Tanja van Mourik

List of Publications by Year in descending order

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71 papers	1,956 citations	257450 24 h-index	254184 43 g-index
72 all docs	72 docs citations	72 times ranked	2034 citing authors

#	Article	IF	Citations
1	A critical note on density functional theory studies on rare-gas dimers. Journal of Chemical Physics, 2002, 116, 9620-9623.	3.0	221
2	Molecular Conformations and Relative Stabilities Can Be as Demanding of the Electronic Structure Method as Intermolecular Calculations. Journal of Physical Chemistry A, 2006, 110, 8-12.	2.5	115
3	Insufficient description of dispersion in B3LYP and large basis set superposition errors in MP2 calculations can hide peptide conformers. Chemical Physics Letters, 2007, 442, 42-46.	2.6	110
4	Ab initio and diffusion Monte Carlo study of uracilâ€“water, thymineâ€“water, cytosineâ€“water, and cytosineâ€“(water)2. Physical Chemistry Chemical Physics, 2000, 2, 1281-1290.	2.8	88
5	First-Principles Calculation of the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules. Journal of Chemical Theory and Computation, 2012, 8, 3322-3337.	5.3	84
6	Density functional theory across chemistry, physics and biology. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120488.	3.4	84
7	Neurotransmitters in the gas phase: a computational and spectroscopic study of noradrenaline. Molecular Physics, 2003, 101, 1239-1248.	1.7	78
8	NMR spectroscopy: quantumâ€chemical calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 634-647.	14.6	76
9	Characterization of the Monovalent Ion Position and Hydrogen-Bond Network in Guanine Quartets by DFT Calculations of NMR Parameters. Chemistry - A European Journal, 2005, 11, 6064-6079.	3.3	65
10	Assessment of Density Functionals for Intramolecular Dispersion-Rich Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1610-1619.	5.3	65
11	Conformational Structure of Tyrosine, Tyrosyl-glycine, and Tyrosyl-glycyl-glycine by Double Resonance Spectroscopy. Journal of Physical Chemistry A, 2011, 115, 6077-6087.	2.5	60
12	The structure of the gas-phase tyrosineâ€“glycine dipeptide. Molecular Physics, 2006, 104, 559-570.	1.7	56
13	H-Densities:â€‰ A New Concept for Hydrated Molecules. Accounts of Chemical Research, 2000, 33, 441-447.	15.6	55
14	Complete conformational space of the potential HIV-1 reverse transcriptase inhibitors d4U and d4C. A quantum chemical study. Physical Chemistry Chemical Physics, 2012, 14, 6787.	2.8	50
15	A theoretical study of uracilâ€“(H2O)n, n = 2 to 4. Physical Chemistry Chemical Physics, 2001, 3, 2886-2892.	2.8	45
16	A theoretical study of the conformational landscape of serotoninElectronic supplementary information (ESI) available: computed harmonic hydride stretch frequencies and intensities of the serotonin (OH-anti) and (OH-syn) conformers. See http://www.rsc.org/suppdata/cp/b2/b207565b/. Physical Chemistry Chemical Physics, 2002, 4, 5863-5871.	2.8	45
17	The shape of neurotransmitters in the gas phase: A theoretical study of adrenaline, pseudoadrenaline, and hydrated adrenalineElectronic supplementary information (ESI) available: Relative energies of all adrenaline and pseudoadrenaline conformers studied. See http://www.rsc.org/suppdata/cp/b3/b315520j/. Physical Chemistry Chemical Physics, 2004, 6, 2827.	2.8	45
18	Neurotransmitters in the gas phase: hydrated noradrenaline. Physical Chemistry Chemical Physics, 2003, 5, 4519-4526.	2.8	44

