Pablo A Denis

List of Publications by Year
in descending order

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159	4,521	94269 37	138251 58
papers	citations	h-index	g-index

162	162	162	4398
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Band gap opening of monolayer and bilayer graphene doped with aluminium, silicon, phosphorus, and sulfur. Chemical Physics Letters, 2010, 492, 251-257.	1.2	391
2	Is It Possible to Dope Singleâ€Walled Carbon Nanotubes and Graphene with Sulfur?. ChemPhysChem, 2009, 10, 715-722.	1.0	215
3	Mechanical properties of graphene nanoribbons. Journal of Physics Condensed Matter, 2009, 21, 285304.	0.7	158
4	Comparative Study of Defect Reactivity in Graphene. Journal of Physical Chemistry C, 2013, 117, 19048-19055.	1.5	149
5	Density Functional Investigation of Thioepoxidated and Thiolated Graphene. Journal of Physical Chemistry C, 2009, 113, 5612-5619.	1.5	104
6	When noncovalent interactions are stronger than covalent bonds: Bilayer graphene doped with second row atoms, aluminum, silicon, phosphorus and sulfur. Chemical Physics Letters, 2011, 508, 95-101.	1.2	85
7	Beryllium doped graphene as an efficient anode material for lithium-ion batteries with significantly huge capacity: A DFT study. Applied Materials Today, 2017, 9, 333-340.	2.3	84
8	Concentration dependence of the band gaps of phosphorus and sulfur doped graphene. Computational Materials Science, 2013, 67, 203-206.	1.4	83
9	Structural characterization and chemical reactivity of dual doped graphene. Carbon, 2015, 87, 106-115.	5.4	83
10	Theoretical characterization of sulfur and nitrogen dual-doped graphene. Computational and Theoretical Chemistry, 2014, 1049, 13-19.	1.1	80
11	Band-gap tuning of graphene by Be doping and Be, B co-doping: a DFT study. RSC Advances, 2015, 5, 55762-55773.	1.7	75
12	Theoretical investigation of the stacking interactions between curved conjugated systems and their interaction with fullerenes. Chemical Physics Letters, 2011, 516, 82-87.	1.2	74
13	Chemical Reactivity and Bandâ€Gap Opening of Graphene Doped with Gallium, Germanium, Arsenic, and Selenium Atoms. ChemPhysChem, 2014, 15, 3994-4000.	1.0	67
14	Magnetism induced by single carbon vacancies in a three-dimensional graphitic network. Physical Review B, 2008, 77, .	1.1	65
15	On the hydrogen addition to graphene. Computational and Theoretical Chemistry, 2009, 907, 93-103.	1.5	57
16	Organic Chemistry of Graphene: The Dielsâ€“Alder Reaction. Chemistry - A European Journal, 2013, 19, 15719-15725.	1.7	57
17	Chemical Reactivity of Lithium Doped Monolayer and Bilayer Graphene. Journal of Physical Chemistry C, 2011, 115, 13392-13398.	1.5	56
18	Band Gap Opening in Dual-Doped Monolayer Graphene. Journal of Physical Chemistry C, 2016, 120, 7103-7112.	1.5	56

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19	Theoretical Characterization of Hydrogen Polyoxides: HOOH, HOOOH, HOOOOH, and HOOO. Journal of Physical Chemistry A, 2009, 113, 499-506.	1.1	53
20	Monolayer and Bilayer Graphene Functionalized with Nitrene Radicals. Journal of Physical Chemistry C, 2011, 115, 195-203.	1.5	53
21	Chemical Reactivity of Electron-Doped and Hole-Doped Graphene. Journal of Physical Chemistry C, 2013, 117, 3895-3902.	1.5	50
22	Methane adsorption inside and outside pristine and N-doped single wall carbon nanotubes. Chemical Physics, 2008, 353, 79-86.	0.9	49
23	Tripleâ€Doped Monolayer Graphene with Boron, Nitrogen, Aluminum, Silicon, Phosphorus, and Sulfur. ChemPhysChem, 2017, 18, 1864-1873.	1.0	49
24	Hexagonal boron phosphide as a potential anode nominee for alkali-based batteries: A multi-flavor DFT study. Applied Surface Science, 2019, 471, 134-141.	3.1	49
