Shmuel Zilberg

List of Publications by Year
in descending order

56	1,249	331259	377514
papers	citations	21 h-index	34 g-index

57	57	57	1187
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Controllable Electron Transfer in Mixed-Valence Bridged Norbornylogous Compounds:Ab InitioCalculation Combined with a Parametric Model and Through-Bond and Through-Space Interpretation. Journal of Physical Chemistry A, 2022, 126, 2855-2878.	1.1	6
2	Insight Into The Spinâ€Vibronic Problem of a Mixed Valence Magnetic Molecular Cell for Quantum Cellular Automata. ChemPhysChem, 2021, 22, 1754-1768.	1.0	1
3	In Search of the Perfect Triple BB Bond: Mechanical Tuning of the Host Molecular Trap for the Triple Bond Bâ‰¡B Fragment. Molecules, 2021, 26, 6428.	1.7	1
4	Can the Double Exchange Cause Antiferromagnetic Spin Alignment?. Magnetochemistry, 2020, 6, 36.	1.0	6
5	A parametric two-mode vibronic model of a dimeric mixed-valence cell for molecular quantum cellular automata and computationalab initioverification. Physical Chemistry Chemical Physics, 2020, 22, 25982-25999.	1.3	15
6	Mixed-Valence Magnetic Molecular Cell for Quantum Cellular Automata: Prospects of Designing Multifunctional Devices through Exploration of Double Exchange. Journal of Physical Chemistry C, 2020, 124, 25602-25614.	1.5	9
7	Long-Range Nâ€“N Bonding by Rydberg Electrons. Journal of Physical Chemistry Letters, 2020, 11, 2284-2290.	2.1	8
8	Design of Lightâ€Induced Molecular Switcher for the Driver of the Quantum Cellular Automata (QCA) Based on the Transition through the Intramolecular Charge Transfer (ICT) Structure. Israel Journal of Chemistry, 2020, 60, 570-576.	1.0	3
9	Double-Dimeric Versus Tetrameric Cells for Quantum Cellular Automata: a Semiempirical Approach to Evaluation of Cellâ€“Cell Responses Combined with Quantum-Chemical Modeling of Molecular Structures. Journal of Physical Chemistry C, 2019, 123, 22614-22623.	1.5	17
10	Stronger Hydrogen Bonds of Less Stable Tautomers in the Ground State and Reversed Stability in the First Excited State: The Role of Electronic Excited States in Hydrogen-Bonding. , 2019, , 239-273.		1
11	Carbonate and carbonate anion radicals in aqueous solutions exist as CO₃(H₂O)₆^{2â¯} and CO₃(H₂O)₆Ë™^{â¯} respectively: the crucial role of the inner hydration sphere of anions in explaining their properties. Physical Chemistry Chemical Physics, 2019, 20, 9429-9435.	1.3	26
12	Triple Bâ‰¡B bond: from a perfect Lewis structure to a dominant Ï€-back-donation. The need for a reference point. Journal of Coordination Chemistry, 2018, 71, 2053-2064.	0.8	5
13	Less stable tautomers form stronger hydrogen bonds: the case of water complexes. Physical Chemistry Chemical Physics, 2017, 19, 25086-25094.	1.3	7
14	Finding structural principles for strong hydrogen-bonds: Less stable tautomers form dimers with stronger hydrogen bonds.. ChemistrySelect, 2016, 1, 195-200.	0.7	2
15	Origin of the Regioselectivity in the Gasâ€Phase Aniline+CH₃⁺ Electrophilic Aromatic Substitution. ChemPhysChem, 2015, 16, 2366-2374.	1.0	0
16	Chemical reaction with two different elementary transition states. International Journal of Quantum Chemistry, 2014, 114, 1162-1168.	1.0	4
17	Gas-phase electrophilic aromatic substitution mechanism with strong electrophiles explained by ab initio non-adiabatic dynamics. Physical Chemistry Chemical Physics, 2014, 16, 18686-18689.	1.3	3
18	The Raman spectrum of dimethylaminophenyl pentazole (DMAPP). Chemical Physics Letters, 2013, 556, 127-131.	1.2	17

#	Article	IF	Citations
19	Nuclear Spin Selective Torsional States: Implications of Molecular Symmetry. Zeitschrift Fur Physikalische Chemie, 2013, 227, 1021-1048.	1.4	9
20	Reply to â€œComment on 'The Frequency Upshift in BO2 and CO2+ upon Electronic Excitation: A Twin-State Model Rationalization'â€• Journal of Physical Chemistry A, 2012, 116, 1318-1318.	1.1	1
21	Role of Rydberg States in the Photostability of Heterocyclic Dimers: The Case of Pyrazole Dimer. Journal of Physical Chemistry A, 2012, 116, 11111-11117.	1.1	2
22	The photo-dissociation of the pyrroleâ€“ammonia complexâ€”the role of hydrogen bonding in Rydberg states photochemistry. Physical Chemistry Chemical Physics, 2012, 14, 8836.	1.3	8
23	Towards experimental determination of conical intersection properties: a twin state based comparison with bound excited states. Physical Chemistry Chemical Physics, 2011, 13, 11872.	1.3	1
24	Frequency Upshift in BO2and CO2+upon Electronic Excitation: A Twin-State Model Rationalization. Journal of Physical Chemistry A, 2011, 115, 10650-10654.	1.1	8
25	Solvent Tuning of a Conical Intersection: Direct Experimental Verification of a Theoretical Prediction. Journal of Physical Chemistry A, 2011, 115, 10854-10861.	1.1	25
26	Electronic structure of 9-mesityl-10-methylacridinium in ground and excited states: charge-shift mechanism introduced by counter anion shift. Physical Chemistry Chemical Physics, 2010, 12, 10292.	1.3	11
27	Stability of Polynitrogen Compounds: The Importance of Separating the Ïƒ and Ï€ Electron Systems. Journal of Physical Chemistry A, 2009, 113, 7376-7382.	1.1	56
28	Predicted stability of the organo-xenon compound HXeCCH above the cryogenic range. Chemical Physics Letters, 2008, 460, 23-26.	1.2	34
29	Locating conical intersections relevant to photochemical reactions. Chemical Physics, 2008, 347, 65-77.	0.9	20
30	Properties of Stable Organic Bond-Stretched Non-Lewis Molecules. Journal of Physical Chemistry A, 2008, 112, 12799-12805.	1.1	2
31			

