BIOVIA TURBOMOLE 関連論文リスト（1/26）

No.	First author	Title	Year	Journal name	Link
1	Erik Van Dyke	Towards detection of molecular parity violation via chiral co-sensing: the 1H/31P model system	2025	Physical Chemistry Chemical Physics	link
2	Josef Tomeček	Metal–Metal Bonding in Tri-Actinide Clusters: A DFT Study of [An3Cl6]z (z=1–6) and [An3Cl6Cp3]z (z=−2–+3; An=Ac, Th, Pa, U, Np, Pu)	2025	ChemPhysChem	link
3	Alessia Giordana	Exploring coinage bonding interactions in [Au(CN)4]− assemblies with silver and zinc complexes: a structural and theoretical study	2025	Physical Chemistry Chemical Physics	link
4	Kristoffer J. M. Lundgren	The CuB site in particulate methane monooxygenase may be used to produce hydrogen peroxide	2025	Dalton Transactions	link
5	Rosa M. Gomila	Noble gas bonds facilitate anion···anion supramolecular assemblies: insights from CSD and DFT analysis	2025	CrystEngComm	link
6	Amin Kiani	Intermolecular interaction potential maps from energy decomposition for interpreting reactivity and intermolecular interactions	2025	Physical Chemistry Chemical Physics	link
7	Seraj A. Ansari	Exploring the complexation behaviour of NpO2+ with diglycolamide in ionic liquid vs. aqueous solution	2025	Dalton Transactions	link
8	Nóra Kovács	An evaluation of local double hybrid density functionals	2025	Chemical Physics Letters	link
9	Jindřich Fanfrlík	Heats of formation on the way from B2H6 to B20H16: thermochemical consequences of multicenter bonding in ab initio and DFT methods	2025	Dalton Transactions	link

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10	Qian Wang	Magnetically Induced Current-Density Susceptibility of Circum[n]coronenes	2025	The Journal of Physical Chemistry A	link
11	Anton Florian Ketzel	Benchmark of Density Functional Theory in the Prediction of 13C Chemical Shielding Anisotropies for Anisotropic Nuclear Magnetic Resonance-Based Structural Elucidation	2025	Journal of Chemical Theory and Computation	link
12	Annasaheb Dhawale	Multifunctional Chemosensors for the Simultaneous Detection of Copper and Mercury Ions: Applications in Test Strip Fabrication, Spiking Studies, and Logic Gate Formulation	2025	ACS Omega	link
13	Julia Rienmüller	Isolation of a planar π-aromatic $Bi5^-$ ring in a cobalt-based inverse-sandwich-type complex	2025	Nature Chemistry	link
14	Sourav Majumdar	Mechanism of the Non-Kasha Fluorescence in Pyrene	2025	Journal of Computational Chemistry	link
15	Ali Al-Jaaidi	Ultrafast Dynamics of Diketopyrrolopyrrole Dimers	2025	Journal of Computational Chemistry	link
16	Simon Metz	Excitonic Coupling of a TADF Assistant Dopant and a Multi-Resonance TADF Emitter	2025	Advanced Optical Materials	link
17	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
18	Mitchell R. Whittam	Circular dichroism of relativistically–moving chiral molecules	2024	Scientific Reports	link

19	Sergi Burguera	Unconventional C—Hlg···H–C (Hlg = Cl, Br, and I) Interactions Involving Organic Halides: A Theoretical Study	2024	Molecules	link
20	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
21	Dang-Bao-An Tran	Continuous-wave cavity ringdown for high-sensitivity polarimetry and magnetometry measurements	2024	The Journal of Chemical Physics	link
22	Danillo Valverde	Computational investigations of the detailed mechanism of reverse intersystem crossing in inverted singlet–triplet gap molecules	2024	ACS Applied Materials & Interfaces	link
23	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
24	Qian Wang	Changing aromatic properties through stacking: the face-to-face dimer of Ni(II) bis(pentafluorophenyl)norcorrole	2024	Physical Chemistry Chemical Physics	link
25	Hao Jiang	H2 formation from the E2–E4 states of nitrogenase	2024	Physical Chemistry Chemical Physics	link
26	Marc Reimann	Rydberg electron stabilizes the charge localized state of the diamine cation	2024	Nature Communications	link
27	Patricia Godermajer	Degradable bispiperidone derivative amine networks with monomer recovery	2024	Polymer Chemistry	link

