Miklos Kertesz

List of Publications by Year
in descending order

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182 papers	10,433 citations	44069 48 h-index	36028 97 g-index
187 all docs	187 docs citations	187 times ranked	9286 citing authors

#	Article	IF	Citations
1	Carbon Nanotube Actuators. Science, 1999, 284, 1340-1344.	12.6	2,343
2	Conjugated Polymers and Aromaticity. Chemical Reviews, 2005, 105, 3448-3481.	47.7	447
3	Conformational Information from Vibrational Spectra of Styrene, trans-Stilbene, and cis-Stilbene. Journal of Physical Chemistry A, 1997, 101, 3823-3831.	2.5	291
4	Performance of the Vienna ab initio simulation package (VASP) in chemical applications. Computational and Theoretical Chemistry, 2003, 624, 37-45.	1.5	275
5	Single-Bond Torsional Potentials in Conjugated Systems:â€‰ A Comparison of ab Initio and Density Functional Results. Journal of Physical Chemistry A, 1997, 101, 7426-7433.	2.5	254
6	Octahedral vs. trigonal-prismatic coordination and clustering in transition-metal dichalcogenides. Journal of the American Chemical Society, 1984, 106, 3453-3460.	13.7	247
7	Electronic Structure of Polymers. Advances in Quantum Chemistry, 1982, , 161-214.	0.8	187
8	Pancake Bonding: An Unusual Piâ€Stacking Interaction. Chemistry - A European Journal, 2019, 25, 400-416.	3.3	171
9	Hypothetical metallic allotrope of carbon. Journal of the American Chemical Society, 1983, 105, 4831-4832.	13.7	165
10	The geometry and the radial breathing mode of carbon nanotubes: beyond the ideal behaviour. New Journal of Physics, 2003, 5, 125-125.	2.9	154
11	Bandgap calculations for conjugated polymers. Synthetic Metals, 2004, 141, 171-177.	3.9	154
12	Evidence of Ïƒ- and Ï€-Dimerization in a Series of Phenalenyls. Journal of the American Chemical Society, 2014, 136, 18009-18022.	13.7	150
13	Intermolecular Covalent Ï€â^'Ï€ Bonding Interaction Indicated by Bond Distances, Energy Bands, and Magnetism in Biphenalenyl Biradicaloid Molecular Crystal. Journal of the American Chemical Society, 2007, 129, 1634-1643.	13.7	145
14	The effects of electron correlation on the degree of bond alternation and electronic structure of oligomers of polyacetylene. Journal of Chemical Physics, 1997, 107, 6712-6721.	3.0	143
15	Intermolecular transfer integrals for organic molecular materials: can basis set convergence be achieved?. Chemical Physics Letters, 2004, 390, 110-115.	2.6	137
16	Bond Length Alternation and Energy Band Gap of Polyyne. Journal of Physical Chemistry A, 2006, 110, 9771-9774.	2.5	123
17	Rotational Barrier in Phenalenyl Neutral Radical Dimer: Separating Pancake and van der Waals Interactions. Journal of the American Chemical Society, 2014, 136, 5539-5542.	13.7	120
18	Metal oligo-yne polymers: electronic structures of [-(L)nMC.tplbond.CRC.tplbond.C-]x polymers. Inorganic Chemistry, 1993, 32, 732-740.	4.0	118

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19	Two helical conformations of polythiophene, polypyrrole, and their derivatives. Physical Review B, 1989, 40, 9661-9670.	3.2	115
20	Theoretical13C NMR Spectra of IPR Isomers of Fullerenes C60, C70, C72, C74, C76, and C78Studied by Density Functional Theory. Journal of Physical Chemistry A, 2000, 104, 7398-7403.	2.5	101
21	Higher order Peierls distortion of one-dimensional carbon skeletons. Solid State Communications, 1983, 47, 97-102.	1.9	97
22	Fluxional Ïƒ-Bonds of the 2,5,8-Trimethylphenalenyl Dimer: Direct Observation of the Sixfold Ïƒ-Bond Shift via a Ï€-Dimer. Journal of the American Chemical Society, 2016, 138, 4665-4672.	13.7	92
