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	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
2	Ultrafast dynamics of the liquid deposited blend film of porphyrin donor and perylene diimide acceptor. Chemical Physics, 2022, 559, 111547.	0.9	1
3	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
4	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
5	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
6	On the electronic properties of defective graphene buffer layer on 6Hâ€“SiC(0001). Computational Condensed Matter, 2021, 26, e00538.	0.9	1
7	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
8	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
9	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
10	Theoretical study of the adsorption of lithium, sodium and potassium on pyridine. Chemical Physics Letters, 2021, 784, 139112.	1.2	2
11	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:mtext></mml:mrow></mml:math>	1.1	11
12	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
13	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
14	On the estimation of the strength of supramolecular complexes of fullerenes. International Journal of Quantum Chemistry, 2019, 119, e25670.	1.0	5
15	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
16	Comparative study of the chemical reactivity of graphene and boron nitride sheets. Computational and Theoretical Chemistry, 2019, 1164, 112538.	1.1	9
17	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
18	Unraveling the electromagnetic structure of the epitaxial graphene buffer layer. Journal of Physics Condensed Matter, 2019, 31, 435001.	0.7	6

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19	Non-trivial band gaps and charge transfer in Janus-like functionalized bilayer boron arsenide. Computational Materials Science, 2019, 170, 109186.	1.4	4
20	Theoretical characterization of hexagonal 2D Be₃N₂ monolayers. New Journal of Chemistry, 2019, 43, 2933-2941.	1.4	20
21	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
22	Cycloaddition reactions on epitaxial graphene. New Journal of Chemistry, 2019, 43, 11251-11257.	1.4	7
23	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
24	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
25	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
26	Theoretical investigation of various aspects of two dimensional holey boroxine, B₃O₃. RSC Advances, 2019, 9, 37526-37536.	1.7	21
27	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
28	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
29	Exploring the effect of substitutional doping on the electronic properties of graphene oxide. Journal of Materials Science, 2018, 53, 7516-7526.	1.7	9
30	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
31	An effective tridental molecular clip for fullerenes. Journal of Physical Organic Chemistry, 2018, 31, e3727.	0.9	4
32	Adsorption of Sodium on Doped Graphene: A vdW-DF Study. Current Graphene Science, 2018, 2, 35-44.	0.5	7
33	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
34	Hydrogenation and Fluorination of 2D Boron Phosphide and Boron Arsenide: A Density Functional Theory Investigation. ACS Omega, 2018, 3, 16416-16423.	1.6	38
35	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
36	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

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37	Theoretical characterization of supramolecular complexes formed by fullerenes and dimeric porphyrins. New Journal of Chemistry, 2018, 42, 9956-9964.	1.4	3
38	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
39	Lithium adsorption on heteroatom mono and dual doped graphene. Chemical Physics Letters, 2017, 672, 70-79.	1.2	34
40	Tripleâ€Doped Monolayer Graphene with Boron, Nitrogen, Aluminum, Silicon, Phosphorus, and Sulfur. ChemPhysChem, 2017, 18, 1864-1873.	1.0	49
41	On the band gaps and effective masses of mono and dual doped monolayer graphene. Computational Materials Science, 2017, 137, 20-29.	1.4	9
42	Cycloaddition Reactions between Graphene and Fluorinated Maleimides. Journal of Physical Chemistry C, 2017, 121, 13218-13222.	1.5	10
43	Rectangular and hexagonal doping of graphene with B, N, and O: a DFT study. RSC Advances, 2017, 7, 16064-16068.	1.7	26
44	Structure and chemical reactivity of lithium-doped graphene on hydrogen-saturated silicon carbide. Journal of Materials Science, 2017, 52, 1348-1356.	1.7	6
45	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
46	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
47	Are [6+4] Cycloadditions onto Graphene Possible?. ChemistrySelect, 2017, 2, 9620-9623.	0.7	5
48	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
49	Diels-Alder reactions onto fluorinated and hydrogenated graphene. Chemical Physics Letters, 2017, 684, 79-85.	1.2	12
50	Triple-Doped Monolayer Graphene with Boron, Nitrogen, Aluminum, Silicon, Phosphorus, and Sulfur. ChemPhysChem, 2017, 18, 1854-1854.	1.0	3
51	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
52	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
53	Porphyrins bearing corannulene pincers: outstanding fullerene receptors. RSC Advances, 2016, 6, 50978-50984.	1.7	18
54	Mono and dual doped monolayer graphene with aluminum, silicon, phosphorus and sulfur. Computational and Theoretical Chemistry, 2016, 1097, 40-47.	1.1	32

