Filip Uhlik

List of Publications by Year
in descending order

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187	3,031	159573	254170
papers	citations	30 h-index	43 g-index

190	190	190	1763
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computing relative stabilities of metallofullerenes by Gibbs energy treatments. Theoretical Chemistry Accounts, 2007, 117, 315-322.	1.4	104
2	Enhanced Relaxation and Intermixing in Ge Islands Grown on Pit-Patterned Si(001) Substrates. Physical Review Letters, 2009, 102, 025502.	7.8	80
3	Simulations of ionization equilibria in weak polyelectrolyte solutions and gels. Soft Matter, 2019, 15, 1155-1185.	2.7	78
4	Zeolite (In)Stability under Aqueous or Steaming Conditions. Advanced Materials, 2020, 32, e2003264.	21.0	75
5	AM1 computations on seven isolated-pentagon-rule isomers of C80. Chemical Physics Letters, 1995, 246, 66-72.	2.6	71
6	Enthalpyâ€“entropy interplay for C[sub 36] cages: B3LYP/6-31G[sup â^—] calculations. Journal of Chemical Physics, 2000, 113, 4933.	3.0	68
7	Intrinsic Viscosity of Cyclic Polystyrene. Macromolecules, 2017, 50, 7770-7776.	4.8	61
8	Computational modeling of the elemental catalysis in the Stoneâ€“Wales fullerene rearrangements. Journal of Organometallic Chemistry, 2000, 599, 57-61.	1.8	60
9	Local pH and effective pK_A of weak polyelectrolytes â€“ insights from computer simulations. Physical Chemistry Chemical Physics, 2017, 19, 14376-14387.	2.8	60
10	Modeling of Ionization and Conformations of Starlike Weak Polyelectrolytes. Macromolecules, 2014, 47, 4004-4016.	4.8	58
11	La2@C72and Sc2@C72:Â Computational Characterizations. Journal of Physical Chemistry A, 2006, 110, 2231-2234.	2.5	57
12	Electron pairing and chemical bonds. On the accuracy of the electron pair model of chemical bond. Computational and Theoretical Chemistry, 1997, 391, 159-168.	1.5	55
13	Polyelectrolyte Behavior of Polystyrene-block-poly(methacrylic acid) Micelles in Aqueous Solutions at Low Ionic Strength. Macromolecules, 2004, 37, 10141-10154.	4.8	53
14	Hiding and Recovering Electrons in a Dimetallic Endohedral Fullerene: Air-Stable Products from Radical Additions. Journal of the American Chemical Society, 2015, 137, 232-238.	13.7	49
15	Computed structure and energetics of La@C60. International Journal of Quantum Chemistry, 2005, 104, 272-277.	2.0	47
16	Facile Synthesis of an Extensive Family of Sc₂O@C_{2n} (n = 35â€“47) and Chemical Insight into the Smallest Member of Sc₂O@C₂(7892)â€“C₇₀. Journal of Physical Chemistry C, 2014, 118, 28883-28889.	3.1	47
17	Experimental Study of Hydrophobically Modified Amphiphilic Block Copolymer Micelles Using Light Scattering and Nonradiative Excitation Energy Transfer,. Macromolecules, 2002, 35, 9487-9496.	4.8	41
18	Sm@C_{2v}(19138)-C₇₆: A Non-IPR Cage Stabilized by a Divalent Metal Ion. Inorganic Chemistry, 2015, 54, 4243-4248.	4.0	39

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19	Isolation and Crystallographic Characterization of the Labile Isomer of Y@C₈₂ Cocrystallized with Ni(OEP): Unprecedented Dimerization of Pristine Metallofullerenes. Angewandte Chemie - International Edition, 2016, 55, 9234-9238.	13.8	38
20	Isomeric Sc₂O@C₇₈ Related by a Single-Step Stoneâ€“Wales Transformation: Key Links in an Unprecedented Fullerene Formation Pathway. Inorganic Chemistry, 2016, 55, 11354-11361.	4.0	37
21	MPWB1K calculations of stepwise encapsulations: Lix@C60. Chemical Physics Letters, 2008, 463, 121-123.	2.6	36