28	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
29	Markus Nyman	A digital twin for a chiral sensing platform	2024	Laser & Photonics Reviews	link
30	Daniel Blasco	The aromatic nature of auracycles and diauracycles based on calculated ring-current strengths	2024	Dalton Transactions	link
31	Robin Grotjahn	Chemically Accurate Singlet–Triplet Gaps of Arylcarbenes from Local Hybrid Density Functionals	2024	The Journal of Physical Chemistry A	link
32	Annina Z. Lieberherr	Optimal transport distances to characterize electronic excitations	2024	Journal of Chemical Theory and Computation	link
33	Raphael I. Petrikat	A Photoswitchable Metallocycle Based on Azobenzene: Synthesis, Characterization, and Ultrafast Dynamics	2024	Chemistry – A European Journal	link
34	Ahmadreza Rajabi	A DFT perspective on organometallic lanthanide chemistry	2024	Dalton Transactions	link
35	Réka A. Horváth	Which model density is best in pair natural orbital local correlation theory?	2024	Chemical Physics Letters	link
36	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
37	Praveen Naik	Exploring optical, electrochemical, thermal, and theoretical aspects of simple carbazole-derived organic dyes	2024	Heliyon	link

38	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
39	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
40	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
41	Zheng-Wang Qu	Mechanism of Alkaline Earth Metal Amide Catalyzed Hydrogenation of Challenging Alkenes and Arenes	2024	ChemSusChem	link
42	Thomas Gasevic	Benchmark Study on the Calculation of 207Pb NMR Chemical Shifts	2024	Inorganic Chemistry	link
43	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
44	Sergi Burguera	Manganese matere bonds in biological systems: PDB inspection and DFT calculations	2024	Physical Chemistry Chemical Physics	link
45	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

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

56	Ahmed Shaalan Alag	Ab initio investigation of excited state charge transfer pathways in differently capped bithiophene cages	2024	Journal of Computational Chemistry	link
57	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
58	Usman Ahmed	The effect of hydrogen bonding on the π depletion and the $\pi-\pi$ stacking interaction	2024	Physical Chemistry Chemical Physics	link
59	Dominique J. Luder	Polar covalent apex - base bonding in borapyramidanes probed by solid - state NMR and DFT calculations	2024	Chemistry – A European Journal	link
60	Matheus Máximo-Canadas	Ab initio electronic absorption spectra of para - nitroaniline in different solvents: Intramolecular charge transfer effects	2024	Journal of Computational Chemistry	link
61	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
62	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
63	Sergi Burguera	A novel approach for estimating the strength of argentophilic and aurophilic interactions using QTAIM parameters	2024	Physical Chemistry Chemical Physics	link
64	Guillaume Bastien	Triptycene - Based Tripodal Molecular Platforms	2024	Chemistry – A European Journal	link

65	María de las Nieves Piña	Diphenylene Iodonium as a Prominent Halogen Bond Donor: The Case of Human Monoamine Oxidase B	2024	ChemPhysChem	link
66	Ariel C. Jones	Exploring non-covalent interactions in excited states: beyond aromatic excimer models	2024	Physical Chemistry Chemical Physics	link
67	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
68	Vitor Angelo Fonseca Deichmann	Design and Synthesis of Red-Absorbing Fluoran Leuco Dyes Supported by Computational Screening	2024	ACS Omega	link
69	Jascha Martini	Vibronic Splitting of the Electronic Origin in Two Conformers of the 3 - Tolunitrile Dimer	2024	ChemPhysChem	link
70	Pierre-François Loos	A mountaineering strategy to excited states: Accurate vertical transition energies and benchmarks for substituted benzenes	2024	Journal of Computational Chemistry	link
71	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
72	Marko Horbatsch	Calculation of Low-Lying Electronic Excitations of Magnesium Monofluoride: How Well Do Coupled-Cluster Methods Work?	2024	Atoms	link
73	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

74	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
75	Mirza Wasif Baig	Relativistic two-component density functional study of ethyl 2-(2-Iodobenzylidenehydrazinyl)thiazole-4-carboxylate	2024	Computational and Theoretical Chemistry	link
76	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
77	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
78	Ryan L. Dempsey	Computational study of the interactions of tetravalent actinides (An = Th–Pu) with the α-Fe13 Keggin cluster	2024	Dalton Transactions	link
79	Hao Jiang	Putative reaction mechanism of nitrogenase with a half-dissociated S2B ligand	2024	Dalton Transactions	link
80	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
81	Laura Galleni	The C1s core levels of polycyclic aromatic hydrocarbons and styrenic polymers: A first-principles study	2024	The Journal of Chemical Physics	link
82	Risa Amano	Optical force and torque in near-field excitation of C3H6: A first-principles study using RT-TDDFT	2024	The Journal of Chemical Physics	link

