

# 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	Molecular investigation of artificial and natural sweeteners as potential anti-inflammatory agents. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 12608-12620.	2.0	7
2	The Effect of Geometry, Spin, and Orbital Optimization in Achieving Accurate, Correlated Results for Iron-Sulfur Cubanes. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 687-702.	2.3	10
3	Molybdenum-Sulfur Bond: Electronic Structure of Low-Lying States of MoS. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1168-1181.	1.1	7
4	Losartan Interactions with 2-Hydroxypropyl- $\beta$ -CD. <i>Molecules</i> , 2022, 27, 2421.	1.7	4
5	3-Input AND Molecular Logic Gate with Enhanced Fluorescence Output: The Key Atom for the Accurate Prediction of the Spectra. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 6436-6448.	2.5	5
6	Conformational Properties of New Thiosemicarbazone and Thiocarbohydrazone Derivatives and Their Possible Targets. <i>Molecules</i> , 2022, 27, 2537.	1.7	8
7	Review on the QM/MM Methodologies and Their Application to Metalloproteins. <i>Molecules</i> , 2022, 27, 2660.	1.7	28
8	Breaking covalent bonds in the context of the many-body expansion (MBE). I. The purported "first row anomaly" in $XH_n$ ( $X = C, Si, Ge, Sn; n = 1-4$ ). <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	4
9	Conformational Properties and Putative Bioactive Targets for Novel Thiosemicarbazone Derivatives. <i>Molecules</i> , 2022, 27, 4548.	1.7	2
10	A DFT Study towards the Amide cis-trans Isomerization Process of the MycMax Inhibitor Mycro 3 and Its Photophysical Properties; Synthesis and NMR Studies of the trans-Conformation. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
11	The role of electric field, peripheral chains, and magnetic effects on significant $^1H$ upfield shifts of the encapsulated molecules in chalcogen-bonded capsules. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19647-19658.	1.3	4
12	N <sub>5</sub> - and N <sub>6</sub> -membered Ring pericyclic Annulation in Naphthalene. Is it a Heteroring or merely a pericyclic Heterobridge?. <i>ChemistrySelect</i> , 2021, 6, 951-961.	0.7	2
13	Quadruple chemical bonding in the diatomic anions $TcN^+$ , $RuC^+$ , $RhB^+$ , and $PdBe^+$ . <i>Journal of Computational Chemistry</i> , 2021, 42, 1126-1137.	1.5	7
14	Quantitative Account of the Bonding Properties of a Rubredoxin Model Complex $[Fe(SCH_3)_3(SCH_2)_4]^+$ , $q = 2, 1, +2, +3$ . <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6080-6091.	2.3	5
15	Structure assignment, conformational properties and discovery of potential targets of the Ugi cinnamic adduct NGI25. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-14.	2.0	3
16	Reactivity and Mechanism of Photo- and Electrocatalytic Hydrogen Evolution by a Diimine Copper(I) Complex. <i>Catalysts</i> , 2020, 10, 1302.	1.6	10
17	Quadruple Bonding in the Ground and Low-Lying Excited States of the Diatomic Molecules TcN, RuC, RhB, and PdBe. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6667-6681.	1.1	13
18	Aromaticity and Chemical Bonding of Chalcogen-Bonded Capsules Featuring Enhanced Magnetic Anisotropy. <i>ChemPhysChem</i> , 2020, 21, 2187-2195.	1.0	5

