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	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
2	Quinonoid versus Aromatic Ï€-Conjugated Oligomers and Polymers and Their Diradical Characters. Journal of Physical Chemistry C, 2022, 126, 5302-5310.	3.1	3
3	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
4	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
5	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
6	Unexpected Charge Effects Strengthen Ï€â€“Stacking Pancake Bonding. Jacs Au, 2021, 1, 1647-1655.	7.9	15
7	Quinonoid vs. aromatic structures of heteroconjugated polymers from oligomer calculations. Physical Chemistry Chemical Physics, 2020, 22, 11431-11439.	2.8	5
8	Linear and Radial Conjugation in Extended Ï€-Electron Systems. Journal of the American Chemical Society, 2020, 142, 2293-2300.	13.7	32
9	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
10	Pancake Bonding: An Unusual Piâ€Stacking Interaction. Chemistry - A European Journal, 2019, 25, 400-416.	3.3	171
11	Molecules under Pressure: The Case of [n]Cycloparaphenylenes. Chemistry of Materials, 2019, 31, 6443-6452.	6.7	5
12	Pancake Bonding in Ï€â€Stacked Trimers in a Salt of Tetrachloroquinone Anion. Chemistry - A European Journal, 2018, 24, 8292-8297.	3.3	26
13	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
14	Sigmaâ€versus Piâ€Dimerization Modes of Triangulene. Chemistry - A European Journal, 2018, 24, 6140-6147.	3.3	15
15	Mechanochemistry in [6]Cycloparaphenylene: A Combined Raman Spectroscopy and Density Functional Theory Study. ChemPhysChem, 2018, 19, 1903-1916.	2.1	9
16	Cethrene: The Chameleon of Woodwardâ€“Hoffmann Rules. Journal of Organic Chemistry, 2018, 83, 4769-4774.	3.2	33
17	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
18	Intramolecular Pancake Bonding in Helical Structures. Chemistry - A European Journal, 2017, 23, 7381-7381.	3.3	0

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19	Pancake Bond Orders of a Series of Ï€â€Stacked Triangulene Radicals. Angewandte Chemie - International Edition, 2017, 56, 10188-10191.	13.8	46
20	Intramolecular Pancake Bonding in Helical Structures. Chemistry - A European Journal, 2017, 23, 7474-7482.	3.3	20
21	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
22	Highâ€Pressure Chemistry and the Mechanochemical Polymerization of [5]â€Cycloâ€pâ€phenylene. Chemistry - A European Journal, 2017, 23, 16593-16604.	3.3	10
23	Pancake Bond Orders of a Series of Ï€â€Stacked Triangulene Radicals. Angewandte Chemie, 2017, 129, 10322-10325.	2.0	8
24	Validation of density functionals for pancake-bonded Ï€-dimers; dispersion is not enough. Physical Chemistry Chemical Physics, 2017, 19, 24761-24768.	2.8	32
25	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
26	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
27	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
28	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
29	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
30	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
31	Heteroâ€Ïâ€Dimers of Phenalenyls. Chemistry - A European Journal, 2015, 21, 18230-18236.	3.3	38
32	Nitrogen Doping Enables Covalent-Like Ïâ€“Ï€ Bonding between Graphenes. Nano Letters, 2015, 15, 5482-5491.	9.1	31
33	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
34	Helical molecular redox actuators with pancake bonds?. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	13
35	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
36	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

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37	Divacancies in diamond: a stepwise formation mechanism. Physical Chemistry Chemical Physics, 2014, 16, 1515-1521.	2.8	19
38	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
39	Evidence of Ïƒ- and Ï€-Dimerization in a Series of Phenalenyls. Journal of the American Chemical Society, 2014, 136, 18009-18022.	13.7	150
40	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
41	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
42	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
43	Binding Interactions in Dimers of Phenalenyl and Closed-Shell Analogues. Journal of Physical Chemistry A, 2013, 117, 3642-3649.	2.5	35
44	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
45	Modeling of Chemical Reactivity of Carbon Nanotubes: A Review. , 2012, , 173-208.		0
46	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
47	Cyclo-biphenalenyl Biradicaloid Molecular Materials: Conformation, Tautomerization, Magnetism, and Thermochromism. Chemistry of Materials, 2011, 23, 874-885.	6.7	17
48	Conformations of Antipyrines. Journal of Physical Chemistry A, 2011, 115, 4832-4839.	2.5	2
49	Charge Shift Bonding Concept in Radical Ï€-Dimers. Journal of Physical Chemistry A, 2011, 115, 13942-13949.	2.5	31
50	Simulations of large multi-atom vacancies in diamond. Diamond and Related Materials, 2010, 19, 1153-1162.	3.9	7
51	Conformational Preferences of Î²-Carotene in the Confined Spaces inside Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 12139-12144.	3.1	13
52	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
53	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
54	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