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55	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
56	Heteroatom Promoted Cycloadditions for Graphene. ChemistrySelect, 2016, 1, 5497-5500.	0.7	13
57	Dual doped monolayer and bilayer graphene: The case of 4p and 2p elements. Chemical Physics Letters, 2016, 658, 152-157.	1.2	20
58	Band Gap Opening in Dual-Doped Monolayer Graphene. Journal of Physical Chemistry C, 2016, 120, 7103-7112.	1.5	56
59	Organic nanotubes and belt shaped molecules based on norbornadiene tethers. New Journal of Chemistry, 2016, 40, 202-208.	1.4	3
60	Buckycatcher polymer versus fullerene-buckycatcher complex: Which is stronger?. International Journal of Quantum Chemistry, 2015, 115, 1668-1672.	1.0	8
61	Structural characterization and chemical reactivity of dual doped graphene. Carbon, 2015, 87, 106-115.	5.4	83
62	Stacked functionalized silicene: a powerful system to adjust the electronic structure of silicene. Physical Chemistry Chemical Physics, 2015, 17, 5393-5402.	1.3	43
63	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
64	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
65	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
66	Strong N-Doped Graphene: The Case of of Physical Chemistry C, 2015, 119, 15103-15111.	1.5	14
67	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
68	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
69	Hydrogen storage in doped biphenylene based sheets. Computational and Theoretical Chemistry, 2015, 1062, 30-35.	1.1	48
70	Subphthalocyanines hydrogen bonded capsules featuring norbornadiene tethers: Promising fullerene receptors. Chemical Physics Letters, 2015, 640, 140-146.	1.2	9
71	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
72	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

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73	Design and characterization of two strong fullerene receptors based on ballâ€“socket interactions. Chemical Physics Letters, 2014, 591, 323-327.	1.2	25
74	Chemical Reactivity and Bandâ€Gap Opening of Graphene Doped with Gallium, Germanium, Arsenic, and Selenium Atoms. ChemPhysChem, 2014, 15, 3994-4000.	1.0	67
75	Stability and Electronic Properties of Biphenylene Based Functionalized Nanoribbons and Sheets. Journal of Physical Chemistry C, 2014, 118, 24976-24982.	1.5	38
76	Theoretical characterization of sulfur and nitrogen dual-doped graphene. Computational and Theoretical Chemistry, 2014, 1049, 13-19.	1.1	80
77	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
78	New trends along hydrogen polyoxides: unusually long oxygenâ€“oxygen bonds in H₂O₆and H₂O₇. Molecular Physics, 2014, 112, 3047-3056.	0.8	4
79	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
80	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
81	C2V or C6V: Which is the most stable structure of the benzeneâ€“lithium complex?. Chemical Physics Letters, 2013, 573, 15-18.	1.2	21
82	Comparative Study of Defect Reactivity in Graphene. Journal of Physical Chemistry C, 2013, 117, 19048-19055.	1.5	149
83	Theoretical characterization of existing and new fullerene receptors. RSC Advances, 2013, 3, 25296.	1.7	38
84	Heat of formation and thermochemical parameters of silole. Chemical Physics Letters, 2013, 588, 17-21.	1.2	2
85	Concentration dependence of the band gaps of phosphorus and sulfur doped graphene. Computational Materials Science, 2013, 67, 203-206.	1.4	83
86	On the encapsulation of halide anions by bambus[6]uril. Computational and Theoretical Chemistry, 2013, 1023, 5-9.	1.1	10
87	Theoretical characterization of hydrogen pentoxide, H₂O₅. International Journal of Quantum Chemistry, 2013, 113, 2206-2212.	1.0	5
88	Chemical Reactivity of Electron-Doped and Hole-Doped Graphene. Journal of Physical Chemistry C, 2013, 117, 3895-3902.	1.5	50
89	Organic Chemistry of Graphene: The Dielsâ€“Alder Reaction. Chemistry - A European Journal, 2013, 19, 15719-15725.	1.7	57
90	On the Addition of Aryl Radicals to Graphene: The Importance of Nonbonded Interactions. ChemPhysChem, 2013, 14, 3271-3277.	1.0	24

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91	Coupled cluster investigation of the axial and equatorial isomers of pyrrolidine. Molecular Physics, 2013, 111, 9-17.	0.8	5
92	[2 + 2] Cycloadditions onto graphene. Journal of Materials Chemistry, 2012, 22, 5470.	6.7	43
93	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
94	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
95	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
96	Chemical reactivity of lithiumâ€doped fullerenes. Journal of Physical Organic Chemistry, 2012, 25, 322-326.	0.9	16
97	Interaction between alkyl radicals and single wall carbon nanotubes. Journal of Computational Chemistry, 2012, 33, 1511-1516.	1.5	4
98	A Firstâ€Principles Study on the Interaction between Alkyl Radicals and Graphene. Chemistry - A European Journal, 2012, 18, 7568-7574.	1.7	37
99	Improving the Chemical Reactivity of Single-Wall Carbon Nanotubes with Lithium Doping. Journal of Physical Chemistry C, 2011, 115, 20282-20288.	1.5	19
100	Monolayer and Bilayer Graphene Functionalized with Nitrene Radicals. Journal of Physical Chemistry C, 2011, 115, 195-203.	1.5	53
101	Tuning the electronic properties of doped bilayer graphene with small structural changes. Computational and Theoretical Chemistry, 2011, 974, 21-25.	1.1	17
102	Chemical Reactivity of Lithium Doped Monolayer and Bilayer Graphene. Journal of Physical Chemistry C, 2011, 115, 13392-13398.	1.5	56
103	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
104	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
105	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
106	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
107	Addition of sulfur radicals to fullerenes. International Journal of Quantum Chemistry, 2011, 111, 4266-4275.	1.0	6
108	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