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19	Chalcogen Bonding and Hydrophobic Effects Force Molecules into Small Spaces. <i>Journal of the American Chemical Society</i> , 2020, 142, 5876-5883.	6.6	54
20	The solvent effect on a styryl- <i>bodipy</i> derivative functioning as an AND molecular logic gate. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26181.	1.0	8
21	Theoretical investigation on the binding of alkyl halides and cyclohexyl halides in water-soluble cavitands. <i>Chemical Physics Letters</i> , 2019, 728, 174-180.	1.2	4
22	Theoretical study of the photophysical processes of a styryl- <i>bodipy</i> derivative eliciting an AND molecular logic gate response. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25958.	1.0	6
23	Physical Insights into Molecular Sensors, Molecular Logic Gates, and Photosensitizers in Photodynamic Therapy. <i>Journal of Chemistry</i> , 2019, 2019, 1-9.	0.9	7
24	The activation of carbon dioxide by first row transition metals (Sc-Zn). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25495-25505.	1.3	12
25	Naphthalene Peri-Annulated N, N- and N, O-Heterocycles: The Effect of Heteroatom-Guided <i>Peri-Fusion</i> on Their Structure and Reactivity Profiles-A Theoretical Endoscopy. <i>ChemistrySelect</i> , 2018, 3, 9743-9752.	0.7	6
26	Intramolecular single H bonding vs bifurcation in tuning the conformation of 2,2'-dihydroxybenzophenone and its derivatives: a DFT insight. <i>Structural Chemistry</i> , 2017, 28, 925-943.	1.0	5
27	Time-evolution study of photoinduced charge-transfer in tertiary amine-fluorophore systems. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 197-207.	1.1	5
28	Experimental and theoretical spectroscopic studies of branchlet-like SrCO <sub>3</sub> superarchitecture. <i>AIP Conference Proceedings</i> , 2016, . .	0.3	1
29	2, 2'-Dihydroxybenzophenones and Derivatives. Efficient Synthesis and Structure Endoscopy by DFT and NMR. Credentials as Potent Antiinflammatory Agents.. <i>ChemistrySelect</i> , 2016, 1, 2426-2438.	0.7	6
30	Molecular logic gates based on benzo-18-crown-6 ether of styrylquinoline: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32132-32145.	1.3	8
31	Encapsulation of monomers, homodimers and heterodimers of amides and carboxylic acids in three non-covalent assemblies. <i>Structural Chemistry</i> , 2015, 26, 1585-1601.	1.0	5
32	Reversible encapsulation in a covalent capsule. <i>Chemical Physics Letters</i> , 2015, 633, 99-104.	1.2	3
33	Intramolecular cyclization of $\hat{I}^2$ -nitroso-o-quinone methides. A theoretical endoscopy of a potentially useful innate <i>reclusive</i> <sup>TM</sup> reaction. <i>Tetrahedron</i> , 2015, 71, 359-369.	1.0	17
34	Arene-fused 1,2-oxazole N-oxides and derivatives. The impact of the N=O dipole and substitution on their aromatic character and reactivity profile. Can it be a useful structure in synthesis? A theoretical insight. <i>Structural Chemistry</i> , 2014, 25, 1837-1846.	1.0	4
35	The role of the host-guest interactions in the relative stability of compressed encapsulated homodimers and heterodimers of amides and carboxylic acids. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	3
36	$\hat{I}^2$ -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. <i>Structural Chemistry</i> , 2014, 25, 1711-1723.	1.0	7

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37	Theoretical study of free and encapsulated carboxylic acid and amide dimers. International Journal of Quantum Chemistry, 2013, 113, 734-739.	1.0	19
38	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
39	Compression in encapsulated carboxylic acid homodimers. Chemical Physics Letters, 2013, 573, 48-55.	1.2	8
40	A Theoretical Study of Complexes of Crown Ethers with Substituted Ammonium Cations. Progress in Theoretical Chemistry and Physics, 2012, , 599-610.	0.2	0
41	Encapsulated hydrogen-bonded dimers of amide and carboxylic acid. Chemical Physics Letters, 2012, 548, 55-59.	1.2	10
42	Conformations and Fluorescence of Encapsulated Stilbene. Journal of the American Chemical Society, 2012, 134, 4346-4354.	6.6	40
43	Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with $(CH_3)_xNH_4^{+x}$ , $x = 0-4$ . Physical Chemistry Chemical Physics, 2011, 13, 954-965.	1.3	10
44	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
45	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
46	Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a $\pi$ -extended TTF derivative. Physical Chemistry Chemical Physics, 2011, 13, 11965.	1.3	17
47	Theoretical study on the electronic structure and the absorption spectra of complexes of C <sub>60</sub> and C <sub>59</sub> N with $\pi$ -extended derivatives of tetrathiafulvalene. Computational and Theoretical Chemistry, 2011, 965, 168-175.	1.1	11
48	Mind the basis set superposition error. Chemical Physics Letters, 2010, 496, 42-45.	1.2	9
49	Accurate <i>ab initio</i> calculations of the ground states of FeC, FeC <sup>+</sup> , and FeC <sup>2+</sup> . Journal of Chemical Physics, 2010, 132, 194312.	1.2	26
50	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
51	Theoretical Study of Adsorption of Group IIIA Nitrides on Si(111). Journal of Physical Chemistry C, 2009, 113, 5563-5567.	1.5	6
52	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
53	Structure and energetics of InN and GaN dimers. Chemical Physics, 2008, 349, 98-108.	0.9	3
54	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 <i>ab initio</i> calculations. Journal of Chemical Physics, 2008, 128, 034309.	1.2	41

