus Bursch	Theoretical study on conformational energies of transition metal complexes	2021	Physical Chemistry Chemical Physics	link
25	Arjeta Rushiti	Activation of Molecular O2 on CoFe2O4 (001) Surfaces: An Embedded Cluster Study	2021	Chemistry–A European Journal	link
26	Lin Yang	High coordination number actinide-noble gas complexes; a computational study	2021	Physical Chemistry Chemical Physics	link
27	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
28	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

29	Naveenchandra Pilicode	New cyanopyridine based conjugated polymers carrying auxiliary electron donors: from molecular design to blue emissive PLEDs	2020	Dyes and Pigments	link
30	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
31	Rama Mohana Rao Dumpala	Aquatic interaction of uranium with two naturally ubiquitous pyrazine compounds: Speciation studies by experiment and theory	2020	Chemosphere	link
32	S. A. Khan	Palladium (II) complexes based on N, S-donor ligands: synthesis and molecular structures	2019	Journal of Structural Chemistry	link
33	Emily R. Draper	Insight into the self-assembly of water-soluble perylene bisimide derivatives through a combined computational and experimental approach	2019	Nanoscale	link
34	Matthias Stein	Intermolecular interactions in molecular organic crystals upon relaxation of lattice parameters	2019	Crystals	link
35	Lili Cao	Extremely large differences in DFT energies for nitrogenase models	2019	Physical Chemistry Chemical Physics	link
36	Octav Caldararu	Mechanism of hydrogen peroxide formation by lytic polysaccharide monooxygenase	2019	Chemical Science	link
37	Hannes Konrad Buchholz	Accurate lattice energies of organic molecular crystals from periodic turbomole calculations	2018	Journal of Computational Chemistry	link

38	Samuel Bouvron	Charge transport in a single molecule transistor probed by scanning tunneling microscopy	2018	Nanoscale	link
39	Mirko Matthias Lindic	Excited state dipole moments of anisole in gas phase and solution	2018	Journal of Photochemistry and Photobiology A: Chemistry	link
40	Praveen Naik	Investigation of new carbazole based metal-free dyes as active photo-sensitizers/co-sensitizers for DSSCs	2018	Dyes and Pigments	link
41	Gang Feng	Hydrogen Spillover to Copper Clusters on Hydroxylated γ-Al2O3	2018	The Journal of Physical Chemistry C	link
42	Praveen Naik	Molecular Engineering of a New Organic Chromophore with D-π-A Architecture for Dye-Sensitized Solar Cells	2018	Materials Today: Proceedings	link
43	Rashid R. Valiev	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34] octaphyrins	2018	Physical Chemistry Chemical Physics	link
44	Praveen Naik	Synthesis, characterization and performance studies of a new metal-free organic sensitizer for DSSC application	2018	Materials Today: Proceedings	link
45	Mohd. Athar	Investigation of structural and conformational equilibrium of Oxacalix [4] arene: A density functional theory approach	2017	Journal of Molecular Liquids	link
46	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

47	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
48	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
49	Yannick J. Franzke	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays	2017	Physical Chemistry Chemical Physics	link
50	Shailja Jain	The Unusual Role of Aromatic Solvent in Single - Site AluminumI Chemistry: Insights from Theory	2017	Chemistry–A European Journal	link
51	Shuming Bai	On the decay of the triplet state of thionucleobases	2017	Physical Chemistry Chemical Physics	link
52	Michael Dommett	Excited state proton transfer in 2'-hydroxychalcone derivatives	2017	Physical Chemistry Chemical Physics	link
53	Antonio Prlj	Rationalizing fluorescence quenching in meso-BODIPY dyes	2016	Physical Chemistry Chemical Physics	link
54	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
55	Kasper P. Kepp	Theoretical study of spin crossover in 30 iron complexes	2016	Inorganic Chemistry	link
56	Petr Štěpánek	Magnetic circular dichroism of chlorofullerenes: Experimental and computational study	2016	Chemical Physics Letters	link

57	Raviraj M. Kulkarni	Experimental and theoretical studies on the oxidation of lomefloxacin by alkaline permanganate	2016	Desalination and Water Treatment	link
58	Vincent Baijot	Effect of temperature and O2 pressure on the gaseous species produced during combustion of aluminum	2016	Chemical Physics Letters	link
59	Florian H. Hodel	What Influences the Water Oxidation Activity of a Bioinspired Molecular CoII4O4 Cubane? An In-Depth Exploration of Catalytic Pathways	2016	Acs Catalysis	link
60	Andreas J. Achazi	Theoretical and experimental investigation of crown/ammonium complexes in solution	2016	Journal of Computational Chemistry	link
61	Dickson D. Babu	Molecular engineering and theoretical investigation of metal-free organic Chromophores for dye-sensitized solar cells	2016	Advanced Science Letters	link
62	Mario Barbatti	Effects of different initial condition samplings on photodynamics and spectrum of pyrrole	2016	International Journal of Quantum Chemistry	link
63	Antonio Prlj	Low-lying $\pi\pi^*$ states of heteroaromatic molecules: a challenge for excited state methods	2016	Journal of Chemical Theory and Computation	link
64	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
65	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