22	Evidence for fullerenes in solid bitumen from pillow lavas of Proterozoic age from MÃ†ov (Bohemian) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	3.9	35
23	La₂@C_s(17â€‰490)â€C₇₆: A New Nonâ€IPR Dimetallic Metallofullerene Featuring Unexpectedly Weak Metalâ€“Pentalene Interactions. Chemistry - A European Journal, 2013, 19, 17125-17130.	3.3	35
24	Computing enthalpy-entropy interplay for isomeric fullerenes. International Journal of Quantum Chemistry, 2004, 99, 640-653.	2.0	34
25	Computed Structures of Two Known Yb@C74Isomers. Journal of Physical Chemistry A, 2006, 110, 12860-12863.	2.5	34
26	Computed stabilities in metallofullerene series: Al@C₈₂, Sc@C₈₂, Y@C₈₂, and La@C₈₂. International Journal of Quantum Chemistry, 2011, 111, 2712-2718.	2.0	34
27	Charge-controlled nano-structuring in partially collapsed star-shaped macromolecules. Soft Matter, 2016, 12, 4846-4852.	2.7	34
28	Isolation and Structural Characterization of Er@C_{2v}(9)-C₈₂ and Er@C_s(6)-C₈₂: Regioselective Dimerization of a Pristine Endohedral Metallofullerene Induced by Cage Symmetry. Inorganic Chemistry, 2019, 58, 2177-2182.	4.0	33
29	Ho₂O@C₇₄: Ho₂O Cluster Expands within a Small Non-IPR Fullerene Cage of C₂(13333)-C₇₄. Inorganic Chemistry, 2019, 58, 4774-4781.	4.0	32
30	Temperature dependence of the Gibbs energy ordering of isomers of chlorine oxide (Cl2O2). The Journal of Physical Chemistry, 1991, 95, 5432-5434.	2.9	31
31	Ab InitioSCF Nonlinear Pair Population Analysis. A New Means of Detection and Localization of Multicenter Bonding. Inorganic Chemistry, 1997, 36, 5363-5368.	4.0	31
32	Polyelectrolyte shells of copolymer micelles in aqueous solutions: A Monte Carlo study. Journal of Chemical Physics, 2004, 121, 2367-2375.	3.0	31
33	Intermixing in heteroepitaxial islands: fast, self-consistent calculation of the concentration profile minimizing the elastic energy. New Journal of Physics, 2008, 10, 083039.	2.9	31
34	Computing the relative gas-phase populations of C60 and C70: beyond the traditional Î”Hf,298o scale. Journal of Molecular Graphics and Modelling, 2001, 19, 216-221.	2.4	29
35	Synthesis and photophysical properties of Î±,Ï‰-bis(terpyridine)oligothiophenes. Tetrahedron, 2011, 67, 75-79.	1.9	28
36	Popular C₈₂ Fullerene Cage Encapsulating a Divalent Metal Ion Sm²⁺: Structure and Electrochemistry. Inorganic Chemistry, 2015, 54, 2103-2108.	4.0	28

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37	Silver(<scp>i</scp>) complexes with 1â€²-(diphenylphosphino)-1-cyanoferrocene: the art of improvisation in coordination. Dalton Transactions, 2016, 45, 10655-10671.	3.3	28
38	Mg@C72 MNDO/d evaluation of the isomeric composition. Journal of Molecular Graphics and Modelling, 2001, 19, 252-255.	2.4	27
39	Tuning intramolecular electron and energy transfer processes in novel conjugates of La₂@C₈₀ and electron accepting subphthalocyanines. Chemical Communications, 2015, 51, 330-333.	4.1	26
40	Computational modelling for the clustering degree in the saturated steam and the water-containing complexes in the atmosphere. Journal of Quantitative Spectroscopy and Radiative Transfer, 2006, 97, 415-423.	2.3	25
41	Computational evaluation of the relative production yields in the X@C74 series (X=Ca, Sr, Ba). Chemical Physics Letters, 2007, 440, 259-262.	2.6	25
42	Eu@C72: Computed Comparable Populations of Two Non-IPR Isomers. Molecules, 2017, 22, 1053.	3.8	25
43	Computed stabilization for a giant fullerene endohedral: Y2C2@C1(1660)-C108. Chemical Physics Letters, 2018, 710, 147-149.	2.6	25