#	Article	IF	Citations
37	The nature of the S1/S0 conical intersection of fulvene. Chemical Physics, 2006, 325, 251-256.	0.9	15
38	The use of elementary reaction coordinates in the search for conical intersections. International Journal of Quantum Chemistry, 2005, 102, 961-970.	1.0	33
39	Charge Separation in Ground-State 1,2,4,5-Tetra-Substituted Benzene Derivatives. Journal of the American Chemical Society, 2004, 126, 8991-8998.	6.6	27
40	Formation of the cyclo-Pentazolate N5- Anion by High-Energy Dissociation of Phenylpentazole Anions. Journal of Physical Chemistry A, 2004, 108, 11715-11720.	1.1	35
41	Electronic Degeneracies in Symmetric (Jahnâ^'Teller) and Nonsymmetric Aliphatic Radical Cations:Â Global Topology of Ïƒ-Bonded Molecules. Journal of the American Chemical Society, 2003, 125, 1810-1820.	6.6	17
42	Isomerization around a Cî€N double bond and a Cî€C double bond with a nitrogen atom attached: thermal and photochemical routes. Photochemical and Photobiological Sciences, 2003, 2, 1256-1263.	1.6	31
43	A Valence Bond Analysis of Electronic Degeneracies in Jahnâ^'Teller Systems:â€‰ Low-Lying States of the Cyclopentadienyl Radical and Cation. Journal of the American Chemical Society, 2002, 124, 10683-10691.	6.6	35
44	The Nature of the Intramolecular Charge Transfer Excited State in p-Pyrrolocyanobenzene (PBN) and Other Derivatives of Benzene Substituted by Electron Donor and Acceptor Groups. Journal of Physical Chemistry A, 2002, 106, 1-11.	1.1	97
45	The photochemistry of 1,4-cyclohexadiene in solution and in the gas phase: conical intersections and the origin of the â€˜helicopter-typeâ€™ motion of H2 photo-generated in the isolated molecule. Physical Chemistry Chemical Physics, 2002, 4, 34-42.	1.3	10
46	Photochemistry by conical intersections: a practical guide for experimentalists. Journal of Photochemistry and Photobiology A: Chemistry, 2001, 144, 221-228.	2.0	20
47	Conical intersections in molecular photochemistry â€“ the role of phase change. Chemical Physics, 2000, 259, 249-261.	0.9	14
48	The electron-pair origin of antiaromaticity: Spectroscopic manifestations. International Journal of Quantum Chemistry, 1999, 71, 133-145.	1.0	33
49	Molecular Photochemistry: A General Method for Localizing Conical Intersections Using the Phase-Change Rule. Chemistry - A European Journal, 1999, 5, 1755-1765.	1.7	45
50	The Singlet-State Photophysics and Photochemistry of Polyenes:â€‰ Application of the Twin-State Model and of the Phase-Change Theorem. Journal of Physical Chemistry A, 1999, 103, 2364-2374.	1.1	27
51	The Twin-Excited State as a Probe for the Transition State in Concerted Unimolecular Reactions: The Semibullvalene Rearrangement. Angewandte Chemie - International Edition, 1998, 37, 1394-1397.	7.2	32
52	Two-State Model of Antiaromaticity:Â The Low Lying Singlet States. Journal of Physical Chemistry A, 1998, 102, 10843-10850.	1.1	49
53	Two-State Model of Antiaromaticity:Â The Triplet State. Is Hund's Rule Violated?. Journal of Physical Chemistry A, 1998, 102, 10851-10859.	1.1	29
54	A KekulÃ©-Crossing Model for the â€œAnomalousâ€•Behavior of the b2u Modes of Aromatic Hydrocarbons in the Lowest Excited 1B2u State. Accounts of Chemical Research, 1996, 29, 211-218.	7.6	86

#	Article	IF	Citations
55	Ab initiostudy of styrene and Î²â€methyl styrene in the ground and in the two lowest excited singlet states. Journal of Chemical Physics, 1995, 103, 20-36.	1.2	68
56	The .nu.14(b2u) Mode of Benzene in S0 and S1 and the Distortive Nature of the .pi. Electron System: Theory and Experiment. Journal of the American Chemical Society, 1995, 117, 5387-5388.	6.6	71