

Sven Stafström

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

197
papers

8,390
citations

46
h-index

85
g-index

207
ext. papers

8,863
ext. citations

4.6
avg, IF

6
L-index

#	Paper	IF	Citations
197	Polaron dynamics in anisotropic Holstein-Peierls systems. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 4078-4084	3.6	9
196	Effect of Polarization on the Mobility of C60: A Kinetic Monte Carlo Study. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 812-24	6.4	22
195	Impact of the electron-phonon coupling symmetry on the polaron stability and mobility in organic molecular semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1386-91	3.6	17
194	Unfolding spinor wave functions and expectation values of general operators: Introducing the unfolding-density operator. <i>Physical Review B</i> , 2015 , 91,	3.3	200
193	Visualization and thermodynamic encoding of single-molecule partition function projections. <i>Nature Communications</i> , 2015 , 6, 6210	17.4	20
192	Polaron stability in molecular semiconductors: theoretical insight into the impact of the temperature, electric field and the system dimensionality. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 8973-82	3.6	30
191	Bonding, charge rearrangement and interface dipoles of benzene, graphene, and PAH molecules on Au(1 1 1) and Cu(1 1 1). <i>Carbon</i> , 2015 , 81, 620-628	10.4	33
190	Transition fields in organic materials: from percolation to inverted Marcus regime. A consistent Monte Carlo simulation in disordered PPV. <i>Journal of Chemical Physics</i> , 2015 , 142, 094503	3.9	14
189	Transport of Polarons in Graphene Nanoribbons. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 510-4	6.4	36
188	Unraveling the Mechanism of the Covalent Coupling Between Terminal Alkynes on a Noble Metal. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 3181-3187	3.8	65
187	Dynamics of charge separation at an organic donor-acceptor interface. <i>Physical Review B</i> , 2014 , 90,	3.3	18
186	Carbon Fluoride, CF _x : Structural Diversity as Predicted by First Principles. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 6514-6521	3.8	35
185	Effects of extrinsic and intrinsic perturbations on the electronic structure of graphene: Retaining an effective primitive cell band structure by band unfolding. <i>Physical Review B</i> , 2014 , 89,	3.3	313
184	Adsorption of large hydrocarbons on coinage metals: a van der Waals density functional study. <i>ChemPhysChem</i> , 2014 , 15, 2851-8	3.2	40
183	Reactivity of adducts relevant to the deposition of hexagonal BN from first-principles calculations. <i>Chemical Physics Letters</i> , 2013 , 583, 119-124	2.5	34
182	Mechanisms of halogen-based covalent self-assembly on metal surfaces. <i>Journal of the American Chemical Society</i> , 2013 , 135, 5768-75	16.4	181
181	Dynamics of exciton dissociation in donor-acceptor polymer heterojunctions. <i>Journal of Chemical Physics</i> , 2013 , 138, 164905	3.9	28

