Sven Stafstrm

List of Publications by Citations

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 lattice in highly conducting polyaniline: Theoretical and optical studies. *Physical Review Letters*, **1987**, 59, 1464-1467	7.4	775
196	Superhard and elastic carbon nitride thin films having fullerenelike microstructure. *Physical Review Letters*, **1995**, 75, 1336-1339	7.4	603
195	Negative Poissons ratios as a common feature of cubic metals. *Nature*, **1998**, 392, 362-365	50.4	516
194	Effects of extrinsic and intrinsic perturbations on the electronic structure of graphene: Retaining an effective primitive cell band structure by band unfolding. *Physical Review B*, **2014**, 89,	3.3	313
193	Materials with negative compressibilities in one or more dimensions. *Science*, **1998**, 279, 1522-4	33.3	277
192	Unfolding spinor wave functions and expectation values of general operators: Introducing the unfolding-density operator. *Physical Review B*, **2015**, 91,	3.3	200
191	Mechanisms of halogen-based covalent self-assembly on metal surfaces. *Journal of the American Chemical Society*, **2013**, 135, 5768-75	16.4	181
190	Cross-linked nano-onions of carbon nitride in the solid phase: existence of a novel C(48)N(12) aza-fullerene. *Physical Review Letters*, **2001**, 87, 225503	7.4	167
189	The chemical and electronic structure of the interface between aluminum and polythiophene semiconductors. *Journal of Chemical Physics*, **1993**, 99, 664-672	3.9	156
188	Polaron dynamics in a system of coupled conjugated polymer chains. *Physical Review Letters*, **2001**, 86, 3602-5	7.4	153
187	Evolution of the electronic structure of polyacetylene and polythiophene as a function of doping level and lattice conformation. *Physical Review B*, **1988**, 38, 4180-4191	3.3	133
186	Electronic structure of tris(8-hydroxyquinoline) aluminum thin films in the pristine and reduced states. *Journal of Chemical Physics*, **1999**, 111, 2157-2163	3.9	125
185	Optical absorption of poly(3-alkylthiophenes) at low temperatures. *Solid State Communications*, **1989**, 71, 435-439	1.6	120
184	Electron localization and the transition from adiabatic to nonadiabatic charge transport in organic conductors. *Chemical Society Reviews*, **2010**, 39, 2484-99	58.5	113
183	Direct observation of charge-induced pi -electronic structural changes in a conjugated polymer. *Physical Review Letters*, **1989**, 63, 1841-1844	7.4	112
182	Nonadiabatic simulations of polaron dynamics. *Physical Review B*, **2004**, 69,	3.3	110
181	Zipping up: cooperativity drives the synthesis of graphene nanoribbons. *Journal of the American Chemical Society*, **2011**, 133, 14884-7	16.4	99

180	Tuning the supramolecular chirality of one- and two-dimensional aggregates with the number of stereogenic centers in the component porphyrins. *Journal of the American Chemical Society*, **2010**, 132, 9350-62	16.4	89
179	Reactivity of curved and planar carbon nitride structures. *Applied Physics Letters*, **2000**, 77, 3941-3943	3.4	78
178	Effect of bending and vacancies on the conductance of carbon nanotubes. *Physical Review B*, **2000**, 62, 7639-7644	3.3	77
177	Band resonant tunneling in DNA molecules. *Physical Review Letters*, **2001**, 87, 228101	7.4	77
176	Predicted stability of a new aza[60]fullerene molecule, C48N12. *Chemical Physics Letters*, **2001**, 340, 227-231	2.3	75
175	Dynamics of molecular self-ordering in tetraphenyl porphyrin monolayers on metallic substrates. *Nanotechnology*, **2009**, 20, 275602	3.4	72
174	Efficient spin injection through exchange coupling at organic semiconductor/ferromagnet heterojunctions. *Advanced Materials*, **2010**, 22, 1626-30	24	69