25	The 1,3 dipolar cycloaddition of azomethine ylides to graphene, single wall carbon nanotubes, and C60. International Journal of Quantum Chemistry, 2010, 110, 1764-1771.	1.0	48
26	Hydrogen storage in doped biphenylene based sheets. Computational and Theoretical Chemistry, 2015, 1062, 30-35.	1.1	48
27	Density functional investigation of atmospheric sulfur chemistry. I. Enthalpy of formation of HSO and related molecules. International Journal of Quantum Chemistry, 2000, 80, 439-453.	1.0	44
28	First-principles study of dual-doped graphene: towards promising anode materials for Li/Na-ion batteries. New Journal of Chemistry, 2018, 42, 10842-10851.	1.4	44
29	[2 + 2] Cycloadditions onto graphene. Journal of Materials Chemistry, 2012, 22, 5470.	6.7	43
30	Stacked functionalized silicene: a powerful system to adjust the electronic structure of silicene. Physical Chemistry Chemical Physics, 2015, 17, 5393-5402.	1.3	43
31	Thiophene adsorption on Single Wall Carbon Nanotubes and graphene. Computational and Theoretical Chemistry, 2010, 957, 114-119.	1.5	41
32	Basis Set Requirements for Sulfur Compounds in Density Functional Theory:Â a Comparison between Correlation-Consistent, Polarized-Consistent, and Pople-Type Basis Sets. Journal of Chemical Theory and Computation, 2005, 1, 900-907.	2.3	40
33	Fine tuning the band-gap of graphene by atomic and molecular doping: a density functional theory study. RSC Advances, 2016, 6, 55990-56003.	1.7	40
34	Complete basis set and density functional determination of the enthalpy of formation of the controversial HO3 radical: a discrepancy between theory and experiment. Chemical Physics Letters, 2002, 365, 440-449.	1.2	39
35	Investigation of H₂ Physisorption on Corannulene (C₂₀H₁₀), Tetraindenocorannulene (C₄₄H₁₈), Pentaindenocorannulene (C₅₀H₂₀), C₆₀, and Their Nitrogen Derivatives. Journal of Physical Chemistry C, 2008, 112, 2791-2796.	1.5	38
36	Theoretical characterization of existing and new fullerene receptors. RSC Advances, 2013, 3, 25296.	1.7	38

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37	Stability and Electronic Properties of Biphenylene Based Functionalized Nanoribbons and Sheets. Journal of Physical Chemistry C, 2014, 118, 24976-24982.	1.5	38
38	Hydrogenation and Fluorination of 2D Boron Phosphide and Boron Arsenide: A Density Functional Theory Investigation. ACS Omega, 2018, 3, 16416-16423.	1.6	38
39	A Firstâ€Principles Study on the Interaction between Alkyl Radicals and Graphene. Chemistry - A European Journal, 2012, 18, 7568-7574.	1.7	37
40	Cooperative behavior in functionalized graphene: Explaining the occurrence of 1,3 cycloaddition of azomethine ylides onto graphene. Chemical Physics Letters, 2012, 550, 111-117.	1.2	34
41	Lithium adsorption on heteroatom mono and dual doped graphene. Chemical Physics Letters, 2017, 672, 70-79.	1.2	34
42	Systematic Coupled Cluster, Brueckner Coupled Cluster, G3, CBS-QB3, and DFT Investigation of SX Diatomics; X = First- or Second-Row Atom. Journal of Physical Chemistry A, 2004, 108, 11092-11100.	1.1	33
43	The enthalpy of formation of the HSO radical revisited. Chemical Physics Letters, 2005, 402, 289-293.	1.2	33
44	Assessment of density functional methods for the study of vanadium and rhenium complexes with thiolato ligands. Computational and Theoretical Chemistry, 2010, 941, 1-9.	1.5	32
45	Mono and dual doped monolayer graphene with aluminum, silicon, phosphorus and sulfur. Computational and Theoretical Chemistry, 2016, 1097, 40-47.	1.1	32
46	Density functional investigation of atmospheric sulfur chemistry II. The heat of formation of the XSO2 radicals X=H,CH3. Chemical Physics Letters, 2001, 344, 221-228.	1.2	31