180	Polaron dynamics in a two-dimensional Holstein-Peierls system. <i>Journal of Chemical Physics</i> , 2013 , 138, 184104	3.9	29
179	Polaron stability in molecular crystals. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 1807-1811	2.3	16
178	Benzene, coronene, and circumcoronene adsorbed on gold, and a gold cluster adsorbed on graphene: Structural and electronic properties. <i>Physical Review B</i> , 2012 , 85,	3.3	51
177	Monte Carlo simulations of charge transport in organic systems with true off-diagonal disorder. <i>Journal of Chemical Physics</i> , 2012 , 137, 114901	3.9	16
176	Structural Patterns Arising during Synthetic Growth of Fullerene-Like Sulfocarbide. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 21124-21131	3.8	31
175	Spin-dependent polaron recombination in conjugated polymers. <i>Journal of Chemical Physics</i> , 2012 , 136, 244901	3.9	21
174	Zippering up: cooperativity drives the synthesis of graphene nanoribbons. <i>Journal of the American Chemical Society</i> , 2011 , 133, 14884-7	16.4	99
173	Polaron effects and electric field dependence of the charge carrier mobility in conjugated polymers. <i>Journal of Chemical Physics</i> , 2011 , 135, 134902	3.9	16
172	Intercalation of P atoms in Fullerene-like CPx. <i>Chemical Physics Letters</i> , 2011 , 501, 400-403	2.5	34
171	Fullerene-like CSx: A first-principles study of synthetic growth. <i>Chemical Physics Letters</i> , 2011 , 506, 86-91	2.5	34
170	Complex polarization propagator approach in the restricted open-shell, self-consistent field approximation: the near K-edge X-ray absorption fine structure spectra of allyl and copper phthalocyanine. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 5096-102	3.4	18
169	Effect of dynamic disorder on charge transport along a pentacene chain. <i>Physical Review B</i> , 2011 , 83,	3.3	18
168	Scattering process between polaron and exciton in conjugated polymers. <i>Journal of Chemical Physics</i> , 2011 , 134, 044906	3.9	20
167	Bipolaron recombination in conjugated polymers. <i>Journal of Chemical Physics</i> , 2011 , 135, 074902	3.9	15
166	Tuning the supramolecular chirality of one- and two-dimensional aggregates with the number of stereogenic centers in the component porphyrins. <i>Journal of the American Chemical Society</i> , 2010 , 132, 9350-62	16.4	89
165	Electron localization and the transition from adiabatic to nonadiabatic charge transport in organic conductors. <i>Chemical Society Reviews</i> , 2010 , 39, 2484-99	58.5	113
164	Efficient spin injection through exchange coupling at organic semiconductor/ferromagnet heterojunctions. <i>Advanced Materials</i> , 2010 , 22, 1626-30	24	69
163	Impact of ring torsion dynamics on intrachain charge transport in conjugated polymers. <i>Physical Review B</i> , 2009 , 79,	3.3	18

162	Dynamics of molecular self-ordering in tetraphenyl porphyrin monolayers on metallic substrates. <i>Nanotechnology</i> , 2009 , 20, 275602	3.4	72
161	Effects of pi-stacking interactions on the near carbon K-edge x-ray absorption fine structure: a theoretical study of the ethylene pentamer and the phthalocyanine dimer. <i>Journal of Chemical Physics</i> , 2009 , 130, 104305	3.9	11
160	Water adsorption on phosphorous-carbide thin films. <i>Surface and Coatings Technology</i> , 2009 , 204, 1035-1039	4.1	15
159	Dangling bond energetics in carbon nitride and phosphorus carbide thin films with fullerene-like and amorphous structure. <i>Chemical Physics Letters</i> , 2009 , 482, 110-113	2.5	34
158	The effect of lattice dynamics on electron localization in poly-(para-phenylenevinylene). <i>Synthetic Metals</i> , 2009 , 159, 2219-2221	3.6	5
157	Hole mobility and transport mechanisms in lambda-DNA. <i>Journal of Chemical Physics</i> , 2009 , 131, 155102	3.9	2
156	A Monte Carlo study of charge transfer in DNA. <i>Journal of Chemical Physics</i> , 2008 , 129, 125102	3.9	14
155	TDAE chemisorbed on gold. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 315008	1.8	2
154	Integer charge transfer at the tetrakis(dimethylamino)ethylene/Au interface. <i>Applied Physics Letters</i> , 2008 , 92, 163302	3.4	40
153	Water adsorption on fullerene-like carbon nitride overcoats. <i>Thin Solid Films</i> , 2008 , 517, 1106-1110	2.2	33
152	Nonradiative relaxation processes in molecular crystals. <i>Journal of Luminescence</i> , 2008 , 128, 2019-2026	3.8	3
151	Nano-wire formation by self-assembly of silicon-metal cage-like molecules. <i>Chemical Physics Letters</i> , 2008 , 458, 170-174	2.5	19
150	Synthesis of phosphorus-carbide thin films by magnetron sputtering. <i>Physica Status Solidi - Rapid Research Letters</i> , 2008 , 2, 191-193	2.5	35
149	Monte Carlo simulations of charge carrier mobility in semiconducting polymer field-effect transistors. <i>Physical Review B</i> , 2007 , 76,	3.3	39
148	Monte Carlo simulation of controlled charge carriers diffusion in highly ordered iodine doped pentacene film. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2007 , 204, 3545-3555	1.6	
147	Impact of ring torsion on the intrachain mobility in conjugated polymers. <i>Physical Review B</i> , 2007 , 75,	3.3	46
146	Structural and electronic transitions in potassium-doped pentacene. <i>Physical Review B</i> , 2006 , 73,	3.3	16
145	Electronic structure calculations of the phenalenyl-based neutral radical conductor bis(9-cyclohexylimino-1-phenalenyl) boron. <i>Physical Review B</i> , 2006 , 74,	3.3	16