23	Bond length alternation and aromaticity in large annulenes. Journal of Chemical Physics, 1998, 108, 6681-6688.	3.0	90
24	Ab initio Hartreeâ€“Fock crystal orbital studies. Energy bands in polyene reconsidered. Journal of Chemical Physics, 1977, 67, 1180.	3.0	88
25	Variations of the Geometries and Band Gaps of Single-Walled Carbon Nanotubes and the Effect of Charge Injection. Journal of Physical Chemistry B, 2003, 107, 6924-6931.	2.6	88
26	Dimensional Changes as a Function of Charge Injection in Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2002, 124, 15076-15080.	13.7	87
27	Vibrational Assignment of All 46 Fundamentals of C60and C606-:Â Scaled Quantum Mechanical Results Performed in Redundant Internal Coordinates and Compared to Experiments. Journal of Physical Chemistry A, 2000, 104, 102-112.	2.5	86
28	Bond-length alternation and charge transfer in a linear carbon chain encapsulated within a single-walled carbon nanotube. Physical Review B, 2005, 72, .	3.2	83
29	Is There a Lower Limit to the CC Bonding Distances in Neutral Radical Ï€-Dimers? The Case of Phenalenyl Derivatives. Journal of the American Chemical Society, 2010, 132, 10648-10649.	13.7	83
30	Properties of Sizeable [n]Cycloparaphenylenes as Molecular Models of Singleâ€Wall Carbon Nanotubes Elucidated by Raman Spectroscopy: Structural and Electronâ€Transfer Responses under Mechanical Stress. Angewandte Chemie - International Edition, 2014, 53, 7033-7037.	13.8	77
31	Validation of intermolecular transfer integral and bandwidth calculations for organic molecular materials. Journal of Chemical Physics, 2005, 122, 234707.	3.0	76
32	Double Pancake Bonds: Pushing the Limits of Strong Ï€â€“Ï€ Stacking Interactions. Journal of the American Chemical Society, 2014, 136, 12958-12965.	13.7	74
33	Bonds or not bonds? Pancake bonding in 1,2,3,5-dithiadiazolyl and 1,2,3,5-diselenadiazolyl radical dimers and their derivatives. Physical Chemistry Chemical Physics, 2012, 14, 10713.	2.8	72
34	Ab Initio Oligomer Approach to Vibrational Spectra of Polymers: Comparison of Helical and Planar Poly(p-phenylene). Macromolecules, 1994, 27, 762-770.	4.8	66
35	Identification for IPR Isomers of Fullerene C82by Theoretical13C NMR Spectra Calculated by Density Functional Theory. Journal of Physical Chemistry A, 2001, 105, 5468-5472.	2.5	66
36	Isomer Identification for Fullerene C84by13C NMR Spectrum:Â A Density-Functional Theory Study. Journal of Physical Chemistry A, 2001, 105, 5212-5220.	2.5	65

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37	Energy gap and bond length alternation in heterosubstituted narrow gap semiconducting polymers. The Journal of Physical Chemistry, 1987, 91, 2690-2692.	2.9	61
38	Crystal packing of TCNQ anion Ï€-radicals governed by intermolecular covalent Ï€â€“Ï€ bonding: DFT calculations and statistical analysis of crystal structures. Physical Chemistry Chemical Physics, 2008, 10, 2625.	2.8	61
39	Inorganic rings, intact and cleaved, between two metal fragments. Journal of the American Chemical Society, 1989, 111, 2030-2039.	13.7	59
40	13C NMR spectra for IPR isomers of fullerene C86. Chemical Physics, 2002, 276, 107-114.	1.9	58
41	Application of a Novel Linear/Exponential Hybrid Force Field Scaling Scheme to the Longitudinal Raman Active Mode of Polyyne. Journal of Physical Chemistry A, 2007, 111, 2434-2441.	2.5	56
42	Localization and delocalization: Distinction between through space and through bond interactions. Journal of Chemical Physics, 1982, 77, 2454-2459.	3.0	55