47	Density functional study of the decomposition pathways of nitroethane and 2-nitropropaneElectronic supplementary information (ESI) available: The structure of minima on the PES of nitroethane (Fig. S1) and 2-nitropropane (Fig. S2). See http://www.rsc.org/suppdata/cp/b3/b300275f/. Physical Chemistry Chemical Physics, 2003, 5, 1730-1738.	1.3	31
48	Theoretical characterization of thioepoxidated single wall carbon nanotubes. Chemical Physics Letters, 2008, 460, 486-491.	1.2	31
49	On the performance of CCSD(T) and CCSDT in the study of molecules with multiconfigurational character: halogen oxides, HSO, BN and O3. Chemical Physics Letters, 2004, 395, 12-20.	1.2	29
50	Theoretical characterization of the thiosulfeno radical, HS2. Chemical Physics Letters, 2006, 422, 434-438.	1.2	29
51	Hydrogenated double wall carbon nanotubes. Journal of Chemical Physics, 2009, 130, 194704.	1.2	27
52	Pristine Graphene-Based Catalysis: Significant Reduction of the Inversion Barriers of Adsorbed and Confined Corannulene, Sumanene, and Dibenzo[a,g]corannulene. Journal of Physical Chemistry A, 2015, 119, 5770-5777.	1.1	27
53	Theoretical investigation of the stability, electronic and magnetic properties of thiolated singleâ€wall carbon nanotubes. International Journal of Quantum Chemistry, 2009, 109, 772-781.	1.0	26
54	Rectangular and hexagonal doping of graphene with B, N, and O: a DFT study. RSC Advances, 2017, 7, 16064-16068.	1.7	26

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55	Theoretical investigation of nitrogen disubstituted corannulenes. Computational and Theoretical Chemistry, 2008, 865, 8-13.	1.5	25
56	Design and characterization of two strong fullerene receptors based on ballâ€“socket interactions. Chemical Physics Letters, 2014, 591, 323-327.	1.2	25
57	On the Addition of Aryl Radicals to Graphene: The Importance of Nonbonded Interactions. ChemPhysChem, 2013, 14, 3271-3277.	1.0	24
58	A theoretical study on the interaction between well curved conjugated systems and fullerenes smaller than C60or larger than C70. Journal of Physical Organic Chemistry, 2014, 27, 918-925.	0.9	24
59	Bond dissociation energies and enthalpies of formation of flavonoids: A G4 and M06-2X investigation. Computational and Theoretical Chemistry, 2016, 1091, 18-23.	1.1	24
60	Hydroxamic chelates of boric acid, a density functional study. Computational and Theoretical Chemistry, 2001, 537, 173-180.	1.5	23
61	High order correlation effects in the calculation of enthalpies of formation of sulfur compounds, CCSDT vs CCSD[T]. Chemical Physics Letters, 2003, 382, 65-70.	1.2	23
62	Ab Initio and Density Functional Study of Thionitroso XNS and Thiazyl Isomers XSN, X = H, F, Cl, Br, OH, SH, NH2, CH3, CF3, and SiF3. Journal of Physical Chemistry A, 2004, 108, 5073-5080.	1.1	23
63	Thermochemistry of the Hypobromous and Hypochlorous Acids, HOBr and HOCl. Journal of Physical Chemistry A, 2006, 110, 5887-5892.	1.1	23
64	Tunable optoelectronic properties in h-BP/h-BAs bilayers: The effect of an external electrical field. Applied Surface Science, 2019, 493, 308-319.	3.1	23
65	Studies of trypanocidal (inhibitory) power of naphthoquinones: Evaluation of quantum chemical molecular descriptors for structureâ€“activity relationships. European Journal of Medicinal Chemistry, 2008, 43, 2238-2246.	2.6	22
66	Thermochemistry of 35 selected sulfur compounds, a comparison between experiment and theory. Journal of Sulfur Chemistry, 2008, 29, 327-352.	1.0	22
67	Coupled cluster, B2PLYP and M06-2X investigation of the thermochemistry of five-membered nitrogen containing heterocycles, furan, and thiophene. Theoretical Chemistry Accounts, 2011, 129, 219-227.	0.5	22