144	Effect of long-range correlation on the metal-insulator transition in a disordered molecular crystal. <i>Physical Review B</i> , 2006 , 74,	3.3	8
143	First-principles calculations on the structural evolution of solid fullerene-like CPx. <i>Chemical Physics Letters</i> , 2006 , 426, 374-379	2.5	39
142	Polaron dynamics in highly ordered molecular crystals. <i>Chemical Physics Letters</i> , 2006 , 428, 446-450	2.5	52
141	AlGaInN metal-organic-chemical-vapor-deposition gas-phase chemistry in hydrogen and nitrogen diluents: First-principles calculations. <i>Chemical Physics Letters</i> , 2006 , 431, 346-351	2.5	33
140	Silicon-metal clusters: Nano-templates for cluster assembled materials. <i>Thin Solid Films</i> , 2006 , 515, 1192-1196	3.1	31
139	Fullerene-like CPx: A first-principles study of the relative stability of precursors and defect energetics during synthetic growth. <i>Thin Solid Films</i> , 2006 , 515, 1028-1032	2.2	34
138	Electronic structure calculations of potassium-intercalated single-walled carbon nanotubes. <i>Physical Review B</i> , 2005 , 72,	3.3	11
137	Dynamical simulation of exciton dissociation in poly(para-phenylenevinylene) systems. <i>Journal of Luminescence</i> , 2005 , 112, 357-362	3.8	4
136	First-principles calculations on the role of CN precursors for the formation of fullerene-like carbon nitride. <i>Chemical Physics Letters</i> , 2005 , 401, 288-295	2.5	58
135	First-principles calculations on the curvature evolution and cross-linkage in carbon nitride. <i>Chemical Physics Letters</i> , 2005 , 410, 228-234	2.5	50
134	Charge and energy dynamics in photo-excited poly(para-phenylenevinylene) systems. <i>Journal of Chemical Physics</i> , 2004 , 121, 1601-8	3.9	5
133	Nonadiabatic simulations of polaron dynamics. <i>Physical Review B</i> , 2004 , 69,	3.3	110
132	Split gate nanoscale Coulomb driven stochastic resonance mechanism for separating like-charged impurities in semiconductors. <i>Physical Review B</i> , 2004 , 69,	3.3	2
131	Coulomb interactions in rubidium-doped tetracyanoethylene: A model system for organometallic magnets. <i>Physical Review B</i> , 2004 , 69,	3.3	31
130	Fullerene-like BCN thin films: a computational and experimental study. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2004 , 113, 242-247	3.1	36
129	Characterization of aza-fullerene C ₅₈ N ₂ isomers by X-ray spectroscopy. <i>Chemical Physics Letters</i> , 2003 , 371, 98-104	2.5	14
128	Electron Localization in DNA. <i>Nano Letters</i> , 2003 , 3, 1417-1420	11.5	25
127	Self-consistent drift-diffusion model of nanoscale impurity profiles in semiconductor layers, quantum wires, and quantum dots. <i>Physical Review B</i> , 2003 , 67,	3.3	30

