Demeter Tzeli

List of Publications by Year
in descending order

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79 papers	1,090 citations	430442 18 h-index	476904 29 g-index
82 all docs	82 docs citations	82 times ranked	983 citing authors

#	Article	IF	Citations
1	Theoretical investigation of iron carbide, FeC. Journal of Chemical Physics, 2002, 116, 4901.	1.2	75
2	On the dipole moment of the ground state Xâ€Š3Î” of iron carbide, FeC. Journal of Chemical Physics, 2003, 118, 4984-4986.	1.2	63
3	Chalcogen Bonding and Hydrophobic Effects Force Molecules into Small Spaces. Journal of the American Chemical Society, 2020, 142, 5876-5883.	6.6	54
4	First principles study of the electronic structure and bonding of Mn2. Journal of Chemical Physics, 2008, 129, 154310.	1.2	51
5	First Principles Examination of the Acetyleneâ^'Water Clusters, HCCHâ^'(H2O)x,x= 2, 3, and 4. Journal of Physical Chemistry A, 2002, 106, 11327-11337.	1.1	49
6	Theoretical Study of Hydrogen Bonding in Homodimers and Heterodimers of Amide, Boronic Acid, and Carboxylic Acid, Free and in Encapsulation Complexes. Journal of the American Chemical Society, 2011, 133, 16977-16985.	6.6	42
7	Electronic structure and bonding of the 3d transition metal borides, MB, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu through all electron ab initio calculations. Journal of Chemical Physics, 2008, 128, 034309.	1.2	41
8	Conformations and Fluorescence of Encapsulated Stilbene. Journal of the American Chemical Society, 2012, 134, 4346-4354.	6.6	40
9	First-Principles Investigation of the Boron and Aluminum Carbides BC and AlC and Their Anions BC-and AlC-. 1. Journal of Physical Chemistry A, 2001, 105, 1175-1184.	1.1	39
10	A first principles study of the acetyleneâ€“water interaction. Journal of Chemical Physics, 2000, 112, 6178-6189.	1.2	34
11	Review on the QM/MM Methodologies and Their Application to Metalloproteins. Molecules, 2022, 27, 2660.	1.7	28
12	Electronic Structure of Cobalt Carbide, CoC. Journal of Physical Chemistry A, 2006, 110, 8952-8962.	1.1	26
13	Accurate ab initio calculations of the ground states of FeC, FeC+, and FeCâ^'. Journal of Chemical Physics, 2010, 132, 194312.	1.2	26
14	Theoretical study on the electronic states of NaLi. Journal of Chemical Physics, 2008, 129, 054306.	1.2	23
15	Accurate Theoretical Study of the Excited States of Boron and Aluminum Carbides, BC, AlC. 2. Journal of Physical Chemistry A, 2001, 105, 7672-7685.	1.1	22
16	Theoretical investigation of the ground and low-lying excited states of nickel carbide, NiC. Journal of Chemical Physics, 2007, 126, 194304.	1.2	20
17	Theoretical study of free and encapsulated carboxylic acid and amide dimers. International Journal of Quantum Chemistry, 2013, 113, 734-739.	1.0	19
18	A molecular level study of the aqueous microsolvation of acetylene. Chemical Physics Letters, 2001, 340, 538-546.	1.2	18

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19	The dipole moments of the excited states of FeC. Journal of Chemical Physics, 2005, 122, 056101.	1.2	18
20	The electron affinity of gallium nitride (GaN) and digallium nitride (GaNGa): The importance of the basis set superposition error in strongly bound systems. Journal of Chemical Physics, 2008, 128, 144103.	1.2	18
21	First Principles Investigation of the Electronic Structure of the Iron Carbide Cation, FeC+. Journal of Physical Chemistry A, 2005, 109, 9249-9258.	1.1	17
22	Computational Insight into the Electronic Structure and Absorption Spectra of Lithium Complexes of N-Confused Tetraphenylporphyrin. Journal of Physical Chemistry A, 2011, 115, 11749-11760.	1.1	17
23	Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a Ї€-extended TTF derivative. Physical Chemistry Chemical Physics, 2011, 13, 11965.	1.3	17
24	Intramolecular cyclization of Î²-nitroso-o-quinone methides. A theoretical endoscopy of a potentially useful innate â€˜reclusiveâ€™ reaction. Tetrahedron, 2015, 71, 359-369.	1.0	17
25	Theoretical Study of Adsorption and Diffusion of Group IIIA Metals on Si(111). Journal of Physical Chemistry C, 2009, 113, 13924-13932.	1.5	14
26	Quadruple Bonding in the Ground and Low-Lying Excited States of the Diatomic Molecules TcN, RuC, RhB, and PdBe. Journal of Physical Chemistry A, 2020, 124, 6667-6681.	1.1	13
27	The activation of carbon dioxide by first row transition metals (Scâ€“Zn). Physical Chemistry Chemical Physics, 2018, 20, 25495-25505.	1.3	12
28	Theoretical study on the electronic structure and the absorption spectra of complexes of C60 and C59N with Ї€-extended derivatives of tetrathiafulvalene. Computational and Theoretical Chemistry, 2011, 965, 168-175.	1.1	11
29	Ab Initio Investigation of the Electronic and Geometric Structure of Magnesium Diboride, MgB2. Journal of Physical Chemistry A, 2005, 109, 10663-10674.	1.1	10
30	Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with (CH₃)_xNH+4â^'x, x = 0â€“4. Physical Chemistry Chemical Physics, 2011, 13, 954-965.	1.3	10
31	Encapsulated hydrogen-bonded dimers of amide and carboxylic acid. Chemical Physics Letters, 2012, 548, 55-59.	1.2	10
32	Reactivity and Mechanism of Photo- and Electrocatalytic Hydrogen Evolution by a Diimine Copper(I) Complex. Catalysts, 2020, 10, 1302.	1.6	10
33	The Effect of Geometry, Spin, and Orbital Optimization in Achieving Accurate, Correlated Results for Ironâ€“Sulfur Cubanes. Journal of Chemical Theory and Computation, 2022, 18, 687-702.	2.3	10
34	Mind the basis set superposition error. Chemical Physics Letters, 2010, 496, 42-45.	1.2	9
35	On the electronic structure of the ground (X3Î£â^') and some low-lying excited states (A3Î, a1Î”, b1â^'+, B3Î£â^') of the isovalent species Pî—¸Li and Pî—¸Na. Computational and Theoretical Chemistry, 1997, 417, 277-287.	1.5	8
36	Theoretical Investigation on the Electronic and Geometric Structure of GaN2+and GaN4+. Journal of Physical Chemistry A, 2007, 111, 8892-8902.	1.1	8