68	Theoretical investigation on the interaction between beryllium, magnesium and calcium with benzene, coronene, cirumcoronene and graphene. Chemical Physics, 2014, 430, 1-6.	0.9	22
69	Theoretical characterization of the HSOH, H2SO and H2OS isomers. Molecular Physics, 2008, 106, 2557-2567.	0.8	21
70	C2V or C6V: Which is the most stable structure of the benzeneâ€“lithium complex?. Chemical Physics Letters, 2013, 573, 15-18.	1.2	21
71	A comparative study on the performance of subphthalocyanines and corannulene derivatives as receptors for fullerenes. New Journal of Chemistry, 2014, 38, 5608-5616.	1.4	21
72	Theoretical investigation of various aspects of two dimensional holey boroxine, B₃O₃. RSC Advances, 2019, 9, 37526-37536.	1.7	21

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73	The effect of the dopant nature on the reactivity, interlayer bonding and electronic properties of dual doped bilayer graphene. Physical Chemistry Chemical Physics, 2016, 18, 24693-24703.	1.3	20
74	Dual doped monolayer and bilayer graphene: The case of 4p and 2p elements. Chemical Physics Letters, 2016, 658, 152-157.	1.2	20
75	Theoretical characterization of hexagonal 2D Be₃N₂ monolayers. New Journal of Chemistry, 2019, 43, 2933-2941.	1.4	20
76	Density functional computational thermochemistry: solving the discrepancy between MO and DFT calculations on the enthalpy of formation of sulfine, CH2ĩ…Sĩ…O. Chemical Physics Letters, 2002, 355, 207-213.	1.2	19
77	Improving the Chemical Reactivity of Single-Wall Carbon Nanotubes with Lithium Doping. Journal of Physical Chemistry C, 2011, 115, 20282-20288.	1.5	19
78	New Approach to Accomplish the Covalent Functionalization of Boron Nitride Nanosheets: Cycloaddition Reactions. Journal of Physical Chemistry C, 2018, 122, 18583-18587.	1.5	19
79	How is the stacking interaction of bilayer graphene affected by the presence of defects?. Computational and Theoretical Chemistry, 2012, 995, 1-7.	1.1	18
80	Porphyrins bearing corannulene pincers: outstanding fullerene receptors. RSC Advances, 2016, 6, 50978-50984.	1.7	18
81	Density Functional Computational Thermochemistry:Â Isomerization of Sulfine and Its Enthalpy of Formation. Journal of Physical Chemistry A, 2001, 105, 9912-9916.	1.1	17
82	Spectroscopic constants and potential energy curves of gallium nitride (GaN) and ions: GaN+ and GaNâ^'. Chemical Physics Letters, 2006, 423, 247-253.	1.2	17
83	Tuning the electronic properties of doped bilayer graphene with small structural changes. Computational and Theoretical Chemistry, 2011, 974, 21-25.	1.1	17
84	Spin contamination in XOO radicals X=F, Cl, Br, HO: How is the investigation of the HOOO radical affected. Chemical Physics Letters, 2008, 464, 150-154.	1.2	16
85	Chemical reactivity of lithiumâ€doped fullerenes. Journal of Physical Organic Chemistry, 2012, 25, 322-326.	0.9	16
86	Electronic properties and vibrational spectra of (NH4)2Mâ€³(SO4)2Â·6H2O (Mâ€¯=â€¯Ni, Cu) Tutton's salt: DFT and experimental study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 218, 281-292.	2.0	16
87	Adsorption and diffusion of alkaliâ€atoms (Li, Na, and K) on BeN dual doped graphene. International Journal of Quantum Chemistry, 2019, 119, e25900.	1.0	16
88	Unusual Enhancement of the Adsorption Energies of Sodium and Potassium in Sulfurâ^'Nitrogen and Siliconâ^'Boron Codoped Graphene. ACS Omega, 2018, 3, 15821-15828.	1.6	15
89	Monolayer boronâ€arsenide as a perfect anode for alkaliâ€based batteries with large storage capacities and fast mobilities. International Journal of Quantum Chemistry, 2019, 119, e25975.	1.0	15
90	CCSDT study of the fluoroperoxyl radical, FOO. Chemical Physics Letters, 2004, 385, 292-297.	1.2	14