126	Charge transport in π -conjugated systems. <i>Synthetic Metals</i> , 2003 , 137, 1397-1399	3.6	8
125	Anderson localization in two-dimensional disordered systems. <i>Synthetic Metals</i> , 2003 , 139, 239-244	3.6	11
124	Modeling of the dynamics of charge separation in an excited poly(phenylene vinylene)/C60 system. <i>Physical Review B</i> , 2003 , 68,	3.3	13
123	Intershell conductance in multiwall carbon nanotubes. <i>Physical Review B</i> , 2003 , 67,	3.3	59
122	High intercalation levels in lithium perylene stoichiometric compounds. <i>Chemical Physics Letters</i> , 2002 , 354, 389-394	2.5	33
121	Soliton and polaron transport in trans-polyacetylene. <i>Physical Review B</i> , 2002 , 65,	3.3	37
120	Interchain charge transport in disordered π -conjugated chain systems. <i>Physical Review B</i> , 2002 , 66,	3.3	14
119	An effective hopping model for weakly interacting π -systems: Electronic structure of stacked polyaromatic hydrocarbons. <i>International Journal of Quantum Chemistry</i> , 2001 , 84, 216-225	2.1	18
118	Predicted stability of a new aza[60]fullerene molecule, C ₄₈ N ₁₂ . <i>Chemical Physics Letters</i> , 2001 , 340, 227-231	2.3	75
117	Cross-linked nano-onions of carbon nitride in the solid phase: existence of a novel C(48)N(12) aza-fullerene. <i>Physical Review Letters</i> , 2001 , 87, 225503	7.4	167
116	Theoretical investigation of the role of π -interactions for the stability of phenylene ethynylene aggregates. <i>Chemical Physics</i> , 2001 , 270, 245-251	2.3	17
115	Disorder-induced electron localization in metallic carbon nanotubes. <i>Physical Review B</i> , 2001 , 63,	3.3	33
114	Polaron dynamics in a system of coupled conjugated polymer chains. <i>Physical Review Letters</i> , 2001 , 86, 3602-5	7.4	153
113	Self-consistent-field study of conduction through conjugated molecules. <i>Physical Review B</i> , 2001 , 64,	3.3	47
112	Band resonant tunneling in DNA molecules. <i>Physical Review Letters</i> , 2001 , 87, 228101	7.4	77
111	Interactions between molecular wires and a gold surface. <i>Chemical Physics Letters</i> , 2000 , 322, 301-306	2.5	57
110	Theoretical study of electron transport along self-assembled graphitic nanowires. <i>Journal of Physics Condensed Matter</i> , 2000 , 12, 9433-9440	1.8	7
109	Enhanced thermal dissociation of optically excited C ₆₀ chains. <i>Europhysics Letters</i> , 2000 , 49, 631-636	1.6	9

108	Effect of bending and vacancies on the conductance of carbon nanotubes. <i>Physical Review B</i> , 2000 , 62, 7639-7644	3.3	77
107	Reactivity of curved and planar carbon nitride structures. <i>Applied Physics Letters</i> , 2000 , 77, 3941-3943	3.4	78
106	Negative Poisson's ratios for extreme states of matter. <i>Science</i> , 2000 , 288, 2018-22	33.3	67
105	Modeling vacancies in graphite via the Hückel method. <i>Physical Review B</i> , 2000 , 61, 14089-14094	3.3	65
104	Influence of the Morphology on the Electronic Structure of Hexa-peri-hexabenzocoronene Thin Films <i>Journal of Physical Chemistry B</i> , 2000 , 104, 3967-3975	3.4	38
103	Localization in quasi-one-dimensional systems. <i>Physical Review B</i> , 2000 , 62, 5245-5250	3.3	30
102	Effect of charge state on bonding in fulleride polymers. <i>Europhysics Letters</i> , 1999 , 46, 382-388	1.6	4
101	Conductance manipulation at the molecular level. <i>Journal of Physics Condensed Matter</i> , 1999 , 11, 3555-3562	3.6	23
100	Effects of doping and interchain interactions on the metal-insulator transition in trans-polyacetylene. <i>Physical Review B</i> , 1999 , 60, 7939-7943	3.3	15
99	Electronic structure of tris(8-hydroxyquinoline) aluminum thin films in the pristine and reduced states. <i>Journal of Chemical Physics</i> , 1999 , 111, 2157-2163	3.9	125
98	Electronic and vibrational structure of thin films of bithiophene: Undoped and alkali-doped states. <i>Journal of Chemical Physics</i> , 1999 , 110, 8060-8069	3.9	12
97	A self-consistent-field study of the nitrogen 1s binding energies in carbon nitrides. <i>Journal of Chemical Physics</i> , 1999 , 111, 3203-3208	3.9	39
96	Controlling inter-chain and intra-chain excitations of a poly(thiophene) derivative in thin films. <i>Chemical Physics Letters</i> , 1999 , 304, 84-90	2.5	41
95	Studies of Polaron and/or Bipolaron Formation in Short Segments of Polymers. <i>Synthetic Metals</i> , 1999 , 101, 287-290	3.6	3
94	Effect of charge state on bonding in fulleride polymers. <i>Synthetic Metals</i> , 1999 , 103, 2422-2423	3.6	1
93	Interactions between molecular wires and a gold surface. <i>Synthetic Metals</i> , 1999 , 101, 429-430	3.6	1
92	Conductance through a C60 molecule. <i>Synthetic Metals</i> , 1999 , 101, 469-470	3.6	
91	Materials with negative compressibilities in one or more dimensions. <i>Science</i> , 1998 , 279, 1522-4	33.3	277