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37	Compression in encapsulated carboxylic acid homodimers. Chemical Physics Letters, 2013, 573, 48-55.	1.2	8
38	Molecular logic gates based on benzo-18-crown-6 ether of styrylquinoline: a theoretical study. Physical Chemistry Chemical Physics, 2016, 18, 32132-32145.	1.3	8
39	The solvent effect on a styrylâ€bodipy derivative functioning as an AND molecular logic gate. International Journal of Quantum Chemistry, 2020, 120, e26181.	1.0	8
40	Conformational Properties of New Thiosemicarbazone and Thiocarbohydrazone Derivatives and Their Possible Targets. Molecules, 2022, 27, 2537.	1.7	8
41	Theoretical study on the electronic structure, formation and absorption spectra of lithium, sodium and potassium complexes of N-confused tetraphenylporphyrin. Computational and Theoretical Chemistry, 2013, 1020, 38-50.	1.1	7
42	Î²-Nitroso-o-quinone methides: potent intermediates in organic chemistry and biology. The impact of the NO group on their structure and reactivity profile: a theoretical insight. Structural Chemistry, 2014, 25, 1711-1723.	1.0	7
43	Physical Insights into Molecular Sensors, Molecular Logic Gates, and Photosensitizers in Photodynamic Therapy. Journal of Chemistry, 2019, 2019, 1-9.	0.9	7
44	Quadruple chemical bonding in the diatomic anions <scp>TcN</scp>^{â^'}, <scp>RuC</scp>^{â^'}, <scp>RhB</scp>^{â^'}, and <scp>PdBe</scp>^{â^'}. Journal of Computational Chemistry, 2021, 42, 1126-1137.	1.5	7
45	Molecular investigation of artificial and natural sweeteners as potential anti-inflammatory agents. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12608-12620.	2.0	7
46	Molybdenumâ€“Sulfur Bond: Electronic Structure of Low-Lying States of MoS. Journal of Physical Chemistry A, 2022, 126, 1168-1181.	1.1	7
47	On the ground state of titanium phosphide, TiP: A theoretical investigation. Journal of Chemical Physics, 2004, 121, 2646.	1.2	6
48	Theoretical Study of Adsorption of Group IIIA Nitrides on Si(111). Journal of Physical Chemistry C, 2009, 113, 5563-5567.	1.5	6
49	2, 2â€²â€Dihydroxybenzophenones and Derivatives. Efficient Synthesis and Structure Endoscopy by DFT and NMR. Credentials as Potent Antiinflammatory Agents.. ChemistrySelect, 2016, 1, 2426-2438.	0.7	6
50	Naphthalene Periâ€…Annelated N,Nâ€•and N,Oâ€Heterocycles: The Effect of Heteroatomâ€Guided Periâ€Fusion on Their Structure and Reactivity Profilesâ€A Theoretical Endoscopy. ChemistrySelect, 2018, 3, 9743-9752.	0.7	6
51	Theoretical study of the photophysical processes of a styrylâ€bodipy derivative eliciting an AND molecular logic gate response. International Journal of Quantum Chemistry, 2019, 119, e25958.	1.0	6
52	Theoretical study of adsorption of gallium and gallium nitrides on Si(111). Chemical Physics Letters, 2007, 448, 88-92.	1.2	5
53	Encapsulation of monomers, homodimers and heterodimers of amides and carboxylic acids in three non-covalent assemblies. Structural Chemistry, 2015, 26, 1585-1601.	1.0	5
54	Intramolecular single H bonding vs bifurcation in tuning the conformation of 2,2â€²-dihydroxybenzophenone and its derivatives: a DFT insight. Structural Chemistry, 2017, 28, 925-943.	1.0	5