43	Electronic Structure of Helicenes, C₂S Helicenes, and Thiaheterohelicenes. Chemistry of Materials, 2008, 20, 3266-3277.	6.7	55
44	Limitations of current density functional theories for the description of partial Ï€-bond breaking. Chemical Physics Letters, 1997, 276, 266-268.	2.6	52
45	Low bandgap ladder polymers. Synthetic Metals, 1995, 69, 699-700.	3.9	50
46	Structure and electronic structure of polyacene. International Journal of Quantum Chemistry, 1989, 35, 305-313.	2.0	49
47	Linear C_n Clusters:â€‰ Are They Acetylenic or Cumulenic?. Journal of Physical Chemistry A, 2008, 112, 146-151.	2.5	49
48	Energetics and geometry of conducting polymers from oligomers. The Journal of Physical Chemistry, 1991, 95, 7680-7681.	2.9	48
49	Reversible Dimerization and Polymerization of a Janus Diradical To Produce Labile Câ”C Bonds and Large Chromic Effects. Angewandte Chemie - International Edition, 2016, 55, 14563-14568.	13.8	47
50	Pancake Bond Orders of a Series of Ï€â€Stacked Triangulene Radicals. Angewandte Chemie - International Edition, 2017, 56, 10188-10191.	13.8	46
51	Importance of energetics in the design of small bandgap conducting polymers. Chemistry of Materials, 1990, 2, 526-530.	6.7	45
52	Theoretical prediction of the vibrational spectrum of fluorene and planarized poly(p-phenylene). The Journal of Physical Chemistry, 1994, 98, 12223-12231.	2.9	44
53	Study of the Diradicaloid Character in a Prototypical Pancakeâ€Bonded Dimer: The Stacked Tetracyanoethylene (TCNE) Anion Dimer and the Neutral K₂TCNE₂ Complex. ChemPhysChem, 2014, 15, 165-176.	2.1	43
54	Change of geometry of polyacetylene upon charge transfer. Chemical Physics Letters, 1982, 90, 430-433.	2.6	42

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55	Spin Crossover of Spiro-Biphenalenyl Neutral Radical Molecular Conductors. Journal of the American Chemical Society, 2003, 125, 13334-13335.	13.7	42
56	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
57	Different orbitals for different spins for solids: Fully variationalab initiostudies on hydrogen and carbon atomic chains, polyene, and poly(sulphur nitride). Physical Review B, 1979, 19, 2034-2040.	3.2	41
58	The graphite-to-diamond transformation. Journal of Solid State Chemistry, 1984, 54, 313-319.	2.9	41
59	Do Localized Structures of [14]- and [18]Annulenes Exist?. Journal of the American Chemical Society, 1997, 119, 11994-11995.	13.7	41
60	Concave or convex Ï€-dimers: the role of the pancake bond in substituted phenalenyl radical dimers. Physical Chemistry Chemical Physics, 2015, 17, 23963-23969.	2.8	40
61	Structure and Electronic Structure of Low-Band-Gap Ladder Polymers. Macromolecules, 1995, 28, 1475-1480.	4.8	39
62	Theoretical Analysis of Intermolecular Covalent Ï€â^'Ï€ Bonding and Magnetic Properties of Phenalenyl and spiro-Biphenalenyl Radical Ï€-Dimers. Journal of Physical Chemistry A, 2007, 111, 6304-6315.	2.5	39
63	Extraction of polymer properties from oligomer calculations. The Journal of Physical Chemistry, 1990, 94, 5172-5179.	2.9	38
64	Bonding in crystals containing one-dimensional bridged and unbridged group 11 and 12 linear, zigzag and helical chains. Inorganic Chemistry, 1990, 29, 2568-2575.	4.0	38
65	Heteroâ€Ïâ€Dimers of Phenalenyls. Chemistry - A European Journal, 2015, 21, 18230-18236.	3.3	38
66	Ab initio crystal orbital studies on linear chains of H atoms. Theoretica Chimica Acta, 1976, 41, 89-91.	0.8	35