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19	New Class of Metal Bound Molecular Switches Involving H-Tautomerism. Nano Letters, 2014, 14, 634-639.	9.1	37
20	A DFT study of uracil and 5-bromouracil in nanodroplets. Theoretical Chemistry Accounts, 2010, 125, 233-244.	1.4	31
21	Structural and energetic properties of the potential HIV-1 reverse transcriptase inhibitors d4A and d4G: a comprehensive theoretical investigation. Journal of Biomolecular Structure and Dynamics, 2014, 32, 730-740.	3.5	31
22	DNA base stacking: The stacked uracil/uracil and thymine/thymine minima. Journal of Computational Chemistry, 2012, 33, 2161-2172.	3.3	28
23	Are the Sublimation Thermodynamics of Organic Molecules Predictable?. Journal of Chemical Information and Modeling, 2016, 56, 2162-2179.	5.4	28
24	Simulation of electrochemical properties of naturally occurring quinones. Scientific Reports, 2020, 10, 13571.	3.3	28
25	Indication of water droplet formation in hydrated clusters of cytosine and adenine: An electronic structure study using B3LYP, LMP2 and PM6. Chemical Physics Letters, 2007, 445, 303-308.	2.6	23
26	Competition between hydrogen and halogen bonding in halogenated 1â€methyluracil: Water systems. Journal of Computational Chemistry, 2016, 37, 763-770.	3.3	21
27	Quinoneâ€based switches for candidate building blocks of molecular junctions with QTAIM and the stress tensor. International Journal of Quantum Chemistry, 2018, 118, e25676.	2.0	21
28	Characterizing the Cooperativity in H-Bonded Amino Structures. Journal of Physical Chemistry A, 2007, 111, 11350-11358.	2.5	19
29	Comment on â€œAromaticâ€Backbone Interactions in Model Î±â€Helical Peptidesâ€•[Palermo et al., J Comput Chem 2007, 28, 1208]. Journal of Computational Chemistry, 2008, 29, 1-3.	3.3	17
30	Density functional theory reveals an increase in the amino H1 chemical shift in guanine due to hydrogen bonding with water. Journal of Chemical Physics, 2006, 125, 191101.	3.0	15
31	DNA base stacking involving adenine and 2-aminopurine. Structural Chemistry, 2016, 27, 145-158.	2.0	15
32	The destabilization of hydrogen bonds in an external Eâ€field for improved switch performance. Journal of Computational Chemistry, 2019, 40, 1881-1891.	3.3	15
33	The potential energy landscape of noradrenaline: An electronic structure study. Molecular Physics, 2005, 103, 1641-1654.	1.7	14
34	Performance of the M06-L density functional for a folded Tyrâ€“Gly conformer. Chemical Physics Letters, 2010, 485, 40-44.	2.6	13
35	Nextâ€generation QTAIM for scoring molecular wires in Eâ€fields for molecular electronic devices. Journal of Computational Chemistry, 2020, 41, 913-921.	3.3	12
36	Firstâ€“principles quantum chemistry in the life sciences. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2004, 362, 2653-2670.	3.4	11

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37	Modelling Zwitterions in Solution: 3â€Fluoroâ€Î³â€aminobutyric Acid (3Fâ€GABA). Chemistry - A European Journal, 2012, 18, 184-195.	3.3	11
38	A QTAIM exploration of the competition between hydrogen and halogen bonding in halogenated 1-methyluracil: Water systems. Chemical Physics Letters, 2016, 662, 67-72.	2.6	10
39	Comment on â€˜To stack or not to stack: Performance of a new density functional for the uracil and thymine dimersâ€™ [Chem. Phys. Lett. 459 (2008) 164]. Chemical Physics Letters, 2009, 473, 206-208.	2.6	9
40	Stacking of the mutagenic DNA base analog 5-bromouracil. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	9
41	Next generation QTAIM for the design of quinone-based switches. Chemical Physics Letters, 2019, 722, 110-118.	2.6	9
42	PM6 quantum chemical study of the H-bonded and stacked associates of the adenine and thymine DNA bases: The nature of base stacking. Molecular Physics, 2008, 106, 1487-1494.	1.7	8
43	Stacking of the mutagenic base analogue 5-bromouracil: energy landscapes of pyrimidine dimers in gas phase and water. Physical Chemistry Chemical Physics, 2015, 17, 30364-30370.	2.8	8
44	A DFT study of 2-aminopurine-containing dinucleotides: prediction of stacked conformations with B-DNA structure. Physical Chemistry Chemical Physics, 2016, 18, 14691-14700.	2.8	8
45	Halogen and Hydrogen Bonding in Halogenabenzene/NH3 Complexes Compared Using Next-Generation QTAIM. Molecules, 2019, 24, 2875.	3.8	8
46	Control of chirality, bond flexing and anharmonicity in an electric field. International Journal of Quantum Chemistry, 2021, 121, e26793.	2.0	8
47	Chirality without Stereoisomers: Insight fromÂthe Helical Response of Bond Electrons. ChemPhysChem, 2021, 22, 1989-1995.	2.1	8
48	Chiral and steric effects in ethane: A next generation QTAIM interpretation. Chemical Physics Letters, 2022, 800, 139669.	2.6	8
49	Ï€ Interactions Studied with Electronic Structure Methods: The Ethyne Methyl Isocyanide Complex and Thioanisole. Journal of Chemical Theory and Computation, 2010, 6, 2687-2700.	5.3	7
50	The nature of base stacking: a Monte Carlo study. Theoretical Chemistry Accounts, 2011, 130, 859-870.	1.4	7
51	Mixed chiral and achiral character in substituted ethane: A next generation QTAIM perspective. Chemical Physics Letters, 2022, 803, 139762.	2.6	7
52	Tyrosine-glycine revisited: Resolving the discrepancy between theory and experiment. Chemical Physics Letters, 2015, 621, 124-128.	2.6	6
53	Halogen bonding in monoâ€•and dihydrated halobenzene. Journal of Computational Chemistry, 2018, 40, 554-561.	3.3	6
54	Conformational Landscape of the Nucleoside Reverse Transcriptase Inhibitor d4T: a Comprehensive Quantum-Chemical Approach. Current Physical Chemistry, 2013, 3, 83-92.	0.2	6