90	Negative Poisson's ratios as a common feature of cubic metals. <i>Nature</i> , 1998 , 392, 362-365	50.4	516
89	Tunneling across molecular wires: an analytical exactly solvable model. <i>Solid State Communications</i> , 1998 , 108, 555-559	1.6	19
88	Numerical investigation of electron localization in polymer chains. <i>Physical Review B</i> , 1998 , 57, 2197-2203	3.3	4
87	Inter- and intrachain electron-hole recombination in polythiophene. <i>Synthetic Metals</i> , 1997 , 85, 1065-1068	3.6	6
86	Geometrical and optical properties of fullerene polymers. <i>Synthetic Metals</i> , 1997 , 86, 2393-2394	3.6	2
85	Electronic structure and stability of fullerene polymers. <i>Applied Physics A: Materials Science and Processing</i> , 1997 , 64, 307-314	2.6	11
84	The electronic and geometric structures of neutral and potassium-doped poly[3-(4-octylphenyl)thiophene] studied by photoelectron spectroscopy. <i>Synthetic Metals</i> , 1996 , 76, 263-267	3.6	6
83	The electronic structure of neutral and alkali metal-doped poly[3-(4-octylphenyl)thiophene] studied by photoelectron spectroscopy. <i>Synthetic Metals</i> , 1996 , 80, 59-66	3.6	16
82	Theoretical investigations of the interaction between electron and hole polarons in thiophene oligomers. <i>Physical Review B</i> , 1996 , 54, 13713-13720	3.3	9
81	Formation of C60 dimers: A theoretical study of electronic structure and optical absorption. <i>Physical Review B</i> , 1996 , 53, 13150-13158	3.3	42
80	Superhard and Elastic Carbon Nitride Thin Films Having Fullerenelike Microstructure. <i>Physical Review Letters</i> , 1996 , 76, 2205-2205	7.4	18
79	Conductance and localization in a system of coupled conjugated polymer chains. <i>Physical Review B</i> , 1995 , 51, 4137-4142	3.3	12
78	Electronic Properties of Linear C 60 Polyanions. <i>Europhysics Letters</i> , 1995 , 30, 295-300	1.6	18
77	A Delta Self-Consistent-Field Study of Core Electron Binding Energies of Model Molecules for the Aluminum/Polythiophene Interface. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 16597-16601		10
76	Experimental and Theoretical Studies of the Electronic Structure of Poly(p-phenylenevinylene) and Some Ring-Substituted Derivatives. <i>Macromolecules</i> , 1995 , 28, 1959-1965	5.5	61
75	Chemical and electronic aspects of metal/conjugated polymer interfaces. Implications for electronic devices. <i>Synthetic Metals</i> , 1995 , 71, 2159-2162	3.6	39
74	Superhard and elastic carbon nitride thin films having fullerenelike microstructure. <i>Physical Review Letters</i> , 1995 , 75, 1336-1339	7.4	603
73	Electronic structure of trimethylamine alane in the solid state. <i>Chemical Physics Letters</i> , 1995 , 235, 528-534	3.4	7