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91	Labeling the defects of carbon nanotubes with thiol groups. Journal of Materials Science, 2010, 45, 1039-1045.	1.7	14
92	Strong N-Doped Graphene: The Case of of Physical Chemistry C, 2015, 119, 15103-15111.	1.5	14
93	On the vibrational spectra of HSO and SOH. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 720-725.	2.0	13
94	On the enthalpy of formation of thiophene. Theoretical Chemistry Accounts, 2010, 127, 621-626.	0.5	13
95	Heteroatom Promoted Cycloadditions for Graphene. ChemistrySelect, 2016, 1, 5497-5500.	0.7	13
96	Silicon Carbide Induced Doping of Graphene: A New Potential Synthetic Route for SiC₃ Siligraphene. Journal of Physical Chemistry C, 2019, 123, 30341-30350.	1.5	13
97	Theoretical characterization of the low-lying electronic states of NbC. Journal of Chemical Physics, 2005, 123, 054318.	1.2	12
98	Time-Dependent Density Functional Theory Investigation of the Electronic Spectra of Hexanuclear Chalcohalide Rhenium(III) Clusters. Journal of Physical Chemistry A, 2011, 115, 211-218.	1.1	12
99	Bonding and singletâ€“triplet gap of silicon trimer: Effects of protonation and attachment of alkali metal cations. Journal of Computational Chemistry, 2015, 36, 805-815.	1.5	12
100	Diels-Alder reactions onto fluorinated and hydrogenated graphene. Chemical Physics Letters, 2017, 684, 79-85.	1.2	12
101	Coupled cluster investigation of the interaction of beryllium, magnesium, and calcium with pyridine: Implications for the adsorption on nitrogen-doped graphene. Computational and Theoretical Chemistry, 2019, 1150, 57-62.	1.1	12
102	Density Functional Computational Thermochemistry:â€‰ Determination of the Enthalpy of Formation of Methanethial-S,S-dioxide (Sulfene). Journal of Physical Chemistry A, 2003, 107, 518-521.	1.1	11
103	Coupled cluster and density functional investigation of the neutral sodium-benzene and potassium-benzene complexes. Chemical Physics Letters, 2018, 706, 343-347.	1.2	11
104	Electronic properties of substitutional impurities in graphenelike <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> , <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>t</mml:mi><mml:mi>g</mml:mi><mml:mtext>â^’</mml:mi><mml:mi mathvariant="normal">C</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant	1.1	11
105	On the encapsulation of halide anions by bambus[6]uril. Computational and Theoretical Chemistry, 2013, 1023, 5-9.	1.1	10
106	Cycloaddition Reactions between Graphene and Fluorinated Maleimides. Journal of Physical Chemistry C, 2017, 121, 13218-13222.	1.5	10
107	Theoretical Investigation of Carbonâ€“Sulfur Triple Bonds. Chemistry - A European Journal, 2011, 17, 1979-1987.	1.7	9
108	Theoretical investigation of the 9,10-bis(1,3-dithiol-2-ylidene)-9,10-dihydroanthracene (exTTF) dimer. Structural Chemistry, 2015, 26, 171-176.	1.0	9

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109	Subphthalocyanines hydrogen bonded capsules featuring norbornadiene tethers: Promising fullerene receptors. Chemical Physics Letters, 2015, 640, 140-146.	1.2	9
110	On the band gaps and effective masses of mono and dual doped monolayer graphene. Computational Materials Science, 2017, 137, 20-29.	1.4	9
111	Exploring the effect of substitutional doping on the electronic properties of graphene oxide. Journal of Materials Science, 2018, 53, 7516-7526.	1.7	9
112	Comparative study of the chemical reactivity of graphene and boron nitride sheets. Computational and Theoretical Chemistry, 2019, 1164, 112538.	1.1	9
113	Reduction chemistry of hexagonal boron nitride sheets and graphene: a comparative study on the effect of alkali atom doping on their chemical reactivity. New Journal of Chemistry, 2020, 44, 5725-5730.	1.4	9