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55	Geometry Dependence of Spinâ€“Spin Couplings in Cyanamide by DFT Analysis. ChemPhysChem, 2007, 8, 288-296.	2.1	5
56	Intramolecular BSSE and dispersion affect the structure of a dipeptide conformer. Molecular Physics, 2018, 116, 1236-1244.	1.7	4
57	13C-1H coupling constants as a conformational tool for structural assignment of quinic and octulosonic acid. Journal of Molecular Modeling, 2018, 24, 324.	1.8	4
58	Halogen bonding with the halogenabenzene bird structure, halobenzene, and halocyclopentadiene. Journal of Computational Chemistry, 2019, 40, 2111-2118.	3.3	4
59	Halogen-Bonded Guanine Base Pairs, Quartets and Ribbons. International Journal of Molecular Sciences, 2020, 21, 6571.	4.1	4
60	Next generation quantum theory of atoms in molecules for the design of emitters exhibiting thermally activated delayed fluorescence with laser irradiation. Journal of Computational Chemistry, 2022, 43, 206-214.	3.3	4
61	Different substituent effects on the supramolecular arrays in some (E)-halo- and nitro-benzaldehyde oximes: confirmation of attractive Ï€(C=N)Â·Â·Â·Ï€(phenyl) interactions. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2019, 74, 319-334.	0.7	3
62	A quinone based single-molecule switch as building block for molecular electronics. Physical Chemistry Chemical Physics, 2021, 23, 1811-1814.	2.8	3
63	Gaussian basis sets for use in correlated molecular calculations. VIII. Standard and augmented sextuple zeta correlation consistent basis sets for aluminum through argon. , 0, .		3
64	Gaussian basis sets for use in correlated molecular calculations. VIII. Standard and augmented sextuple zeta correlation consistent basis sets for aluminum through argon. International Journal of Quantum Chemistry, 2000, 76, 205.	2.0	3
65	DFT study of polymorphism of the DNA double helix at the level of dinucleoside monophosphates. International Journal of Quantum Chemistry, 2010, 110, 2548-2559.	2.0	2
66	A comment on â€œAccurate ab initio determination of binding energies for rare-gas dimers by basis set extrapolationâ€• Theoretical Chemistry Accounts, 2006, 115, 274-275.	1.4	1
67	Computational Studies of Bridging Structures and Isomerism in Substituted Disilynes. Journal of Chemical Theory and Computation, 2013, 9, 2697-2705.	5.3	1
68	Consequences of theory level choice evaluated with new tools from QTAIM and the stress tensor for a dipeptide conformer. Chemical Physics Letters, 2018, 696, 42-47.	2.6	1
69	Towards a symmetric reversible single-molecule switch: Amino-imino-cyclo-n-enes. Chemical Physics Impact, 2021, 3, 100035.	3.5	1
70	Crystal structures, Hirsfeld surface analysis and a computational study of four ethyl 2-oxo-2H-chromene-3-carboxylate derivatives: a survey of organyl 2-oxo-2H-chromene-3-carboxylate structures. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 85-99.	0.8	0
71	A computational study of TyrGly hydration. Computational and Theoretical Chemistry, 2020, 1190, 113011.	2.5	0