173	Negative Poisson's ratios for extreme states of matter. *Science*, **2000**, 288, 2018-22	33.3	67
172	Unraveling the Mechanism of the Covalent Coupling Between Terminal Alkynes on a Noble Metal. *Journal of Physical Chemistry C*, **2014**, 118, 3181-3187	3.8	65
171	Modeling vacancies in graphite via the Hückel method. *Physical Review B*, **2000**, 61, 14089-14094	3.3	65
170	Polaron-bipolaron-soliton doping in polyacetylene. *Physical Review B*, **1984**, 30, 2098-2103	3.3	64
169	The chemical and electronic structure of the interface between aluminum and conjugated polymers or molecules. *Synthetic Metals*, **1993**, 55, 212-217	3.6	63
168	Experimental and Theoretical Studies of the Electronic Structure of Poly(p-phenylenevinylene) and Some Ring-Substituted Derivatives. *Macromolecules*, **1995**, 28, 1959-1965	5.5	61
167	Evolution of structure and electronic properties in oxidized polyaniline as a function of the torsion angle between adjacent rings. *Synthetic Metals*, **1986**, 14, 297-308	3.6	61
166	Geometry of polyaniline. *Synthetic Metals*, **1986**, 16, 31-39	3.6	60
165	Intershell conductance in multiwall carbon nanotubes. *Physical Review B*, **2003**, 67,	3.3	59
164	First-principles calculations on the role of CN precursors for the formation of fullerene-like carbon nitride. *Chemical Physics Letters*, **2005**, 401, 288-295	2.5	58
163	Soliton pair charge storage in doped polyene molecules: Evidence from photoelectron spectroscopy studies. *Physical Review Letters*, **1993**, 70, 970-973	7.4	58

162	Interactions between molecular wires and a gold surface. *Chemical Physics Letters*, **2000**, 322, 301-306	2.5	57
161	Reactions of low work function metals Na, Al, and Ca on □diphenyltetradecaheptaene. Implications for metal/polymer interfaces. *Journal of Chemical Physics*, **1994**, 100, 6765-6771	3.9	57
160	The poly-3-hexylthiophene/NOPF6 system: A photoelectron spectroscopy study of electronic structural changes induced by the charge transfer in the solid state. *Journal of Chemical Physics*, **1990**, 93, 4433-4439	3.9	54
159	Polaron dynamics in highly ordered molecular crystals. *Chemical Physics Letters*, **2006**, 428, 446-450	2.5	52
158	Benzene, coronene, and circumcoronene adsorbed on gold, and a gold cluster adsorbed on graphene: Structural and electronic properties. *Physical Review B*, **2012**, 85,	3.3	51
157	Theoretical investigations of the aluminum/polythiophene interface. *Journal of Chemical Physics*, **1992**, 97, 9144-9153	3.9	51
156	First-principles calculations on the curvature evolution and cross-linkage in carbon nitride. *Chemical Physics Letters*, **2005**, 410, 228-234	2.5	50
155	One- and Two-Photon Absorption Spectra of Short Conjugated Polyenes. *The Journal of Physical Chemistry*, **1994**, 98, 7782-7789		49
154	Self-consistent-field study of conduction through conjugated molecules. *Physical Review B*, **2001**, 64,	3.3	47
153	Soliton lattice in highly doped trans-polyacetylene. *Physical Review B*, **1991**, 43, 9158-9170	3.3	47
152	Impact of ring torsion on the intrachain mobility in conjugated polymers. *Physical Review B*, **2007**, 75,	3.3	46
151	The chemical and electronic structure of the interface between aluminum and conjugated polymers. *Electrochimica Acta*, **1994**, 39, 235-244	6.7	46
150	Exact numerical investigation of the polaron-soliton generation in polyacetylene. *Physical Review B*, **1984**, 29, 7010-7011	3.3	45
149	Formation of C60 dimers: A theoretical study of electronic structure and optical absorption. *Physical Review B*, **1996**, 53, 13150-13158	3.3	42
148	Controlling inter-chain and intra-chain excitations of a poly(thiophene) derivative in thin films. *Chemical Physics Letters*, **1999**, 304, 84-90	2.5	41