67	Band structure calculation of extended poly(copper phthalocyanine) one-dimensional and two-dimensional polymers. Inorganic Chemistry, 1988, 27, 3672-3675.	4.0	35
68	Electronic structure of small gap polymers. Synthetic Metals, 1989, 28, 545-552.	3.9	35
69	Geometrical and electronic structures of a benzimidazobenzophenanthroline-type ladder polymer (BBL). Macromolecules, 1992, 25, 5424-5429.	4.8	35
70	Binding Interactions in Dimers of Phenalenyl and Closed-Shell Analogues. Journal of Physical Chemistry A, 2013, 117, 3642-3649.	2.5	35
71	Role of charge transfer and quinonoid structure in the Raman spectrum of doped poly(p-phenylene). Journal of the American Chemical Society, 1994, 116, 9269-9274.	13.7	34
72	Conformational Studies of Vibrational Properties and Electronic States of Leucoemeraldine Base and Its Oligomers. Macromolecules, 1997, 30, 620-630.	4.8	34

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73	Theoretical 13C NMR spectra of IPR isomers of fullerene C80: a density functional theory study. Chemical Physics Letters, 2000, 328, 387-395.	2.6	34
74	Confinement effects on site-preferences for cycloadditions into carbon nanotubes. Chemical Physics Letters, 2007, 444, 155-160.	2.6	34
75	Quantumâ€mechanical oligomer approach for the calculation of vibrational spectra of polymers. Journal of Chemical Physics, 1990, 93, 5257-5266.	3.0	33
76	On the Anisotropy of van der Waals Atomic Radii of O, S, Se, F, Cl, Br, and I. Journal of Physical Chemistry A, 2013, 117, 14184-14190.	2.5	33
77	Cethrene: The Chameleon of Woodwardâ€“Hoffmann Rules. Journal of Organic Chemistry, 2018, 83, 4769-4774.	3.2	33
78	Electronic structures of heterocyclic ladder polymers; polyphenothiazine, polyphenoxazine, and polyphenoquinoxaline. Chemistry of Materials, 1992, 4, 378-383.	6.7	32
79	Individualities and average behavior in the physical properties of small diameter single-walled carbon nanotubes. Carbon, 2004, 42, 971-978.	10.3	32
80	Local Modifications of Single-Wall Carbon Nanotubes Induced by Bond Formation with Encapsulated Fullerenes. Journal of Physical Chemistry B, 2007, 111, 1099-1109.	2.6	32
81	Cooperative Behaviors in Carbene Additions through Local Modifications of Nanotube Surfaces. Chemistry of Materials, 2007, 19, 1028-1034.	6.7	32
82	Fluxional Ïƒ-bonds of 2,5,8-tri-tert-butyl-1,3-diazaphenalenyl dimers: stepwise [3,3], [5,5] and [7,7] sigmatropic rearrangements viaÏ€-dimer intermediates. Physical Chemistry Chemical Physics, 2010, 12, 5084.	2.8	32
83	Validation of density functionals for pancake-bonded Ï€-dimers; dispersion is not enough. Physical Chemistry Chemical Physics, 2017, 19, 24761-24768.	2.8	32
84	Linear and Radial Conjugation in Extended Ï€-Electron Systems. Journal of the American Chemical Society, 2020, 142, 2293-2300.	13.7	32
85	Charge Shift Bonding Concept in Radical Ï€-Dimers. Journal of Physical Chemistry A, 2011, 115, 13942-13949.	2.5	31
86	Nitrogen Doping Enables Covalent-Like Ï€â€“Ï€ Bonding between Graphenes. Nano Letters, 2015, 15, 5482-5491.	9.1	31
87	The [Vâ¯Câ•Câ¯V] Divacancy and the Interstitial Defect in Diamond: Vibrational Properties. Journal of Physical Chemistry C, 2010, 114, 9563-9567.	3.1	30
88	Chameleon-like behaviour of cyclo[n]paraphenylenes in complexes with C₇₀: on their impressive electronic and structural adaptability as probed by Raman spectroscopy. Faraday Discussions, 2014, 173, 157-171.	3.2	30
89	From linear to cyclic oligoparaphenylenes: electronic and molecular changes traced in the vibrational Raman spectra and reformulation of the bond length alternation pattern. Physical Chemistry Chemical Physics, 2016, 18, 11683-11692.	2.8	30