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55	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
56	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
57	Bimolecular hydrogen transfer in phenalene by a stepwise ene-like reaction mechanism. Chemical Communications, 2010, 46, 4282.	4.1	5
58	Energetics of linear carbon chains in one-dimensional restricted environment. Physical Chemistry Chemical Physics, 2009, 11, 425-430.	2.8	28
59	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
60	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
61	Molecular Actuators Designed with Sâˆ’N(sp²) Hemibonds Attached to a Conformationally Flexible Pivot. Chemistry of Materials, 2009, 21, 2149-2157.	6.7	4
62	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
63	Linear C_n Clusters:â€‰ Are They Acetylenic or Cumulenic?. Journal of Physical Chemistry A, 2008, 112, 146-151.	2.5	49
64	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
65	Electronic Structure of Helicenes, C₂S Helicenes, and Thiaheterohelicenes. Chemistry of Materials, 2008, 20, 3266-3277.	6.7	55
66	Single-Walled Carbon Nanotubes. , 2008, , 4085-4095.		0
67	Intermolecular Covalent Ï€âˆ’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
68	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
69	Theoretical Design of Low Band Gap Conjugated Polymers through Ladders with Acetylenic Crosspieces. Macromolecules, 2007, 40, 6740-6747.	4.8	15
70	Theoretical Analysis of Intermolecular Covalent Ï€âˆ’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
71	Confinement effects on site-preferences for cycloadditions into carbon nanotubes. Chemical Physics Letters, 2007, 444, 155-160.	2.6	34
72	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

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73	Cooperative Behaviors in Carbene Additions through Local Modifications of Nanotube Surfaces. Chemistry of Materials, 2007, 19, 1028-1034.	6.7	32
74	Bond Length Alternation and Energy Band Gap of Polyyne. Journal of Physical Chemistry A, 2006, 110, 9771-9774.	2.5	123
75	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
76	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
77	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
78	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
79	Conjugated Polymers and Aromaticity. ChemInform, 2006, 37, no.	0.0	0
80	Covalent Bond Formation in Defected Nanopeapods Induces Local Deformations on Nanotube Walls. Materials Research Society Symposia Proceedings, 2006, 963, 1.	0.1	0
81	Simulations of Multi-atom Vacancies in Diamond. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	0
82	Linear carbon chain in the interior of a single walled carbon nanotube. AIP Conference Proceedings, 2005, , .	0.4	0
83	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
84	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
85	Conjugated Polymers and Aromaticity. Chemical Reviews, 2005, 105, 3448-3481.	47.7	447
86	Validation of intermolecular transfer integral and bandwidth calculations for organic molecular materials. Journal of Chemical Physics, 2005, 122, 234707.	3.0	76
87	Intermolecular transfer integrals for organic molecular materials: can basis set convergence be achieved?. Chemical Physics Letters, 2004, 390, 110-115.	2.6	137
88	Individualities and average behavior in the physical properties of small diameter single-walled carbon nanotubes. Carbon, 2004, 42, 971-978.	10.3	32
89	Bandgap calculations for conjugated polymers. Synthetic Metals, 2004, 141, 171-177.	3.9	154
90	Performance of the Vienna ab initio simulation package (VASP) in chemical applications. Computational and Theoretical Chemistry, 2003, 624, 37-45.	1.5	275