114	Photoinduced Symmetry Breaking-Charge Separation in the Aggregated State of Perylene Diimide: Effect of Hydrophobicity. Journal of Physical Chemistry C, 2022, 126, 3872-3880.	1.5	9
115	Electronic spectra of oxocomplexes of Re(V) with thiolato ligands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 76, 348-355.	2.0	8
116	Buckycatcher polymer versus fullerene-buckycatcher complex: Which is stronger?. International Journal of Quantum Chemistry, 2015, 115, 1668-1672.	1.0	8
117	Tunable and sizeable band gaps in strained SiC3/hBN vdW heterostructures: A potential replacement for graphene in future nanoelectronics. Computational Materials Science, 2021, 188, 110233.	1.4	8
118	Theoretical investigation of ionized HSO and SOH. Molecular Physics, 2010, 108, 1739-1747.	0.8	7
119	Structural, electronic, and magnetic properties of non-planar doping of BeO in graphene: a DFT study. New Journal of Chemistry, 2017, 41, 10780-10789.	1.4	7
120	Adsorption of Sodium on Doped Graphene: A vdW-DF Study. Current Graphene Science, 2018, 2, 35-44.	0.5	7
121	Cycloaddition reactions on epitaxial graphene. New Journal of Chemistry, 2019, 43, 11251-11257.	1.4	7
122	Structural and magnetic properties of a defective graphene buffer layer grown on SiC(0001): a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 16096-16106.	1.3	7
123	Theoretical characterisation of the SSO, cyclic SOS and SOS isomers. Molecular Physics, 2010, 108, 171-179.	0.8	6
124	Addition of sulfur radicals to fullerenes. International Journal of Quantum Chemistry, 2011, 111, 4266-4275.	1.0	6
125	On the applicability of cluster models to study the chemical reactivity of carbon nanotubes. Journal of Computational Chemistry, 2011, 32, 2397-2403.	1.5	6
126	Relative affinity of bambus[6]uril towards halide ions: A DFT/GIAO approach in the gas phase, and in the presence of the solvent employing discrete and discrete-continuum models. Computational and Theoretical Chemistry, 2015, 1064, 35-44.	1.1	6

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127	Structure and chemical reactivity of lithium-doped graphene on hydrogen-saturated silicon carbide. Journal of Materials Science, 2017, 52, 1348-1356.	1.7	6
128	Exotic impurity-induced states in single-layer h -BN: The role of sublattice structure and intervalley interactions. Physical Review B, 2019, 100, .	1.1	6
129	Unraveling the electromagnetic structure of the epitaxial graphene buffer layer. Journal of Physics Condensed Matter, 2019, 31, 435001.	0.7	6
130	Unveiling the multilevel structure of midgap states in Sb-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi>X</mml:mi><mml:m <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>(</mml:mo><mml:mi>X</mml:mi><mml:mo>=</mml:mo><mml:mi) Tj Physical Review B, 2021, 104, .	1.1	6
131	Electronic states and potential energy curves of molybdenum carbide and its ions. Journal of Chemical Physics, 2006, 125, 024306.	1.2	5
132	Multireference configuration interaction study of the electronic states of ZrC. Journal of Chemical Physics, 2006, 124, 174312.	1.2	5
133	Theoretical characterization of hydrogen pentoxide, H₂O₅. International Journal of Quantum Chemistry, 2013, 113, 2206-2212.	1.0	5
134	Coupled cluster investigation of the axial and equatorial isomers of pyrrolidine. Molecular Physics, 2013, 111, 9-17.	0.8	5
135	Coupled cluster and density functional investigation of the hydrogen bond between halides, paraffines, olefins, and alkynes. Structural Chemistry, 2014, 25, 903-908.	1.0	5
136	Band gap opening in bilayer graphene by the simultaneous adsorption of electron donating and electron acceptor molecules. Computational and Theoretical Chemistry, 2017, 1120, 96-101.	1.1	5