72	One- and Two-Photon Absorption Spectra of Short Conjugated Polyenes. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 7782-7789		49
71	Interacting Bipolarons in n -Doped Sexiphenyl Films. <i>Europhysics Letters</i> , 1994 , 28, 85-90	1.6	25
70	Reactions of low work function metals Na, Al, and Ca on π -diphenyltetradecaheptaene. Implications for metal/polymer interfaces. <i>Journal of Chemical Physics</i> , 1994 , 100, 6765-6771	3.9	57
69	Metal/conjugated polymer interfaces: Sodium, magnesium, aluminum, and calcium on trans-polyacetylene. <i>Journal of Chemical Physics</i> , 1994 , 101, 9137-9142	3.9	21
68	Temperature evolution of the electronic band structure of the undoped and doped regioregular analog of poly(3-alkylthiophenes): A spectroscopic and theoretical study. <i>Journal of Chemical Physics</i> , 1994 , 100, 1731-1741	3.9	23
67	Valence-band structure of PMDA-ODA polyimide studied by x-ray photoelectron spectroscopy and theoretical calculations*. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1994 , 12, 772-782	2.9	7
66	The chemical and electronic structure of the interface between aluminum and conjugated polymers. <i>Electrochimica Acta</i> , 1994 , 39, 235-244	6.7	46
65	Some chemical and electronic structures of the non-conjugated polymer poly(3,3'-phthalidylidene-4,4'-biphenylene). <i>Synthetic Metals</i> , 1994 , 67, 125-128	3.6	13
64	A theoretical study of the chemical structure of the non-conjugated polymer poly(3,3'-phthalidylidene-4,4'-biphenylene). <i>Synthetic Metals</i> , 1994 , 67, 319-322	3.6	34
63	Electronic structure and conductance in heavily doped trans-polyacetylene. <i>Synthetic Metals</i> , 1994 , 65, 185-194	3.6	5
62	Effects of Interchain Interactions on the Localization of Doping Induced Defects in Quasi One-Dimensional Systems. <i>Molecular Crystals and Liquid Crystals</i> , 1994 , 256, 209-216		3
61	Interpretation of Anomalous Absorption Spectra. A Theoretical Study of the Geometric, Electronic and Optical Properties of Poly[3-(4-Octylphenyl)-Thiophene]. <i>Molecular Crystals and Liquid Crystals</i> , 1994 , 256, 705-710		3
60	Charge storage states in polyenes. <i>Journal of Chemical Physics</i> , 1993 , 99, 7938-7945	3.9	19
59	A photoelectron spectroscopy study of the charge-induced electronic structural changes in π -diphenyltetradecaheptaene, a model molecule for polyacetylene. <i>Synthetic Metals</i> , 1993 , 57, 4722-4727 ⁶		3.6
58	Calculation of oscillator strengths with the supercell method sub-bandgap transitions in conjugated polymers. <i>Synthetic Metals</i> , 1993 , 57, 4614-4619	3.6	8
57	Inter-chain coupling effects on the electronic structure of alkali doped trans-polyacetylene. <i>Synthetic Metals</i> , 1993 , 57, 4278-4283	3.6	2
56	The chemical and electronic structure of the interface between aluminum and conjugated polymers or molecules. <i>Synthetic Metals</i> , 1993 , 55, 212-217	3.6	63
55	The chemical and electronic structure of the interface between aluminum and polythiophene semiconductors. <i>Journal of Chemical Physics</i> , 1993 , 99, 664-672	3.9	156