90	Electronic structure of long polyiodide chains. Journal of the American Chemical Society, 1982, 104, 5889-5893.	13.7	29

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91	Geometrical and electronic structures of .pi.-conjugated silicon ring polymers. Organometallics, 1992, 11, 3178-3184.	2.3	29
92	Vibrational Raman Spectra of C70 and C706- Studied by Density Functional Theory. Journal of Physical Chemistry A, 2002, 106, 6381-6386.	2.5	29
93	The effect of additional fused rings on the stabilities and the band gaps of heteroconjugated polymers. International Journal of Quantum Chemistry, 1987, 32, 163-170.	2.0	28
94	Evidence of quinonoid structures in the vibrational spectra of thiophene based conducting polymers: Poly(thiophene), poly(thieno[3,4-b]benzene), and poly(thieno[3,4-b]pyrazine). Journal of Chemical Physics, 1997, 106, 5541-5553.	3.0	28
95	One-Dimensional Metallic Conducting Pathway of Cyclohexyl-Substituted Spiro-Biphenalenyl Neutral Radical Molecular Crystal. Journal of the American Chemical Society, 2006, 128, 1418-1419.	13.7	28
96	Energetics of linear carbon chains in one-dimensional restricted environment. Physical Chemistry Chemical Physics, 2009, 11, 425-430.	2.8	28
97	Electronic structure and metallization of silicon. Physical Review B, 1984, 29, 1791-1797.	3.2	26
98	Argon-matrix-isolation Raman spectra and density functional study of 1,3-butadiene conformers. Theoretical Chemistry Accounts, 1999, 102, 196-206.	1.4	26
99	Pancake Bonding in Ï€â€Stacked Trimers in a Salt of Tetrachloroquinone Anion. Chemistry - A European Journal, 2018, 24, 8292-8297.	3.3	26
100	Changes of Lattice Geometries Upon Charge Transfer. Molecular Crystals and Liquid Crystals, 1985, 126, 103-110.	0.8	25
101	AB initio study of the dynamical properties of polythiophene. Synthetic Metals, 1991, 43, 3491-3496.	3.9	24
102	Consistencies between experiments and quantum calculations of strained Câ€“C single bond lengths. Chemical Communications, 1997, , 2199-2200.	4.1	24
103	Dimensional change as a function of charge injection in graphite intercalation compounds: â€ƒA density functional theory study. Physical Review B, 2003, 68, .	3.2	24
104	Electronic Structures and Charge Transport Properties of the Organic Semiconductor Bis[1,2,5]thiadiazolo-p-quinobis(1,3-dithiole), BTQBT, and Its Derivatives. Journal of Physical Chemistry B, 2005, 109, 12891-12898.	2.6	23
105	New Interpretation of the Valence Tautomerism of 1,6-Methano[10]annulenes and Its Application to Fullerene Derivatives. Journal of Physical Chemistry A, 1998, 102, 3429-3437.	2.5	22
106	Assignment of the vibrational spectra of polysilane and its oligomers. Macromolecules, 1992, 25, 1103-1108.	4.8	21
107	Density Functional Studies of Vibrational Properties of HCN, H2O, CH2O, CH4, and C2H4. The Journal of Physical Chemistry, 1996, 100, 16530-16537.	2.9	21
108	Low-Bandgap Pyrazine Polymers: Ladder-Type Connectivity by Intramolecular SÂ·Â·Â·N(sp²) Interactions and Hydrogen Bonds. Macromolecules, 2009, 42, 2309-2312.	4.8	21

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109	The Raman fingerprint of cyclic conjugation: the case of the stabilization of cations and dications in cycloparaphenylenes. Chemical Science, 2016, 7, 3494-3499.	7.4	21
110	Interpretation of the vibrational spectra of planarized poly-p-phenylene. Synthetic Metals, 1995, 69, 683-684.	3.9	20