44	Endohedrally stabilized C₇₀ isomer with fused pentagons characterized by crystallography. Dalton Transactions, 2016, 45, 8142-8148.	3.3	23
45	The Unanticipated Dimerization of Ce@C_{2v}(9)â€C₈₂ upon Coâ€crystallization with Ni(octaethylporphyrin) and Comparison with Monomeric M@C_{2v}(9)â€C₈₂ (M = La, Sc, and Y). Chemistry - A European Journal, 2016, 22, 18115-18122.	3.3	23
46	Structural and electrochemical studies of Sm@D3h-C74 reveal a weak metalâ€“cage interaction and a small band gap species. Nanoscale, 2013, 5, 10409.	5.6	22
47	Local pH and Effective pK of a Polyelectrolyte Chain: Two Names for One Quantity?. ACS Macro Letters, 2018, 7, 1243-1247.	4.8	22
48	Nonradiative Excitation Energy Transfer in Hydrophobically Modified Amphiphilic Block Copolymer Micelles. Theoretical Model and Monte Carlo Simulations,. Macromolecules, 2002, 35, 9497-9505.	4.8	21
49	A Monte Carlo study of shells of hydrophobically modified amphiphilic copolymer micelles in polar solvents. Journal of Chemical Physics, 2003, 118, 11258-11264.	3.0	21
50	Calculations of Metallofullerene Yields. Journal of Computational and Theoretical Nanoscience, 2011, 8, 2233-2239.	0.4	19
51	C 78 IPR fullerenes: Computed B3LYP/6-31G*//HF/3-21G temperature-dependent relative concentrations. European Physical Journal D, 2001, 16, 349-352.	1.3	18
52	Computed structures and relative stabilities of Be@C74. International Journal of Quantum Chemistry, 2007, 107, 2494-2498.	2.0	18
53	Synthesis, Crystal Structures, and Electrochemical Behavior of Feâ€“Ru Heterobimetallic Complexes with Bridged Metallocene Units. Organometallics, 2014, 33, 5020-5032.	2.3	18
54	Mean squared displacement from fluorescence correlation spectroscopy. Soft Matter, 2016, 12, 3760-3769.	2.7	18

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55	Adamantylidene Addition to M 3 N@ I h â€€ 80 (M=Sc, Lu) and Sc 3 N@ D 5 h â€€ 80 : Synthesis and Crystallographic Characterization of the [5,6]â€Open and [6,6]â€Open Adducts. Chemistry - A European Journal, 2017, 23, 6552-6561.	3.3	18
56	Reaction of Zirconacyclopentadienes with Ethynylferrocenes. Collection of Czechoslovak Chemical Communications, 2004, 69, 351-364.	1.0	17
57	Synthesis and non-conventional structure of square-planar Pd(<scp>ii</scp>) and Pt(<scp>ii</scp>) complexes with an N,C,N-chelated stibinidene ligand. Dalton Transactions, 2018, 47, 5812-5822.	3.3	17
58	Comparing the reactivity of isomeric phosphinoferrocene nitrile and isocyanide in Pd(<scp>ii</scp>) complexes: synthesis of simple coordination compoundsvs. preparation of P-chelated insertion products and Fischer-type carbenes. Dalton Transactions, 2018, 47, 16082-16101.	3.3	17
59	Multivalent counterions accumulate in star-like polyelectrolytes and collapse the polymer in spite of increasing its ionization. Soft Matter, 2020, 16, 1047-1055.	2.7	17
60	Enhancement of fullerene stabilities from excited electronic states. Computing Letters, 2005, 1, 304-312.	0.5	16
61	Excited electronic states and relative stabilities of C80 isomers. International Journal of Quantum Chemistry, 2006, 106, 2222-2228.	2.0	16
62	Computations on three isomers of La@C₇₄. International Journal of Quantum Chemistry, 2008, 108, 2636-2640.	2.0	16
63	Synthesis of phosphinoferrocene amides and thioamides from carbamoyl chlorides and the structural chemistry of Group 11 metal complexes with these mixed-donor ligands. Dalton Transactions, 2015, 44, 3092-3108.	3.3	16
64	Computational studies of atmospheric chemistry species. Computational and Theoretical Chemistry, 1993, 282, 271-275.	1.5	15