54	Fundamental excitations in C60. <i>Physical Review B</i> , 1993 , 48, 11367-11374	3.3	33
53	Soliton pair charge storage in doped polyene molecules: Evidence from photoelectron spectroscopy studies. <i>Physical Review Letters</i> , 1993 , 70, 970-973	7.4	58
52	Effects of interchain interactions on the electronic structure of heavily doped trans-polyacetylene. <i>Physical Review B</i> , 1993 , 47, 12437-12444	3.3	35
51	Theoretical studies of optical absorption spectra of soliton containing polyenes. <i>Chemical Physics Letters</i> , 1993 , 203, 81-87	2.5	4
50	Supercell representation of localized defects: A method for calculating band-gap states in conjugated polymers. <i>Physical Review B</i> , 1992 , 46, 4551-4558	3.3	3
49	Core x-ray photoelectron shake-up states of model molecules for polyaniline. <i>Journal of Chemical Physics</i> , 1992 , 97, 137-144	3.9	14
48	Theoretical investigations of the aluminum/polythiophene interface. <i>Journal of Chemical Physics</i> , 1992 , 97, 9144-9153	3.9	51
47	The electronic structure of β -diphenyltetradecaheptaene, a model molecule for polyacetylene, as studied by photoelectron spectroscopy. <i>Synthetic Metals</i> , 1992 , 51, 187-195	3.6	17
46	GEOMETRICAL AND ELECTRONIC STRUCTURE OF C60 ANIONS. <i>International Journal of Modern Physics B</i> , 1992 , 06, 3853-3858	1.1	4
45	The effect of inter-chain coupling properties of doped trans-polyacetylene. <i>Journal of Magnetism and Magnetic Materials</i> , 1992 , 104-107, 2099-2100	2.8	7
44	Ab initio Hartree-Fock studies of the binding energy of a soliton to a sodium counterion in doped trans-polyacetylene. <i>Chemical Physics Letters</i> , 1992 , 190, 407-412	2.5	7
43	Soliton lattice in highly doped trans-polyacetylene. <i>Physical Review B</i> , 1991 , 43, 9158-9170	3.3	47
42	Electronic properties of highly doped trans-polyacetylene. <i>Physical Review B</i> , 1991 , 44, 12737-12741	3.3	4
41	Photoelectron studies of trans-polyacetylene using synchrotron radiation. <i>Synthetic Metals</i> , 1991 , 41, 1365-1368	3.6	12
40	Soliton-impurity interaction in heavily doped trans-polyacetylene. <i>Synthetic Metals</i> , 1991 , 43, 3657-3662	3.6	4
39	Stretch-oriented poly(3-alkylthiophenes). <i>Synthetic Metals</i> , 1991 , 41, 593-596	3.6	7
38	The evolution of the electronic structure of polyacetylene, poly(p-phenylene), and the copolymer poly(p-phenylenevinylene) as studied by photoelectron spectroscopy. <i>Synthetic Metals</i> , 1991 , 41, 1315-1318	3.6	3
37	Ab initio studies of soliton defects in trans-polyacetylene. <i>Synthetic Metals</i> , 1991 , 43, 3467-3470	3.6	7

36	Ab initio calculations of trans-polyacetylene clusters including sodium counterions. <i>Synthetic Metals</i> , 1991 , 44, 65-74	3.6	7
35	Polaron defects in emeraldine. <i>Synthetic Metals</i> , 1991 , 43, 3697-3700	3.6	2
34	Optical anisotropy of neutral and doped poly(3-octylthiophene). <i>Solid State Communications</i> , 1990 , 76, 203-208	1.6	22
33	Electronic structure of polyimide and related monomers: Theory and experiment. <i>Physical Review B</i> , 1990 , 41, 1645-1656	3.3	34
32	The poly-3-hexylthiophene/NOPF6 system: A photoelectron spectroscopy study of electronic structural changes induced by the charge transfer in the solid state. <i>Journal of Chemical Physics</i> , 1990 , 93, 4433-4439	3.9	54
31	Direct observation of charge-induced pi -electronic structural changes in a conjugated polymer. <i>Physical Review Letters</i> , 1989 , 63, 1841-1844	7.4	112
30	The valence electronic structure of isotactic polystyrene revisited. <i>Chemical Physics Letters</i> , 1989 , 164, 240-246	2.5	13
29	Optical absorption of poly(3-alkylthiophenes) at low temperatures. <i>Solid State Communications</i> , 1989 , 71, 435-439	1.6	120
28	Electronic excitation properties of trans-polyacetylene and polythiophene as a function of doping level. <i>Synthetic Metals</i> , 1989 , 28, D477-D482	3.6	3
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