111	Stepwise Cope Rearrangement of Cyclo-biphenalenyl via an Unusual Multicenter Covalent Ï€-Bonded Intermediate. Journal of the American Chemical Society, 2006, 128, 7277-7286.	13.7	20
112	Intramolecular Pancake Bonding in Helical Structures. Chemistry - A European Journal, 2017, 23, 7474-7482.	3.3	20
113	Structure of infinite polyenes: Ab initio quantum chemical study. Journal of the Chemical Society Chemical Communications, 1978, , 575-576.	2.0	19
114	Dimensional changes as a function of charge injection for trans-polyacetylene: A density functional theory study. Journal of Chemical Physics, 2002, 117, 7691-7697.	3.0	19
115	Divacancies in diamond: a stepwise formation mechanism. Physical Chemistry Chemical Physics, 2014, 16, 1515-1521.	2.8	19
116	Theoretical evidence for the major isomers of fullerene C84 based on 13C NMR chemical shifts. New Journal of Chemistry, 2000, 24, 741-743.	2.8	18
117	Probing semiconductivity in crystals of stable semiquinone radicals: organic salts of 5,6-dichloro-2,3-dicyanosemiquinone (DDQ) radical anions. CrystEngComm, 2018, 20, 1862-1873.	2.6	18
118	Is a 1.90 Ã... Câ€“C bond length in polymeric fullerides possible?. Chemical Physics Letters, 1998, 282, 318-324.	2.6	17
119	Cyclo-biphenalenyl Biradicaloid Molecular Materials: Conformation, Tautomerization, Magnetism, and Thermochromism. Chemistry of Materials, 2011, 23, 874-885.	6.7	17
120	Can carbon monoxide polymerize? A theoretical investigation of polyketone. Chemical Communications, 1997, , 2011.	4.1	16
121	Ladder-Type Polyenazine Based on Intramolecular SÂ·Â·Â·N Interactions: A Theoretical Study of a Small-Bandgap Polymer. Macromolecules, 2009, 42, 6123-6127.	4.8	16
122	Roles of Conformational Restrictions of a Bismalonate in the Interactions with a Carbon Nanotube. Journal of Physical Chemistry C, 2009, 113, 14184-14194.	3.1	16
123	Volume Change during Thermal [4 + 4] Cycloaddition of [2.2] (9,10)Anthracenophane. Journal of the American Chemical Society, 2013, 135, 13720-13727.	13.7	16
124	Conformational information from vibrational spectra of polyaniline. Synthetic Metals, 1997, 85, 1073-1076.	3.9	15
125	Theoretical Design of Low Band Gap Conjugated Polymers through Ladders with Acetylenic Crosspieces. Macromolecules, 2007, 40, 6740-6747.	4.8	15
126	Reversible Dimerization and Polymerization of a Janus Diradical To Produce Labile Câ”C Bonds and Large Chromic Effects. Angewandte Chemie, 2016, 128, 14783-14788.	2.0	15

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127	Sigmaâ€•versus Piâ€Dimerization Modes of Triangulene. Chemistry - A European Journal, 2018, 24, 6140-6147.	3.3	15
128	Unexpected Charge Effects Strengthen Ï€â€“Stacking Pancake Bonding. Jacs Au, 2021, 1, 1647-1655.	7.9	15
129	Ab initionumerical studies on density-matrix asymptotics in extended systems. Physical Review B, 1983, 27, 7583-7588.	3.2	14
130	The effect of side-group substitution on the energy gaps of phenylene and thienylene oligomers and polymers. Synthetic Metals, 1992, 47, 179-186.	3.9	14
131	Dependence of Youngâ€™s modulus oftrans-polyacetylene upon charge transfer. Physical Review Letters, 1990, 64, 3031-3034.	7.8	13
132	Conformational Fingerprints in the IR and Raman Spectra of Oligoanilines:â€‰ A Combined Theoretical and Experimental Study. Chemistry of Materials, 1999, 11, 855-857.	6.7	13
133	Conformational Preferences of Î²-Carotene in the Confined Spaces inside Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 12139-12144.	3.1	13
134	Helical molecular redox actuators with pancake bonds?. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	13