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109	Theoretical Investigation of Carbonâ€“Sulfur Triple Bonds. Chemistry - A European Journal, 2011, 17, 1979-1987.	1.7	9
110	On the enthalpy of formation of thiophene. Theoretical Chemistry Accounts, 2010, 127, 621-626.	0.5	13
111	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
112	Thiophene adsorption on Single Wall Carbon Nanotubes and graphene. Computational and Theoretical Chemistry, 2010, 957, 114-119.	1.5	41
113	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
114	Labeling the defects of carbon nanotubes with thiol groups. Journal of Materials Science, 2010, 45, 1039-1045.	1.7	14
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	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
117	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
118	Theoretical characterisation of the SSO, cyclic SOS and SOS isomers. Molecular Physics, 2010, 108, 171-179.	0.8	6
119	Theoretical investigation of ionized HSO and SOH. Molecular Physics, 2010, 108, 1739-1747.	0.8	7
120	Is It Possible to Dope Singleâ€Walled Carbon Nanotubes and Graphene with Sulfur?. ChemPhysChem, 2009, 10, 715-722.	1.0	215
121	On the hydrogen addition to graphene. Computational and Theoretical Chemistry, 2009, 907, 93-103.	1.5	57
122	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
123	On the vibrational spectra of HSO and SOH. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 720-725.	2.0	13
124	Theoretical Characterization of Hydrogen Polyoxides: HOOH, HOOOH, HOOOOH, and HOOO. Journal of Physical Chemistry A, 2009, 113, 499-506.	1.1	53
125	Hydrogenated double wall carbon nanotubes. Journal of Chemical Physics, 2009, 130, 194704.	1.2	27
126	Density Functional Investigation of Thioepoxidated and Thiolated Graphene. Journal of Physical Chemistry C, 2009, 113, 5612-5619.	1.5	104

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127	Mechanical properties of graphene nanoribbons. Journal of Physics Condensed Matter, 2009, 21, 285304.	0.7	158
128	Thermodynamic study of proton transfer reactions of Re(V) trans-dioxocomplexes in aqueous solution. Dalton Transactions, 2009, , 8257.	1.6	4
129	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
130	Theoretical characterization of thioepoxidated single wall carbon nanotubes. Chemical Physics Letters, 2008, 460, 486-491.	1.2	31
131	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
132	Methane adsorption inside and outside pristine and N-doped single wall carbon nanotubes. Chemical Physics, 2008, 353, 79-86.	0.9	49
133	Theoretical investigation of nitrogen disubstituted corannulenes. Computational and Theoretical Chemistry, 2008, 865, 8-13.	1.5	25
134	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
135	Theoretical characterization of the HSOH, H2SO and H2OS isomers. Molecular Physics, 2008, 106, 2557-2567.	0.8	21
136	Thermochemistry of 35 selected sulfur compounds, a comparison between experiment and theory. Journal of Sulfur Chemistry, 2008, 29, 327-352.	1.0	22
137	Magnetism induced by single carbon vacancies in a three-dimensional graphitic network. Physical Review B, 2008, 77, .	1.1	65
138	Thermochemistry of the Hypobromous and Hypochlorous Acids, HOBr and HOCl. Journal of Physical Chemistry A, 2006, 110, 5887-5892.	1.1	23
139	Theoretical characterization of the thiosulfeno radical, HS2. Chemical Physics Letters, 2006, 422, 434-438.	1.2	29
140	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
141	Electronic states and potential energy curves of molybdenum carbide and its ions. Journal of Chemical Physics, 2006, 125, 024306.	1.2	5
142	Multireference configuration interaction study of the electronic states of ZrC. Journal of Chemical Physics, 2006, 124, 174312.	1.2	5
143	The enthalpy of formation of the HSO radical revisited. Chemical Physics Letters, 2005, 402, 289-293.	1.2	33
144	Theoretical characterization of the low-lying electronic states of NbC. Journal of Chemical Physics, 2005, 123, 054318.	1.2	12

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145	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
146	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
147	CCSDT study of the fluoroperoxyl radical, FOO. Chemical Physics Letters, 2004, 385, 292-297.	1.2	14
148	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
149	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
150	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
151	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
152	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
153	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
154	Density functional computational thermochemistry: solving the discrepancy between MO and DFT calculations on the enthalpy of formation of sulfine, CH2S̃...S̃...O. Chemical Physics Letters, 2002, 355, 207-213.	1.2	19
155	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
156	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
157	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
158	Hydroxamic chelates of boric acid, a density functional study. Computational and Theoretical Chemistry, 2001, 537, 173-180.	1.5	23
159	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