137	Are [6+4] Cycloadditions onto Graphene Possible?. ChemistrySelect, 2017, 2, 9620-9623.	0.7	5
138	On the estimation of the strength of supramolecular complexes of fullerenes. International Journal of Quantum Chemistry, 2019, 119, e25670.	1.0	5
139	Tunable optoelectronic properties in multilayer 1T-TiS2: the effects of strain and an external electric field. Journal of Materials Science, 2021, 56, 6891-6902.	1.7	5
140	Thermodynamic study of proton transfer reactions of Re(V) trans-dioxocomplexes in aqueous solution. Dalton Transactions, 2009, , 8257.	1.6	4
141	Structural and theoretical studies of (E,E)-benzaldehyde azine and its rhenium(IV) complex. Journal of Molecular Structure, 2010, 963, 9-15.	1.8	4
142	Solution Phase Photolysis of 1,2-Dithiane Alone and with Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2012, 116, 8345-8351.	1.1	4
143	Interaction between alkyl radicals and single wall carbon nanotubes. Journal of Computational Chemistry, 2012, 33, 1511-1516.	1.5	4
144	New trends along hydrogen polyoxides: unusually long oxygenâ€“oxygen bonds in H₂O₆and H₂O₇. Molecular Physics, 2014, 112, 3047-3056.	0.8	4

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145	Adsorption of polycyclic aromatic hydrocarbons and inversion barriers of curved conjugated systems inside the molecular cage ExCage⁶⁺. International Journal of Quantum Chemistry, 2018, 118, e25539.	1.0	4
146	An effective tridental molecular clip for fullerenes. Journal of Physical Organic Chemistry, 2018, 31, e3727.	0.9	4
147	Non-trivial band gaps and charge transfer in Janus-like functionalized bilayer boron arsenide. Computational Materials Science, 2019, 170, 109186.	1.4	4
148	Adsorption of organic molecules on graphene and fluorographene: An unresolved discrepancy between experiment and theory. International Journal of Quantum Chemistry, 2021, 121, e26605.	1.0	4
149	Organic nanotubes and belt shaped molecules based on norbornadiene tethers. New Journal of Chemistry, 2016, 40, 202-208.	1.4	3
150	Triple-Doped Monolayer Graphene with Boron, Nitrogen, Aluminum, Silicon, Phosphorus, and Sulfur. ChemPhysChem, 2017, 18, 1854-1854.	1.0	3
151	Theoretical characterization of supramolecular complexes formed by fullerenes and dimeric porphyrins. New Journal of Chemistry, 2018, 42, 9956-9964.	1.4	3
152	Heat of formation and thermochemical parameters of silole. Chemical Physics Letters, 2013, 588, 17-21.	1.2	2
153	Coupled cluster investigation on the thermochemistry of dimethyl sulphide, dimethyl disulphide and their dissociation products: the problem of the enthalpy of formation of atomic sulphur. Molecular Physics, 2014, 112, 1167-1173.	0.8	2
154	Theoretical study of the adsorption of lithium, sodium and potassium on pyridine. Chemical Physics Letters, 2021, 784, 139112.	1.2	2
155	On the electronic properties of defective graphene buffer layer on 6Hâ€“SiC(0001). Computational Condensed Matter, 2021, 26, e00538.	0.9	1
156	Elucidating the electronic and magnetic properties of epitaxial graphene grown on SiC with a defective buffer layer. Journal of Materials Science, 2021, 56, 11386-11401.	1.7	1
157	Ultrafast dynamics of the liquid deposited blend film of porphyrin donor and perylene diimide acceptor. Chemical Physics, 2022, 559, 111547.	0.9	1
158	Ab initio and Density Functional Study of Thionitroso XNS and Thiazyl Isomers XSN, X: H, F, Cl, Br, OH, SH, NH2, CH3, CF3, and SiF3.. ChemInform, 2004, 35, no.	0.1	0
159	Impact of oxygen adsorption on the electronic properties and contact type of a defective epitaxial graphene-SiC interface. Computational and Theoretical Chemistry, 2021, 1203, 113361.	1.1	0