135	Anisotropy of the dielectric constant of polyacetylene. Journal of Polymer Science, Polymer Physics Edition, 1981, 19, 743-747.	1.0	12
136	The electronic structure of BC3. Journal of the Chemical Society Chemical Communications, 1988, , 75.	2.0	12
137	Splitting the Ring: Impact of Ortho and Meta Pi Conjugation Pathways through Disjointed [8]Cycloparaphenylene Electronic Materials. Journal of the American Chemical Society, 2022, 144, 4611-4622.	13.7	12
138	Characterization of large vacancy clusters in diamond from a generational algorithm using tight binding density functional theory. Physical Chemistry Chemical Physics, 2010, 12, 14017.	2.8	11
139	Theoretical evaluation of Youngâ€™s moduli of polymers. Physical Review B, 1990, 41, 11368-11378.	3.2	10
140	The aromatic - quinonoid transition in conducting polymers. Synthetic Metals, 1995, 69, 641-644.	3.9	10
141	Highâ€Pressure Chemistry and the Mechanochemical Polymerization of [5]â€Cycloâ€pâ€phenylene. Chemistry - A European Journal, 2017, 23, 16593-16604.	3.3	10
142	Ionic charge-transfer complexes. 2. Comparative ab initio and semiempirical studies on complexes of An+ (An = aniline). Journal of the American Chemical Society, 1986, 108, 4391-4397.	13.7	9
143	Mechanochemistry in [6]Cycloparaphenylene: A Combined Raman Spectroscopy and Density Functional Theory Study. ChemPhysChem, 2018, 19, 1903-1916.	2.1	9
144	Energy bands in solids: bonding, energy levels and orbitals. International Reviews in Physical Chemistry, 1985, 4, 125-164.	2.3	8

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145	Electronic structure of highly doped conducting polymers. International Journal of Quantum Chemistry, 1986, 29, 1165-1176.	2.0	8
146	Helical Peierls distortion: Formation of helices of polyketone and polyisocyanide. Chemical Physics Letters, 1990, 169, 445-449.	2.6	8
147	Pancake Bond Orders of a Series of Ï€â€Stacked Triangulene Radicals. Angewandte Chemie, 2017, 129, 10322-10325.	2.0	8
148	Bonding and electronic structure of conducting mercury networks: KHgC4n graphite amalgams and Hg3MF6 layers and chains. Inorganic Chemistry, 1987, 26, 2852-2857.	4.0	7
149	Simulations of large multi-atom vacancies in diamond. Diamond and Related Materials, 2010, 19, 1153-1162.	3.9	7
150	Superdegeneracies in Extended Systems; a Prerequisite for Ï€ Ferromagnets?. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1989, 176, 115-123.	0.3	6
151	Chemisorption on metals: the method of moments point of view. The Journal of Physical Chemistry, 1989, 93, 3237-3240.	2.9	6
152	Conformations and electronic structures of poly(ketene) and related conjugated polymers: reduction of the n-.pi.* band gap. Journal of the American Chemical Society, 1991, 113, 4404-4409.	13.7	6
153	Smooth energy-band interpolation with gradient utilization. Physical Review B, 1981, 24, 6870-6879.	3.2	5
154	The gradient of the total energy for metals. Chemical Physics Letters, 1984, 106, 443-446.	2.6	5
155	A new partition of the atomic polar tensor: the benzene molecule. Chemical Physics Letters, 1996, 263, 697-702.	2.6	5
156	Bimolecular hydrogen transfer in phenalene by a stepwise ene-like reaction mechanism. Chemical Communications, 2010, 46, 4282.	4.1	5
157	Molecules under Pressure: The Case of [n]Cycloparaphenylenes. Chemistry of Materials, 2019, 31, 6443-6452.	6.7	5
158	Quinonoid vs. aromatic structures of heteroconjugated polymers from oligomer calculations. Physical Chemistry Chemical Physics, 2020, 22, 11431-11439.	2.8	5