147	Adsorption of large hydrocarbons on coinage metals: a van der Waals density functional study. *ChemPhysChem*, **2014**, 15, 2851-8	3.2	40
146	Integer charge transfer at the tetrakis(dimethylamino)ethylene/Au interface. *Applied Physics Letters*, **2008**, 92, 163302	3.4	40
145	Monte Carlo simulations of charge carrier mobility in semiconducting polymer field-effect transistors. *Physical Review B*, **2007**, 76,	3.3	39

144	First-principles calculations on the structural evolution of solid fullerene-like CPx. *Chemical Physics Letters*, **2006**, 426, 374-379	2.5	39
143	A Self-consistent-field study of the nitrogen 1s binding energies in carbon nitrides. *Journal of Chemical Physics*, **1999**, 111, 3203-3208	3.9	39
142	Chemical and electronic aspects of metal/conjugated polymer interfaces. Implications for electronic devices. *Synthetic Metals*, **1995**, 71, 2159-2162	3.6	39
141	Influence of the Morphology on the Electronic Structure of Hexa-peri-hexabenzocoronene Thin Films *Journal of Physical Chemistry B*, **2000**, 104, 3967-3975	3.4	38
140	Soliton and polaron transport in trans-polyacetylene. *Physical Review B*, **2002**, 65,	3.3	37
139	Transport of Polarons in Graphene Nanoribbons. *Journal of Physical Chemistry Letters*, **2015**, 6, 510-4	6.4	36
138	Fullerene-like BCN thin films: a computational and experimental study. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2004**, 113, 242-247	3.1	36
137	Carbon Fluoride, CFx: Structural Diversity as Predicted by First Principles. *Journal of Physical Chemistry C*, **2014**, 118, 6514-6521	3.8	35
136	Synthesis of phosphorus-carbide thin films by magnetron sputtering. *Physica Status Solidi - Rapid Research Letters*, **2008**, 2, 191-193	2.5	35
135	Effects of interchain interactions on the electronic structure of heavily doped trans-polyacetylene. *Physical Review B*, **1993**, 47, 12437-12444	3.3	35
134	Reactivity of adducts relevant to the deposition of hexagonal BN from first-principles calculations. *Chemical Physics Letters*, **2013**, 583, 119-124	2.5	34
133	Intercalation of P atoms in Fullerene-like CPx. *Chemical Physics Letters*, **2011**, 501, 400-403	2.5	34
132	Fullerene-like CSx: A first-principles study of synthetic growth. *Chemical Physics Letters*, **2011**, 506, 86-91	2.5	34
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125	AlGaInN metal-organic-chemical-vapor-deposition gas-phase chemistry in hydrogen and nitrogen diluents: First-principles calculations. *Chemical Physics Letters*, **2006**, 431, 346-351	2.5	33
124	High intercalation levels in lithium perylene stoichiometric compounds. *Chemical Physics Letters*, **2002**, 354, 389-394	2.5	33
123	Disorder-induced electron localization in metallic carbon nanotubes. *Physical Review B*, **2001**, 63,	3.3	33
122	Fundamental excitations in C60. *Physical Review B*, **1993**, 48, 11367-11374	3.3	33
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120	Silicon–metal clusters: Nano-templates for cluster assembled materials. *Thin Solid Films*, **2006**, 515, 1192-1196	1.9	31
119	Coulomb interactions in rubidium-doped tetracyanoethylene: A model system for organometallic magnets. *Physical Review B*, **2004**, 69,	3.3	31
118	Polaron stability in molecular semiconductors: theoretical insight into the impact of the temperature, electric field and the system dimensionality. *Physical Chemistry Chemical Physics*, **2015**, 17, 8973-82	3.6	30
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115	Polaron dynamics in a two-dimensional Holstein-Peierls system. *Journal of Chemical Physics*, **2013**, 138, 184104	3.9	29
114	Dynamics of exciton dissociation in donor-acceptor polymer heterojunctions. *Journal of Chemical Physics*, **2013**, 138, 164905	3.9	28