83	Jindřich Fanfrlík	Heats of Formation on the Way from B2H6 to B20H16: Thermochemical Consequences of Multicenter Bonding in Ab initio and DFT Methods	2024	Dalton Transactions	link
84	J. T. Kohn	A semi-automated quantum-mechanical workflow for the generation of molecular monolayers and aggregates	2024	The Journal of Chemical Physics	link
85	Daisuke Nishizawa	Near-field induced local excitation dynamics of Na10 and Na10–N2 from real-time TDDFT	2024	The Journal of Chemical Physics	link
86	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
87	Lukas Hehn	Chelate Complexes of 3d Transition Metal Ions—A Challenge for Electronic-Structure Methods?	2024	Journal of Chemical Theory and Computation	link
88	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
89	Zheng-Wang Qu	Mechanism of Borane-Catalyzed Oligomerization of Arylallenes and Arylacetylenes	2024	European Journal of Organic Chemistry	link
90	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
91	Zheng-Wang Qu	Reactivity of Frustrated Lewis Pair: Carbocation versus Radical Intermediates	2024	Chemistry – A European Journal	link
92	Özlem Yönder	A computational chemistry study on the evolution of oxygen functional groups during char burnout	2024	Fuel	link

93	Ismael A. Elayan	Beyond Explored Functionals: A Computational Journey of Two-Photon Absorption	2024	Journal of Chemical Theory and Computation	link
94	Rosendo Valero	Estimating Nonradiative Excited-State Lifetimes in Photoactive Semiconducting Nanostructures	2024	The Journal of Physical Chemistry C	link
95	Frédéric Célerse	Unveiling the Full Dynamical and Reactivity Profiles of Acetylcholinesterase: A Comprehensive All-Atom Investigation	2024	ACS Catalysis	link
96	Eimear Madden	The effect of particle size on the optical and electronic properties of hydrogenated silicon nanoparticles	2024	Physical Chemistry Chemical Physics	link
97	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
98	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
99	Benjamin Peerless	ϕ-Aromaticity in prismatic {Bi6}-based clusters	2023	Nature Chemistry	link
100	Kevin Issler	Time-resolved photoelectron spectroscopy of 4-(dimethylamino) benzethyne–an experimental and computational study	2023	Physical Chemistry Chemical Physics	link
101	Muhammad Naeem Ahmed	Crystal engineering with 1, 3, 4-oxadiazole derivatives: on the importance of CH···N and CH···π interactions	2023	CrystEngComm	link
102	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

103	Markus Nyman	A digital twin for a chiral sensing platform	2023	Laser & Photonics Reviews	link
104	Julia Kohn	Computational study of ground-state properties of μ2-bridged group 14 porphyrinic sandwich complexes	2023	Journal of Computational Chemistry	link
105	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
106	David Yubero Valdivielso	IR spectra and structures of saturated ruthenium cluster carbonyl cations Run(CO)m+ (n = 1–6)	2023	Dalton Transactions	link
107	Ali Ghiami-Shomami	Performance of the COSMO solvation model for photoacidity and basicity in water	2023	Journal of Computational Chemistry	link
108	Probal Nag	Understanding the photodynamics of 3-hydroxypyran-4-one using surface hopping simulations	2023	Journal of Photochemistry and Photobiology A: Chemistry	link
109	Tim Schrader	Performance of common density functionals for excited states of tetraphenyldibenzoperiflanthene	2023	The Journal of Physical Chemistry A	link
110	Maite Nößler	Electrochemistry and Spin-Crossover Behavior of Fluorinated Terpyridine-Based Co(II) and Fe(II) Complexes	2023	European Journal of Inorganic Chemistry	link
111	Sonia Jafari	Two local minima for structures of [4Fe–4S] clusters obtained with density functional theory methods	2023	Scientific Reports	link
112	Christoph Schissler	Marriage of an N-Fused and a Regular Porphyrin in a Cofacial Ligand System	2023	Organometallics	link
113	Zohreh Hashemi	Mapping charge-transfer excitations in Bacteriochlorophyll dimers from first principles	2023	Electronic Structure	link