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91	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
92	Spin Crossover of Spiro-Biphenalenyl Neutral Radical Molecular Conductors. Journal of the American Chemical Society, 2003, 125, 13334-13335.	13.7	42
93	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
94	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
95	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
96	Vibrational Raman Spectra of C70 and C706- Studied by Density Functional Theory. Journal of Physical Chemistry A, 2002, 106, 6381-6386.	2.5	29
97	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
98	13C NMR spectra for IPR isomers of fullerene C86. Chemical Physics, 2002, 276, 107-114.	1.9	58
99	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
100	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
101	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
102	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
103	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
104	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
105	Carbon Nanotube Actuators. Science, 1999, 284, 1340-1344.	12.6	2,343
106	Argon-matrix-isolation Raman spectra and density functional study of 1,3-butadiene conformers. Theoretical Chemistry Accounts, 1999, 102, 196-206.	1.4	26
107	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
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109	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
110	Bond length alternation and aromaticity in large annulenes. Journal of Chemical Physics, 1998, 108, 6681-6688.	3.0	90
111	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
112	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
113	Consistencies between experiments and quantum calculations of strained Câ€“C single bond lengths. Chemical Communications, 1997, , 2199-2200.	4.1	24
114	Conformational Studies of Vibrational Properties and Electronic States of Leucoemeraldine Base and Its Oligomers. Macromolecules, 1997, 30, 620-630.	4.8	34
115	Can carbon monoxide polymerize? A theoretical investigation of polyketone. Chemical Communications, 1997, , 2011.	4.1	16
116	Do Localized Structures of [14]- and [18]Annulenes Exist?. Journal of the American Chemical Society, 1997, 119, 11994-11995.	13.7	41
117	Conformational Information from Vibrational Spectra of Styrene, trans-Stilbene, and cis-Stilbene. Journal of Physical Chemistry A, 1997, 101, 3823-3831.	2.5	291
118	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
119	Conformational information from vibrational spectra of polyaniline. Synthetic Metals, 1997, 85, 1073-1076.	3.9	15
120	Limitations of current density functional theories for the description of partial Ï€-bond breaking. Chemical Physics Letters, 1997, 276, 266-268.	2.6	52
121	A new partition of the atomic polar tensor: the benzene molecule. Chemical Physics Letters, 1996, 263, 697-702.	2.6	5
122	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
123	Structure and Electronic Structure of Low-Band-Gap Ladder Polymers. Macromolecules, 1995, 28, 1475-1480.	4.8	39
124	Interpretation of the vibrational spectra of planarized poly-p-phenylene. Synthetic Metals, 1995, 69, 683-684.	3.9	20
125	The aromatic - quinonoid transition in conducting polymers. Synthetic Metals, 1995, 69, 641-644.	3.9	10
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127	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
128	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
129	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
130	Metal oligo-yne polymers: electronic structures of [-(L)nMC.tplbond.CRC.tplbond.C-]x polymers. Inorganic Chemistry, 1993, 32, 732-740.	4.0	118
131	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
132	Electronic structures of heterocyclic ladder polymers; polyphenothiazine, polyphenoxazine, and polyphenoquinoxaline. Chemistry of Materials, 1992, 4, 378-383.	6.7	32
133	Geometrical and electronic structures of .pi.-conjugated silicon ring polymers. Organometallics, 1992, 11, 3178-3184.	2.3	29
134	Assignment of the vibrational spectra of polysilane and its oligomers. Macromolecules, 1992, 25, 1103-1108.	4.8	21
135	Geometrical and electronic structures of a benzimidazobenzophenanthroline-type ladder polymer (BBL). Macromolecules, 1992, 25, 5424-5429.	4.8	35
136	AB initio study of the dynamical properties of polythiophene. Synthetic Metals, 1991, 43, 3491-3496.	3.9	24
137	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
138	Energetics and geometry of conducting polymers from oligomers. The Journal of Physical Chemistry, 1991, 95, 7680-7681.	2.9	48
139	Extraction of polymer properties from oligomer calculations. The Journal of Physical Chemistry, 1990, 94, 5172-5179.	2.9	38
140	Helical Peierls distortion: Formation of helices of polyketone and polyisocyanide. Chemical Physics Letters, 1990, 169, 445-449.	2.6	8
141	Theoretical evaluation of Youngâ€™s moduli of polymers. Physical Review B, 1990, 41, 11368-11378.	3.2	10
142	Dependence of Youngâ€™s modulus oftrans-polyacetylene upon charge transfer. Physical Review Letters, 1990, 64, 3031-3034.	7.8	13
143	Quantumâ€mechanical oligomer approach for the calculation of vibrational spectra of polymers. Journal of Chemical Physics, 1990, 93, 5257-5266.	3.0	33
144	Importance of energetics in the design of small bandgap conducting polymers. Chemistry of Materials, 1990, 2, 526-530.	6.7	45

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145	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
146	Superdegeneracies in Extended Systems; a Prerequisite for Ï€ Ferromagnets?. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1989, 176, 115-123.	0.3	6
147	Inorganic rings, intact and cleaved, between two metal fragments. Journal of the American Chemical Society, 1989, 111, 2030-2039.	13.7	59
148	Structure and electronic structure of polyacene. International Journal of Quantum Chemistry, 1989, 35, 305-313.	2.0	49
149	Electronic structure of small gap polymers. Synthetic Metals, 1989, 28, 545-552.	3.9	35
150	Two helical conformations of polythiophene, polypyrrole, and their derivatives. Physical Review B, 1989, 40, 9661-9670.	3.2	115
151	Chemisorption on metals: the method of moments point of view. The Journal of Physical Chemistry, 1989, 93, 3237-3240.	2.9	6
152	Helical Conformations of Conducting Polymers. Materials Research Society Symposia Proceedings, 1989, 173, 391.	0.1	0
153	Band structure calculation of extended poly(copper phthalocyanine) one-dimensional and two-dimensional polymers. Inorganic Chemistry, 1988, 27, 3672-3675.	4.0	35
154	The electronic structure of BC3. Journal of the Chemical Society Chemical Communications, 1988, , 75.	2.0	12
155	Energy gap and bond length alternation in heterosubstituted narrow gap semiconducting polymers. The Journal of Physical Chemistry, 1987, 91, 2690-2692.	2.9	61
156	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
157	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
158	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
159	Electronic structure of highly doped conducting polymers. International Journal of Quantum Chemistry, 1986, 29, 1165-1176.	2.0	8
160	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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164	Octahedral vs. trigonal-prismatic coordination and clustering in transition-metal dichalcogenides. Journal of the American Chemical Society, 1984, 106, 3453-3460.	13.7	247
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