65	A Computational Treatment of 35 IPR Isomers of C₈₈. Fullerenes, Nanotubes, and Carbon Nanostructures, 2000, 8, 417-432.	0.6	15
66	Water-Dimer Stability and Its Fullerene Encapsulations. Journal of Computational and Theoretical Nanoscience, 2015, 12, 959-964.	0.4	15
67	Calculations of the water-dimer encapsulations into C84. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 1-7.	2.1	15
68	Ho₂O@C₈₄: Crystallographic Evidence Showing Linear Metallic Oxide Cluster Encapsulated in IPR Fullerene Cage of D_{2d}(51591)-C₈₄. Inorganic Chemistry, 2019, 58, 10905-10911.	4.0	15
69	Computations on C84O: thermodynamic, kinetic and photochemical stability. Computational and Theoretical Chemistry, 2004, 684, 129-133.	1.5	14
70	Calculated relative yields for Sc2S@C82 and Y2S@C82. Theoretical Chemistry Accounts, 2011, 130, 549-554.	1.4	14
71	Evaluation of the relative stabilities of two non-IPR isomers of Sm@C76. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 339-344.	2.1	14
72	A computational characterization of CO@C₆₀. Fullerenes Nanotubes and Carbon Nanostructures, 2017, 25, 624-629.	2.1	14

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73	Antimony(<scp>i</scp>) â†' Pd(<scp>ii</scp>) complexes with the (Î¼-Sb)Pd₂ coordination framework. Dalton Transactions, 2019, 48, 11912-11920.	3.3	14
74	Electronic excited states and stabilities of fullerenes: Isomers of C78and Mg@C72. International Journal of Quantum Chemistry, 2004, 100, 610-616.	2.0	13
75	Probing the Influence of Phosphine Substituents on the Donor andÂCatalytic Properties of Phosphinoferrocene Carboxamides: AÂCombined Experimental and Theoretical Study. Organometallics, 2017, 36, 1828-1841.	2.3	13
76	Calculated relative populations of Sm@C₈₂ isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 233-238.	2.1	13
77	Calculated relative populations for the Eu@C82 isomers. Chemical Physics Letters, 2019, 726, 29-33.	2.6	13
78	Interactions of star-like polyelectrolyte micelles with hydrophobic counterions. Journal of Colloid and Interface Science, 2019, 546, 371-380.	9.4	13
79	Quantum-Chemical Calculations of Model Systems of Interest in Fullerene-Based Superconductivity. Journal of Low Temperature Physics, 2003, 131, 1259-1263.	1.4	12
80	Computations of model narrow nanotubes closed by fragments of smaller fullerenes and quasi-fullerenes. Journal of Molecular Graphics and Modelling, 2003, 21, 517-522.	2.4	12
81	Lix@C60: Calculations of the Encapsulation Energetics and Thermodynamics. International Journal of Molecular Sciences, 2008, 9, 1841-1850.	4.1	12
82	Synthesis and characterisation of Dewar benzeneâ€“ferrocene conjugates. Dalton Transactions, 2009, , 3137.	3.3	12
83	Computed Relative Populations of D₂(22)â€Ć₈₄ Endohedrals with Encapsulated Monomeric and Dimeric Water. ChemPhysChem, 2016, 17, 1109-1111.	2.1	12
84	Ho₂O@D₃(85)-C₉₂: Highly Stretched Cluster Dictated by a Giant Cage and Unexplored Isomerization. Inorganic Chemistry, 2020, 59, 11020-11027.	4.0	12
85	A computational evaluation of the water-dimer populations in saturated steam recommended for applications to the Earth's, planetary and cometary atmospheres. Journal of Molecular Structure, 1992, 270, 1-9.	3.6	11
86	Computational studies of atmospheric chemistry species. Computational and Theoretical Chemistry, 1993, 285, 273-276.	1.5	11
87	A computational thermodynamic evaluation of the altitude profiles of (N2)2, N2-O2 and (O2)2 in the Earth's atmosphere. Thermochimica Acta, 1994, 231, 55-60.	2.7	11