113	Electron Localization in DNA. *Nano Letters*, **2003**, 3, 1417-1420	11.5	25
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111	Conductance manipulation at the molecular level. *Journal of Physics Condensed Matter*, **1999**, 11, 3555-3562	1.8	23
110	Temperature evolution of the electronic band structure of the undoped and doped regioregular analog of poly(3-alkylthiophenes): A spectroscopic and theoretical study. *Journal of Chemical Physics*, **1994**, 100, 1731-1741	3.9	23
109	Effect of Polarization on the Mobility of C60: A Kinetic Monte Carlo Study. *Journal of Chemical Theory and Computation*, **2016**, 12, 812-24	6.4	22

108	Optical anisotropy of neutral and doped poly(3-octylthiophene). *Solid State Communications*, **1990**, 76, 203-208	1.6	22
107	Spin-dependent polaron recombination in conjugated polymers. *Journal of Chemical Physics*, **2012**, 136, 244901	3.9	21
106	Metal/conjugated polymer interfaces: Sodium, magnesium, aluminum, and calcium on trans-polyacetylene. *Journal of Chemical Physics*, **1994**, 101, 9137-9142	3.9	21
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101	Charge storage states in polyenes. *Journal of Chemical Physics*, **1993**, 99, 7938-7945	3.9	19
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99	Soliton states in polyacetylene. *Physical Review B*, **1984**, 29, 2255-2266	3.3	19
98	Dynamics of charge separation at an organic donor-acceptor interface. *Physical Review B*, **2014**, 90,	3.3	18
97	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. *Journal of Physical Chemistry B*, **2011**, 115, 5096-102	3.4	18
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94	An effective hopping model for weakly interacting □systems: Electronic structure of stacked polyaromatic hydrocarbons. *International Journal of Quantum Chemistry*, **2001**, 84, 216-225	2.1	18
93	Electronic Properties of Linear C 60 Polyanions. *Europhysics Letters*, **1995**, 30, 295-300	1.6	18
92	Superhard and Elastic Carbon Nitride Thin Films Having Fullerenelike Microstructure. *Physical Review Letters*, **1996**, 76, 2205-2205	7.4	18
91	Impact of the electron-phonon coupling symmetry on the polaron stability and mobility in organic molecular semiconductors. *Physical Chemistry Chemical Physics*, **2016**, 18, 1386-91	3.6	17

90	Theoretical investigation of the role of π interactions for the stability of phenylene ethynylene aggregates. *Chemical Physics*, **2001**, 270, 245-251	2.3	17
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87	Polaron stability in molecular crystals. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 376, 1807-1811	2.3	16
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83	Electronic structure calculations of the phenalenyl-based neutral radical conductor bis(9-cyclohexylimino-1-phenalenyl) boron. *Physical Review B*, **2006**, 74,	3.3	16
82	The electronic structure of neutral and alkali metal-doped poly[3-(4-octylphenyl)thiophene] studied by photoelectron spectroscopy. *Synthetic Metals*, **1996**, 80, 59-66	3.6	16
81	Water adsorption on phosphorous-carbide thin films. *Surface and Coatings Technology*, **2009**, 204, 1035-1039	1.4	15
80	Bipolaron recombination in conjugated polymers. *Journal of Chemical Physics*, **2011**, 135, 074902	3.9	15
79	Effects of doping and interchain interactions on the metal-insulator transition in trans-polyacetylene. *Physical Review B*, **1999**, 60, 7939-7943	3.3	15
78	Transition fields in organic materials: from percolation to inverted Marcus regime. A consistent Monte Carlo simulation in disordered PPV. *Journal of Chemical Physics*, **2015**, 142, 094503	3.9	14
77	A Monte Carlo study of charge transfer in DNA. *Journal of Chemical Physics*, **2008**, 129, 125102	3.9	14