114	Sergi Burguera	Matere Bonds in Technetium Compounds: CSD Survey and Theoretical Considerations	2023	Crystals	link
115	Moritz Bensberg	Corresponding active orbital spaces along chemical reaction paths	2023	The Journal of Physical Chemistry Letters	link
116	Erik Andris	Can Copper (I) and Silver (I) be Hydrogen Bond Acceptors?	2023	Chemistry – A European Journal	link
117	Adam Šrut	The Marcus dimension: identifying the nuclear coordinate for electron transfer from ab initio calculations	2023	Chemical Science	link
118	Sergi Burguera	Hg(II)·d8[M] Interactions: Are they Metallophilic Interactions or Spodium Bonds?	2023	ChemPhysChem	link
119	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
120	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
121	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
122	Anthony Ferté	ESIPT in the pyrrol pyridine molecule: mechanism, timescale and yield revealed using dynamics simulations	2023	Physical Chemistry Chemical Physics	link

123	Sergi Burguera	Biological noncovalent N/O··· V interactions: insights from theory and protein data bank analyses	2023	Physical Chemistry Chemical Physics	link
124	Ritam Mansour	Temperature effects on the internal conversion of excited adenine and adenosine	2023	Physical Chemistry Chemical Physics	link
125	Paul De Bonfils	Synthesis and Photophysical Characterizations of Pyrroloquinolone Photosensitizers for Singlet Oxygen Production	2023	Photochemistry and Photobiology	link
126	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
127	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
128	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
129	Gloria Tobajas-Curiel	Solvation rules: aromatic interactions outcompete cation–π interactions in synthetic host–guest complexes in water	2023	Chemical Communications	link
130	Jessica Groß	Computational Study on a Transfer Hydrogenation Catalysed by a Ru (II) Bis - Pyrazolyl Pyridine Complex	2023	Israel Journal of Chemistry	link
131	Hao Jiang	N2 binding to the E0–E4 states of nitrogenase	2023	Dalton Transactions	link

132	Sulafa Abdalmageed Saadaldeen Mohammed	Experimental and computational evaluation of 1, 2, 4-triazolium-based ionic liquids for carbon dioxide capture	2023	Separations	link
133	Praveen Naik	Synthesis, optical, electrochemical, and computational investigation of new cyanopyridine-centered organic dyads	2023	Optical Materials	link
134	Nenad Jovanović	Fractal nature of benzene stacking interactions	2023	Journal of Molecular Modeling	link
135	Chengcheng Tang	One Molecule Suffices: Spectroscopy of Yariv Reagents	2023	ChemistrySelect	link
136	Tim Schrader	Koopmans' theorem for acidic protons	2023	Chemical Communications	link
137	Victor P. Vysotskiy	Assessment of DFT functionals for a minimal nitrogenase [Fe(SH)4H]− model employing state-of-the-art ab initio methods	2023	The Journal of Chemical Physics	link
138	Gloria Tobajas-Curiel	Aromatic interactions with heterocycles in water	2023	Chemical Science	link
139	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
140	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
141	Daniel Blasco	Gold (I)-containing light-emitting molecules with an inverted singlet–triplet gap	2023	Chemical Science	link
142	Georgyi Koidan	Straightforward Synthesis of Halopyridine Aldehydes via Diaminomethylation	2023	Chemistry – A European Journal	link

143	Javad Shirazi	Catalytic Reaction Mechanism of Glyoxalase II: A Quantum Mechanics/Molecular Mechanics Study	2023	The Journal of Physical Chemistry B	link
144	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
145	Qian Wang	The magnetically induced current density of the [12] infinitene dianion	2023	Physical Chemistry Chemical Physics	link
146	Atif Mahmood	Current-Density Calculations on Zn-Porphyrin40 Nanorings	2023	The Journal of Physical Chemistry A	link
147	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
148	Gloria Tobajas-Curiel	Solvation rules: aromatic interactions outcompete cation-π interactions in synthetic host–guest complexes in water	2023	Chemical Communications	link
149	Łukasz Wolański	Quadripartite bond length rule applied to two prototypical aromatic and antiaromatic molecules	2023	Journal of Molecular Modeling	link
150	Gloria Tobajas-Curiel	Substituent effects on aromatic interactions in water	2023	Chemical Science	link
151	Praveen Naik	A computational approach for screening carbazole based organic dyes as potential photosensitizers for DSSCs application	2023	Results in Chemistry	link
152	Weiwei Li	Resonance effect in Brunel harmonic generation in thin film organic semiconductors	2023	Advanced Optical Materials	link