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55	Theoretical study on the electronic states of NaLi. Journal of Chemical Physics, 2008, 129, 054306.	1.2	23
56	Theoretical Study of Gallium Nitride Molecules, GaN <sub>2</sub> and GaN <sub>4</sub> . Journal of Physical Chemistry A, 2008, 112, 8858-8867.	1.1	3
57	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
58	First principles study of the electronic structure and bonding of Mn <sub>2</sub> . Journal of Chemical Physics, 2008, 129, 154310.	1.2	51
59	Theoretical investigation of the ground and low-lying excited states of nickel carbide, NiC. Journal of Chemical Physics, 2007, 126, 194304.	1.2	20
60	Theoretical Investigation on the Electronic and Geometric Structure of GaN <sub>2</sub> <sup>+</sup> and GaN <sub>4</sub> <sup>+</sup> . Journal of Physical Chemistry A, 2007, 111, 8892-8902.	1.1	8
61	Theoretical study of adsorption of gallium and gallium nitrides on Si(111). Chemical Physics Letters, 2007, 448, 88-92.	1.2	5
62	Electronic Structure of Cobalt Carbide, CoC. Journal of Physical Chemistry A, 2006, 110, 8952-8962.	1.1	26
63	CH(X <sup>+</sup> ; a <sub>4</sub> <sup>+</sup> ) ↔ OH <sub>2</sub> and CH <sub>2</sub> ( <sup>3</sup> B <sub>1</sub> , <sup>1</sup> A <sub>1</sub> ) ↔ OH <sub>2</sub> interactions. A first principles investigation. International Journal of Quantum Chemistry, 2005, 104, 497-511.	1.0	3
64	The dipole moments of the excited states of FeC. Journal of Chemical Physics, 2005, 122, 056101.	1.2	18
65	Ab Initio Investigation of the Electronic and Geometric Structure of Magnesium Diboride, MgB <sub>2</sub> . Journal of Physical Chemistry A, 2005, 109, 10663-10674.	1.1	10
66	First Principles Investigation of the Electronic Structure of the Iron Carbide Cation, FeC <sup>+</sup> . Journal of Physical Chemistry A, 2005, 109, 9249-9258.	1.1	17
67	On the ground state of titanium phosphide, TiP: A theoretical investigation. Journal of Chemical Physics, 2004, 121, 2646.	1.2	6
68	On the dipole moment of the ground state X <sup>3</sup> Σ <sup>+</sup> of iron carbide, FeC. Journal of Chemical Physics, 2003, 118, 4984-4986.	1.2	63
69	First Principles Examination of the Acetylene <sup>+</sup> Water Clusters, HCCH <sup>+</sup> (H <sub>2</sub> O) <sub>x</sub> , x= 2, 3, and 4. Journal of Physical Chemistry A, 2002, 106, 11327-11337.	1.1	49
70	Theoretical investigation of iron carbide, FeC. Journal of Chemical Physics, 2002, 116, 4901.	1.2	75
71	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
72	First-Principles Investigation of the Boron and Aluminum Carbides BC and AlC and Their Anions BC <sup>-</sup> and AlC <sup>-</sup> . 1. Journal of Physical Chemistry A, 2001, 105, 1175-1184.	1.1	39

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73	A molecular level study of the aqueous microsolvation of acetylene. Chemical Physics Letters, 2001, 340, 538-546.	1.2	18
74	A first principles study of the acetylene-water interaction. Journal of Chemical Physics, 2000, 112, 6178-6189.	1.2	34
75	The Electronic Structure of ScAl <sup>+</sup> . Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 2000, 104, 6861-6870.	1.1	3
76	On the Electronic Structure of NLi <sub>2</sub> and PLi <sub>2</sub> , Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 1998, 102, 2223-2230.	1.1	3
77	On the electronic structure of the ground ( $X^3\hat{\Sigma}^+$ ) and some low-lying excited states ( $A^3\hat{\Sigma}^+$ , $a^1\hat{\Sigma}^+$ , $b^1\hat{\Sigma}^+$ , $B^3\hat{\Sigma}^+$ ) of the isovalent species P <sub>f</sub> -Li and P <sub>f</sub> -Na. Computational and Theoretical Chemistry, 1997, 417, 277-287.	1.5	8
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	Analysis of chemical bonding of the ground and low-lying states of Mo <sub>2</sub> and of Mo <sub>2</sub> Cl <sub>x</sub> complexes, $x = 2 - 10$ . Journal of Chemical Physics, 0, , .	1.2	1