		U(Se2PPh2)4 and Np(Se2PPh2)4 in gas phase, COSMO and PEECM			
66	Junais Habeeb Mokkath	Tunable optical absorption in silicene molecules	2016	Journal of Materials Chemistry C	link
67	Rashid R. Valiev	Predicting the degree of aromaticity of novel carbaporphyrinoids	2015	Physical Chemistry Chemical Physics	link
68	Christoph Bannwarth	The Association of Two “Frustrated” Lewis Pairs by State-of-the-Art Quantum Chemical Methods	2015	Israel Journal of Chemistry	link
69	Hongmei Wu	Novel dengue virus NS2B/NS3 protease inhibitors	2015	Antimicrobial Agents and Chemotherapy	link
70	Kasper P. Kepp	Halide binding and inhibition of laccase copper clusters: the role of reorganization energy	2015	Inorganic Chemistry	link
71	Carina F. Pupim	Spurious phosphorus pyramidalization induced by some DFT functionals	2015	Journal of the Brazilian Chemical Society	link
72	Antonio Prlj	Excited state dynamics of thiophene and bithiophene: new insights into theoretically challenging systems	2015	Physical Chemistry Chemical Physics	link
73	Cina Foroutan-Nejad	Unwilling U-U bonding in U2@C80: cage-driven metal-metal bonds in di-uranium fullerenes	2015	Physical Chemistry Chemical Physics	link
74	Mario Barbatti	Why water makes 2-aminopurine fluorescent?	2015	Physical Chemistry Chemical Physics	link
75	Vangelis Daskalakis	Structure and properties of the catalytic site of nitric oxide reductase at ambient temperature	2015	Biochimica et Biophysica Acta (BBA) - Bioenergetics	link

76	Simon Lobsiger	Intersystem crossing rates of S1 state keto-amino cytosine at low excess energy	2015	The Journal of Chemical Physics	link
77	Rachel Crespo-Otero	Stepwise double excited-state proton transfer is not possible in 7-azaindole dimer	2015	Chemical Science	link
78	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
79	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
80	R. R.Valiev	The computational and experimental investigations of photophysical and spectroscopic properties of BF2 dipyrromethene complexes	2014	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	link
81	Adélia A. J. Aquino	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbon-tetracyanoethylene complexes	2014	Physical Chemistry Chemical Physics	link
82	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
83	Dhananjay Dey	Quantitative Evaluation of C-H···O and C-H···π Intermolecular Interactions in Ethyl-3-benzyl-1-	2014	Journal of Chemical Crystallography	link

		methyl-2-oxoindoline-3-carboxylate and 3-Methyl-but-2-en-1-yl-1,3-dimethyl-2-oxoindoline-3-carboxylate: Insights from PIXEL and Hirshfeld Analysis			
84	Heike Fliegl	Coupled-cluster calculations of the lowest 0-0 bands of the electronic excitation spectrum of naphthalene	2014	Physical Chemistry Chemical Physics	link
85	Gangotri Dey	Copper reduction and atomic layer deposition by oxidative decomposition of formate by hydrazine	2014	RSC advances	link
86	Rahul Shukla	Experimental and theoretical analysis of lp···π intermolecular interactions in derivatives of 1,2,4-triazoles	2014	CrystEngComm	link
87	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
88	Jianwen Liu	Selective oxidation of propene by vanadium oxide monomers supported on silica	2014	Journal of catalysis	link
89	Mats Linder	On the method-dependence of transition state asynchronicity in Diels-Alder reactions	2013	Physical Chemistry Chemical Physics	link
90	Marc Steinmetz	Benchmark study of the performance of density functional theory for bond activations with (Ni, Pd) - based transition - metal catalysts	2013	ChemistryOpen	link

91	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
92	LiHong Hu	Accurate reaction energies in proteins obtained by combining QM/MM and large QM calculations	2013	Journal of Chemical Theory and Computation	link
93	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
94	Raphael J. F. Berger	Relativistic effects in triphenylbismuth and their influence on molecular structure and spectroscopic properties	2012	Physical Chemistry Chemical Physics	link
95	Mario Barbatti	Critical appraisal of excited state nonadiabatic dynamics simulations of 9H-adenine	2012	The Journal of Chemical Physics	link
96	Mikko Kaipio	Effect of fluorine substitution on the aromaticity of polycyclic hydrocarbons	2012	The Journal of Physical Chemistry A	link
97	Raphael J. F. Berger	Prediction of a cyclic helical oligoacetylene showing anapolar ring currents in the magnetic field	2012	Zeitschrift für Naturforschung B	link
98	Patxi García-Novo	Interaction between anions and substituted molecular bowls	2012	Physical Chemistry Chemical Physics	link
99	J.-M. Ducéré	Tail effect on trihydroxysilanes dimerization: A dispersion-corrected density functional theory study	2012	Surface science	link

100	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
101	Jean-Marie Ducéré	A computational chemist approach to gas sensors: Modeling the response of SnO2 to CO, O2, and H2O Gases	2012	Journal of Computational Chemistry	link
102	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
103	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
104	D. Rama Mohana Rao	Thermodynamic study of Eu (III) complexation by pyridine monocarboxylates	2012	The Journal of Chemical Thermodynamics	link
105	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