88	AM1 computed relative equilibrium populations of the ( ) and ( ) methanobuckminsterfullerenes C61H2. Chemical Physics Letters, 1994, 228, 490-494.	2.6	11
89	A fast computational method for determining equilibrium concentration profiles in intermixed nanoislands. Journal of Physics Condensed Matter, 2009, 21, 084217.	1.8	11
90	Stability Computations for Isomers of La@Cn (n = 72, 74, 76). Molecules, 2012, 17, 13146-13156.	3.8	11

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91	Stability calculations for Eu@C₇₄ isomers. International Journal of Quantum Chemistry, 2013, 113, 729-733.	2.0	11
92	Calculated Temperature Development of the Relative Stabilities of Yb@C82 Isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 147-154.	2.1	11
93	Hydrophobically Modified Amphiphilic Block Copolymer Micelles in Non-Aqueous Polar Solvents. Fluorometric, Light Scattering and Computer-Based Monte Carlo Study. Collection of Czechoslovak Chemical Communications, 2002, 67, 531-556.	1.0	11
94	Two C60O Structures and Their Relative Stabilities: AM1 Computations. Fullerenes, Nanotubes, and Carbon Nanostructures, 1993, 1, 537-546.	0.6	10
95	Thermodynamic Properties of He@C60. Fullerenes, Nanotubes, and Carbon Nanostructures, 2000, 8, 453-460.	0.6	10
96	Energyâ€“entropy interplay of C60F36 isomers. Chemical Physics Letters, 2003, 374, 100-103.	2.6	10
97	C94 IPR isomeric set: large-scale computations of relative stabilities based on the Gibbs function. Computational and Theoretical Chemistry, 2003, 630, 205-213.	1.5	10
98	Sc₂O@C₇₈: Calculations of the yield ratio for two observed isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2017, 25, 124-127.	2.1	10
99	Calculations of the relative populations of Lu@C₈₂ isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 710-714.	2.1	10
100	Mg@C74isomers: Calculated relative concentrations and comparison with Ca@C74. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 1905-1910.	1.8	9
101	Computational Modeling of the Ce@C₈₂ Metallofullerene Isomeric Composition. ECS Journal of Solid State Science and Technology, 2019, 8, M118-M121.	1.8	9
102	An estimation of dimerization energetics of the ClO radical. Chemical Physics Letters, 1991, 182, 51-56.	2.6	8
103	Computed gas-phase thermodynamics of the N2î—¸O2 complexes. Thermochimica Acta, 1993, 225, 1-7.	2.7	8
104	Relative Stabilities of C₇₄Isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2007, 15, 195-205.	2.1	8
105	Fluorescence Spectroscopy as a Tool for Investigating the Self-Organized Polyelectrolyte Systems. Advances in Polymer Science, 2010, , 187-249.	0.8	8
106	Double-exponential decay of orientational correlations in semiflexible polyelectrolytes. European Physical Journal E, 2012, 35, 53.	1.6	8
107	Stability issues in computational screening of carbon nanostructures: illustrations on La endohedrals. Molecular Simulation, 2017, 43, 1472-1479.	2.0	8
108	Calculated Relative Thermodynamic Stabilities of the Gd@C₈₂ Isomers. ECS Journal of Solid State Science and Technology, 2021, 10, 071013.	1.8	8

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109	Gas-phase association of O2: a computational thermodynamic study. Thermochimica Acta, 1993, 228, 9-14.	2.7	7
110	Isomeric C60F36(g) species: Computed structures and heats of formation. Physics of the Solid State, 2002, 44, 534-535.	0.6	7
111	Mean-Field Study of Poly(methacrylic acid) Shells in Partly Hydrophobically Modified Amphiphilic Block Copolymer Micelles in Polar Solventsâ€. Journal of Physical Chemistry B, 2003, 107, 8241-8247.	2.6	7