76	Characterization of aza-fullerene C58N2 isomers by X-ray spectroscopy. *Chemical Physics Letters*, **2003**, 371, 98-104	2.5	14
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74	Core x-ray photoelectron shake-up states of model molecules for polyaniline. *Journal of Chemical Physics*, **1992**, 97, 137-144	3.9	14
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69	Electronic and vibrational structure of thin films of bithiophene: Undoped and alkali-doped states. *Journal of Chemical Physics*, **1999**, 110, 8060-8069	3.9	12
68	Conductance and localization in a system of coupled conjugated polymer chains. *Physical Review B*, **1995**, 51, 4137-4142	3.3	12
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65	Electronic structure and stability of fullerene polymers. *Applied Physics A: Materials Science and Processing*, **1997**, 64, 307-314	2.6	11
64	Electronic structure calculations of potassium-intercalated single-walled carbon nanotubes. *Physical Review B*, **2005**, 72,	3.3	11
63	Anderson localization in two-dimensional disordered systems. *Synthetic Metals*, **2003**, 139, 239-244	3.6	11
62	Defect states in polyaniline. *Synthetic Metals*, **1987**, 18, 387-392	3.6	11
61	A Delta Self-Consistent-Field Study of Core Electron Binding Energies of Model Molecules for the Aluminum/Polythiophene Interface. *The Journal of Physical Chemistry*, **1995**, 99, 16597-16601		10
60	Localization of kinks in a system of commensurability 3. *Physical Review B*, **1985**, 31, 6058-6062	3.3	10
59	Polaron dynamics in anisotropic Holstein-Peierls systems. *Physical Chemistry Chemical Physics*, **2017**, 19, 4078-4084	3.6	9
58	Enhanced thermal dissociation of optically excited C 60 chains. *Europhysics Letters*, **2000**, 49, 631-636	1.6	9
57	Theoretical investigations of the interaction between electron and hole polarons in thiophene oligomers. *Physical Review B*, **1996**, 54, 13713-13720	3.3	9
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55	Charge transport in □conjugated systems. *Synthetic Metals*, **2003**, 137, 1397-1399	3.6	8

54	Calculation of oscillator strengths with the supercell method sub-bandgap transitions in conjugated polymers. *Synthetic Metals*, **1993**, 57, 4614-4619	3.6	8
53	Theoretical study of electron transport along self-assembled graphitic nanowires. *Journal of Physics Condensed Matter*, **2000**, 12, 9433-9440	1.8	7
52	Valence-band structure of PMDA-ODA polyimide studied by x-ray photoelectron spectroscopy and theoretical calculations*. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1994**, 12, 772-782	2.9	7
51	Electronic structure of trimethylamine alane in the solid state. *Chemical Physics Letters*, **1995**, 235, 528-534	2.5	7
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35	Effect of charge state on bonding in fulleride polymers. *Europhysics Letters*, **1999**, 46, 382-388	1.6	4
34	Electronic properties of highly doped trans-polyacetylene. *Physical Review B*, **1991**, 44, 12737-12741	3.3	4
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29	Electron Correlation Vs Peierls Distortion In Polyacetylene. *Molecular Crystals and Liquid Crystals*, **1985**, 118, 45-48		4
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27	Studies of Polaron and/or Bipolaron Formation in Short Segments of Polymers. *Synthetic Metals*, **1999**, 101, 287-290	3.6	3
26	Effects of Interchain Interactions on the Localization of Doping Induced Defects in Quasi One-Dimensional Systems. *Molecular Crystals and Liquid Crystals*, **1994**, 256, 209-216		3
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1	Electron Lattice Dynamics as a Method to Study Charge Transport in Conjugated Polymers207-238		