159	Change of Câ€“C Bond Length in Layers of Graphite Upon Charge Transfer. Materials Research Society Symposia Proceedings, 1982, 20, 141.	0.1	4
160	Application of the linear/exponential hybrid force field scaling scheme to the bond length alternation modes of polyacetylene. Chemical Physics Letters, 2006, 432, 356-361.	2.6	4
161	Molecular Actuators Designed with Sâˆ’N(sp²) Hemibonds Attached to a Conformationally Flexible Pivot. Chemistry of Materials, 2009, 21, 2149-2157.	6.7	4
162	Impact of the Aryl Amphiphile Hydrophobe Size on Controlling the Ï€-Conjugated Microcrystal Growth along the Ï€-Stack Direction. Crystal Growth and Design, 2021, 21, 2465-2473.	3.0	4

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163	Double walled carbon nanotube with the smallest inner diameter: a first principles study. Physica Status Solidi (B): Basic Research, 2006, 243, 3464-3467.	1.5	3
164	Why is there no in-plane H-atom transfer from aryloxy radicals? A theoretical and experimental investigation. Photochemical and Photobiological Sciences, 2010, 9, 1203-1211.	2.9	3
165	NMR spectral fingerprint patterns as diagnostics for the unambiguous configurational analysis of the classic organoâ€gelator 1,3:2,4â€dibenzylideneâ€‹scp›d‹/scp›â€sorbitol (DBS) and its derivatives. Magnetic Resonance in Chemistry, 2021, 59, 608-613.	1.9	3
166	Quinonoid versus Aromatic Ï€-Conjugated Oligomers and Polymers and Their Diradical Characters. Journal of Physical Chemistry C, 2022, 126, 5302-5310.	3.1	3
167	Conformations of Antipyrines. Journal of Physical Chemistry A, 2011, 115, 4832-4839.	2.5	2
168	Molecular tetrominoes: selective masking of the donor Ï€-face to control the configuration of donorâ€“acceptor complexes. Organic and Biomolecular Chemistry, 2022, 20, 375-386.	2.8	2
169	Interpolation of singular energy bands. Physical Review B, 1982, 25, 7834-7835.	3.2	1
170	Xe-bearing hydrocarbon ions: Observation of Xe.acetylene+ and Xe.benzene+ radical cations and calculations of their ground state structures. Chemical Physics Letters, 2016, 649, 8-14.	2.6	1
171	Multicentric two-electron covalent bonding (pancake bonding) between semiquinone radicals determines bulk properties. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e80-e80.	0.1	1
172	Helical Conformations of Conducting Polymers. Materials Research Society Symposia Proceedings, 1989, 173, 391.	0.1	0
173	Linear carbon chain in the interior of a single walled carbon nanotube. AIP Conference Proceedings, 2005, , .	0.4	0
174	Conjugated Polymers and Aromaticity. ChemInform, 2006, 37, no.	0.0	0
175	Covalent Bond Formation in Defected Nanopeapods Induces Local Deformations on Nanotube Walls. Materials Research Society Symposia Proceedings, 2006, 963, 1.	0.1	0
176	Simulations of Multi-atom Vacancies in Diamond. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	0
177	Single-Walled Carbon Nanotubes. , 2008, , 4085-4095.		0
178	Need for electronic correlation calculations in polymers. International Journal of Quantum Chemistry, 1980, 18, 463-466.	2.0	0
179	Modeling of Chemical Reactivity of Carbon Nanotubes: A Review. , 2012, , 173-208.		0
180	Intramolecular Pancake Bonding in Helical Structures. Chemistry - A European Journal, 2017, 23, 7381-7381.	3.3	0

#	Article	IF	Citations
181	Photophysics of N,N-dimethyl-3-(1-indolyl)propan-1-ammonium chloride and related derivatives. Photochemical and Photobiological Sciences, 2017, 16, 1546-1555.	2.9	0
182	Single-Walled Carbon Nanotubes: Geometries, Electronic Properties, and Actuation. , 0, , 4512-4521.		0