112	Computations of production yields for Ba@C₇₄ and Yb@C₇₄. Molecular Simulation, 2007, 33, 563-568.	2.0	7
113	SCF Study of Amphiphilic Micellar Shells Containing Polyelectrolyte and Hydrophobic Sequences. Macromolecules, 2007, 40, 7656-7664.	4.8	7
114	Computational screening of metallofullerenes for nanoscience: Sr@C₇₄. Molecular Simulation, 2008, 34, 17-21.	2.0	7
115	Towards Relative Populations of Non-Isomeric Metallofullerenes: La@C76( ) vs. La2@C76(,17490). Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 299-306.	2.1	7
116	Thermodynamics of Small Alkali Metal Halide Cluster Ions: Comparison of Classical Molecular Simulations with Experiment and Quantum Chemistry. Journal of Physical Chemistry A, 2015, 119, 488-500.	2.5	7
117	Computational Comparison of the Water-Dimer Encapsulations intoD2(22)-C84andD2d(23)-C84. ECS Journal of Solid State Science and Technology, 2017, 6, M3113-M3115.	1.8	7
118	Cyclic water-trimer encapsulation into D2(22)-C84 fullerene. Chemical Physics Letters, 2018, 695, 245-248.	2.6	7
119	Eu@C86 isomers: Calculated relative populations. Fullerenes Nanotubes and Carbon Nanostructures, 2020, 28, 565-570.	2.1	7
120	AM1 Computations of C60O2. Fullerenes, Nanotubes, and Carbon Nanostructures, 1994, 2, 73-88.	0.6	6
121	Electron Pairing and Chemical Bonds. Physical Meaning of Effective Pairs. Collection of Czechoslovak Chemical Communications, 1994, 59, 2567-2578.	1.0	6
122	Stimuli-Responsive Amphiphilic Shells of Kinetically Frozen Polymeric Micelles in Aqueous Media: Monte Carlo Simulations and Comparison to Self-Consistent Field Calculations. Macromolecules, 2008, 41, 3711-3719.	4.8	6
123	Synthesis, molecular structure, electrochemistry and DFT study of a ferrocenyl-substituted 4-quinazolinone and related heterocycles. New Journal of Chemistry, 2013, 37, 2019.	2.8	6
124	Isolation and Crystallographic Characterization of the Labile Isomer of Y@C₈₂ Cocrystallized with Ni(OEP): Unprecedented Dimerization of Pristine Metallofullerenes. Angewandte Chemie, 2016, 128, 9380-9384.	2.0	6
125	Calculations of the Lu₃N@C₈₀ two-isomer equilibrium. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 382-386.	2.1	6
126	Rotameric Isomers of La₂@C₈₀ & Dodecafluoro-Subphthalocyanine Conjugate: Computational Characterization. ECS Journal of Solid State Science and Technology, 2020, 9, 061014.	1.8	6

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127	Computed gas-phase thermodynamics of N2 association. Thermochimica Acta, 1993, 223, 1-6.	2.7	5
128	COMPUTING NARROW NANOTUBES AND THEIR DERIVATIVES. International Journal of Nanoscience, 2002, 01, 303-312.	0.7	5
129	Computations of the catalytic effects in the stone-wales fullerene isomerizations: N and CN agents. International Journal of Quantum Chemistry, 2004, 99, 634-639.	2.0	5
130	Depletion profiles for dilute solutions of linear chains, stars and H-branched molecules by self-consistent field calculations and Monte Carlo simulations. Soft Matter, 2011, 7, 10258.	2.7	5
131	Predicted stabilities of endohedral metalloâ€fullerenes La@C₇₆. Physica Status Solidi (B): Basic Research, 2012, 249, 2585-2587.	1.5	5
132	Unprecedented Chemical Reactivity of a Paramagnetic Endohedral Metallofullerene La@C_s-C₈₂ that Leads Hydrogen Addition in the 1,3-Dipolar Cycloaddition Reaction. Journal of the American Chemical Society, 2014, 136, 17537-17546.	13.7	5