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55	Time-evolution study of photoinduced charge-transfer in tertiary amine-fluorophore systems. Computational and Theoretical Chemistry, 2017, 1115, 197-207.	1.1	5
56	Aromaticity and Chemical Bonding of Chalcogenâ€Bonded Capsules Featuring Enhanced Magnetic Anisotropy. ChemPhysChem, 2020, 21, 2187-2195.	1.0	5
57	Quantitative Account of the Bonding Properties of a Rubredoxin Model Complex [Fe(SCH₃)₄]^q, q = â^'2, â^'1, +2, +3. Journal of Chemical Theory and Computation, 2021, 17, 6080-6091.	2.3	5
58	3-Input AND Molecular Logic Gate with Enhanced Fluorescence Output: The Key Atom for the Accurate Prediction of the Spectra. Journal of Chemical Information and Modeling, 2022, 62, 6436-6448.	2.5	5
59	Arene-fused 1,2-oxazole N-oxides and derivatives. The impact of the Nâ€“O dipole and substitution on their aromatic character and reactivity profile. Can it be a useful structure in synthesis? A theoretical insight. Structural Chemistry, 2014, 25, 1837-1846.	1.0	4
60	Theoretical investigation on the binding of alkyl halides and cyclohexyl halides in water-soluble cavitands. Chemical Physics Letters, 2019, 728, 174-180.	1.2	4
61	The role of electric field, peripheral chains, and magnetic effects on significant ¹H upfield shifts of the encapsulated molecules in chalcogen-bonded capsules. Physical Chemistry Chemical Physics, 2021, 23, 19647-19658.	1.3	4
62	Losartan Interactions with 2-Hydroxypropyl-Î²-CD. Molecules, 2022, 27, 2421.	1.7	4
63	Breaking covalent bonds in the context of the many-body expansion (MBE). I. The purported â€œfirst row anomalyâ€•in XHn (X = C, Si, Ge, Sn; n = 1â€“4). Journal of Chemical Physics, 2022, 156, .	1.2	4
64	On the Electronic Structure of NLi2and PLi2, Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 1998, 102, 2223-2230.	1.1	3
65	The Electronic Structure of ScAl+. Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 2000, 104, 6861-6870.	1.1	3
66	CH(X2â^¸a4â^'â^') â€¦ OH2 and CH2(??3B1, Ã£1A1) â€¦ OH2 interactions. A first principles investigation. International Journal of Quantum Chemistry, 2005, 104, 497-511.	1.0	3
67	Structure and energetics of InN and GaN dimers. Chemical Physics, 2008, 349, 98-108.	0.9	3
68	Theoretical Study of Gallium Nitride Molecules, GaN2 and GaN4.. Journal of Physical Chemistry A, 2008, 112, 8858-8867.	1.1	3
69	The role of the hostâ€“guest interactions in the relative stability of compressed encapsulated homodimers and heterodimers of amides and carboxylic acids. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	3
70	Reversible encapsulation in a covalent capsule. Chemical Physics Letters, 2015, 633, 99-104.	1.2	3
71	Structure assignment, conformational properties and discovery of potential targets of the Ugi cinnamic adduct NGI25. Journal of Biomolecular Structure and Dynamics, 2021, , 1-14.	2.0	3
72	Theoretical investigation of the ground and low-lying excited states of gallium and indium silicides, GaSi and InSi. Journal of Chemical Physics, 2009, 131, 234301.	1.2	2

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73	N,Nâ€•and N,Oâ€6â€membered Ring peri â€Annelation in Naphthalene. Is it a Heteroring or merely a peri â€• Heterobridge?. ChemistrySelect, 2021, 6, 951-961.	0.7	2
74	Conformational Properties and Putative Bioactive Targets for Novel Thiosemicarbazone Derivatives. Molecules, 2022, 27, 4548.	1.7	2
75	Experimental and theoretical spectroscopic studies of branchlet-like SrCO3 superarchitecture. AIP Conference Proceedings, 2016, , .	0.3	1
76	Analysis of chemical bonding of the ground and low-lying states of Mo₂ and of Mo₂Cl_x complexes, x = 2 - 10.. Journal of Chemical Physics, 0, , .	1.2	1
77	A Theoretical Study of Complexes of Crown Ethers with Substituted Ammonium Cations. Progress in Theoretical Chemistry and Physics, 2012, , 599-610.	0.2	0
78	A DFT Study of Adsorption of Gallium and Gallium Nitrides on Si(111). Progress in Theoretical Chemistry and Physics, 0, , 341-350.	0.2	0
79	A DFT Study towards the Amide cisâ€trans Isomerization Process of the Mycâ€Max Inhibitor Mycro 3â€‰and Its Photophysical Properties;ÂSynthesis and NMR Studies of the transâ€Conformation. ChemistrySelect, 2022, 7, .	0.7	0