153	Jessica Groß	Computational Study on a Transfer Hydrogenation Catalysed by a Ru (II) Bis-Pyrazolyl Pyridine Complex	2023	Israel Journal of Chemistry	link
154	Ritam Mansour	Pre-Dewar structure modulates protonated azaindole photodynamics	2022	Physical Chemistry Chemical Physics	link
155	Raphael J. F. Berger	Integration of global ring currents using the Ampère–Maxwell law	2022	Physical Chemistry Chemical Physics	link
156	Lewis Hutton	Photodynamics of Gas-Phase Pyruvic Acid Following Light Absorption in the Actinic Region	2022	ChemPhotoChem	link
157	Keisuke Hirata	Excited state dynamics of protonated dopamine: hydration and conformation effects	2022	Physical Chemistry Chemical Physics	link
158	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
159	Markus Bursch	Theoretical study on conformational energies of transition metal complexes	2021	Physical Chemistry Chemical Physics	link
160	Arjeta Rushiti	Activation of Molecular O2 on CoFe2O4 (001) Surfaces: An Embedded Cluster Study	2021	Chemistry–A European Journal	link
161	Lin Yang	High coordination number actinide-noble gas complexes; a computational study	2021	Physical Chemistry Chemical Physics	link
162	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

163	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
164	Naveenchandra Pilicode	New cyanopyridine based conjugated polymers carrying auxiliary electron donors: from molecular design to blue emissive PLEDs	2020	Dyes and Pigments	link
165	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
166	Rama Mohana Rao Dumpala	Aquatic interaction of uranium with two naturally ubiquitous pyrazine compounds: Speciation studies by experiment and theory	2020	Chemosphere	link
167	S. A. Khan	Palladium (II) complexes based on N, S-donor ligands: synthesis and molecular structures	2019	Journal of Structural Chemistry	link
168	Emily R. Draper	Insight into the self-assembly of water-soluble perylene bisimide derivatives through a combined computational and experimental approach	2019	Nanoscale	link
169	Matthias Stein	Intermolecular interactions in molecular organic crystals upon relaxation of lattice parameters	2019	Crystals	link
170	Lili Cao	Extremely large differences in DFT energies for nitrogenase models	2019	Physical Chemistry Chemical Physics	link
171	Octav Caldararu	Mechanism of hydrogen peroxide formation by lytic polysaccharide monooxygenase	2019	Chemical Science	link

172	Hannes Konrad Buchholz	Accurate lattice energies of organic molecular crystals from periodic turbomole calculations	2018	Journal of Computational Chemistry	link
173	Samuel Bouvron	Charge transport in a single molecule transistor probed by scanning tunneling microscopy	2018	Nanoscale	link
174	Mirko Matthias Lindic	Excited state dipole moments of anisole in gas phase and solution	2018	Journal of Photochemistry and Photobiology A: Chemistry	link
175	Praveen Naik	Investigation of new carbazole based metal-free dyes as active photo-sensitizers/co-sensitizers for DSSCs	2018	Dyes and Pigments	link
176	Gang Feng	Hydrogen Spillover to Copper Clusters on Hydroxylated γ-Al2O3	2018	The Journal of Physical Chemistry C	link
177	Praveen Naik	Molecular Engineering of a New Organic Chromophore with D-π-A Architecture for Dye-Sensitized Solar Cells	2018	Materials Today: Proceedings	link
178	Rashid R. Valiev	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34] octaphyrins	2018	Physical Chemistry Chemical Physics	link
179	Praveen Naik	Synthesis, characterization and performance studies of a new metal-free organic sensitizer for DSSC application	2018	Materials Today: Proceedings	link
180	Mohd. Athar	Investigation of structural and conformational equilibrium of Oxacalix [4] arene: A density functional theory approach	2017	Journal of Molecular Liquids	link
181	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

182	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
183	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
184	Yannick J. Franzke	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays	2017	Physical Chemistry Chemical Physics	link
185	Shailja Jain	The Unusual Role of Aromatic Solvent in Single - Site Aluminuml Chemistry: Insights from Theory	2017	Chemistry–A European Journal	link
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