133	Computations on Metallofullerenes Derivatized during Extraction: La@C80-C6H3Cl2 and La@C82-C6H3Cl2. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 173-181.	2.1	5
134	Intramolecular micellization and nanopatterning in pH- and thermo-responsive molecular brushes. Soft Matter, 2020, 16, 208-218.	2.7	5
135	Calculated relative populations for the Eu@C84 isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2021, 29, 144-148.	2.1	5
136	The drag of the tails: Diffusion of sticky nanoparticles in dilute polymer solutions. Journal of Chemical Physics, 2015, 143, 243129.	3.0	5
137	Computational Treatment of Alkaline Earth Encapsulations in C₇₄: Relative Thermodynamic Production Abundances. Fullerenes Nanotubes and Carbon Nanostructures, 2008, 16, 507-516.	2.1	4
138	Monte Carlo simulation of fluorescence correlation spectroscopy data. Collection of Czechoslovak Chemical Communications, 2011, 76, 207-222.	1.0	4
139	Stability Computations for Fullerenes and Metallofullerenes. World Scientific Series on Carbon Nanoscience, 2012, , 381-429.	0.1	4
140	Polyelectrolyte Hydrogels as Draw Agents for Desalination of Solutions with Multivalent Ions. Macromolecules, 2022, 55, 1763-1770.	4.8	4
141	Ho@C₈₂ Metallofullerene: Calculated Isomeric Composition. ECS Journal of Solid State Science and Technology, 2022, 11, 053018.	1.8	4
142	A refined evaluation of the gas-phase dimerization thermodynamics of the ClO radical. International Journal of Thermophysics, 1992, 13, 303-313.	2.1	3
143	A computational evaluation of relative stabilities of the open C2v and cyclic D3h forms of ozone. Thermochimica Acta, 1992, 196, 459-465.	2.7	3
144	AM1 Computed Vibrations in Two C60O Structures. Spectroscopy Letters, 1993, 26, 1785-1796.	1.0	3

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145	A Computational Study of ClONO₂H⁺: Structure and Vibrations. Spectroscopy Letters, 1994, 27, 563-571.	1.0	3
146	An analytical solution of isotopomeric enumerations for C2v cyclic odd-numbered carbon clusters Cn. Journal of Radioanalytical and Nuclear Chemistry, 1997, 219, 69-71.	1.5	3
147	B3LYP/6-31Gâ^—//SAM1 Calculations of C36Fullerene andquasi-Fullerene Cages. Fullerenes, Nanotubes, and Carbon Nanostructures, 2000, 8, 433-447.	0.6	3
148	Computations of Low-Energy Non-Icosahedral Structures of C^{6â^'}₆₀. Fullerenes, Nanotubes, and Carbon Nanostructures, 2000, 8, 403-415.	0.6	3
149	Metal-Coated Fullerenes C₆₀M_n: Calculations for M = Be, Mg, Al AND n = 12, 20, 32. Fullerenes, Nanotubes, and Carbon Nanostructures, 2000, 8, 385-402.	0.6	3
150	Model narrow nanotubes related to C36, C32 and C20: initial computational structural sampling. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2002, 96, 164-168.	3.5	3
151	Two Isomers of C60F48: Computed Interâ€isomeric Equilibrium. Fullerenes Nanotubes and Carbon Nanostructures, 2003, 11, 219-226.	2.1	3
152	Amphiphilic Block Copolymer Micelles with Hydrophobically Modified Shells. Molecular Simulation, 2003, 29, 655-660.	2.0	3
153	Sm@C74: Computed Relative Isomeric Populations. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 235-242.	2.1	3
154	Water-Dimer Stability and Its Fullerene Encapsulations. Journal of Computational and Theoretical Nanoscience, 2015, 12, 2622-2622.	0.4	3
155	Computer modeling of polymer stars in variable solvent conditions: a comparison of MD simulations, self-consistent field (SCF) modeling and novel hybrid Monte Carlo SCF approach. Soft Matter, 2021, 17, 580-591.	2.7	3
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