

Zoltan G Soos

List of Publications by Year in descending order

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138
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138
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2401
citing authors

#	ARTICLE	IF	CITATIONS
1	Theory of π -Molecular Charge-Transfer Crystals. Annual Review of Physical Chemistry, 1974, 25, 121-153.	4.8	273
2	Valence-bond theory of linear Hubbard and Pariser-Parr-Pople models. Physical Review B, 1984, 29, 5410-5422.	1.1	261
3	Electronic polarization at surfaces and thin films of organic molecular crystals: PTCDA. Chemical Physics Letters, 2002, 360, 47-52.	1.2	261
4	Valence bond approach to exact nonlinear optical properties of conjugated systems. Journal of Chemical Physics, 1989, 90, 1067-1076.	1.2	226
5	Spin Excitations in Ionic Molecular Crystals. Annual Review of Physical Chemistry, 1966, 17, 237-260.	4.8	168
6	Electrostatic phenomena in organic semiconductors: fundamentals and implications for photovoltaics. Journal of Physics Condensed Matter, 2016, 28, 433002.	0.7	131
7	Correlated states in linear polyenes, radicals, and ions: Exact PPP transition moments and spin densities. Journal of Chemical Physics, 1984, 80, 3278-3287.	1.2	127
8	Spin Densities and Correlations in Regular Polyene Radicals. Physical Review Letters, 1983, 51, 2374-2377.	2.9	122
9	Electronic polarization in pentacene crystals and thin films. Physical Review B, 2003, 68, .	1.1	120
10	Charge redistribution and polarization energy of organic molecular crystals. Physical Review B, 2001, 64, .	1.1	116
11	Excitation and relaxation energies of trans-stilbene: Confined singlet, triplet, and charged bipolarons. Physical Review B, 1993, 47, 1742-1753.	1.1	101
12	Diagrammatic valence-bond theory for finite model Hamiltonians. International Journal of Quantum Chemistry, 1984, 25, 1003-1021.	1.0	97
13	Theory of Charge Transfer in Aromatic Donor-Acceptor Crystals. Journal of Chemical Physics, 1970, 53, 4077-4090.	1.2	94
14	Neutral-ionic interface in organic charge-transfer salts. Physical Review B, 1978, 18, 1991-2003.	1.1	84
15	Dimensionality of spin fluctuations in highly anisotropic TCNQ salts. Journal of Chemical Physics, 1976, 64, 3592-3601.	1.2	83
16	Charge-transfer states in dense hydrogen. Nature, 1994, 369, 384-387.	13.7	81
17	Weak exchange in the Heisenberg linear chain: Structure and EPR of $[N(\text{n-Bu})_4]_2[\text{Cu}(\text{mnt})_2]$. Journal of Chemical Physics, 1975, 63, 1926-1942.	1.2	76
18	Quantum Spin Liquid in Frustrated One-Dimensional LiCuSbO_4 . Physical Review Letters, 2012, 108, 187206.	2.9	76

#	ARTICLE	IF	CITATIONS
19	Electronic Polarization in Organic Crystals: A Comparative Study of Induced Dipoles and Intramolecular Charge Redistribution Schemes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4959-4971.	2.3	76
20	Correlated states in finite polyenes: Exact PPP results. <i>Journal of Chemical Physics</i> , 1982, 76, 4094-4104.	1.2	75
21	Frenkel and Wannier Spin Excitons in Organic Free-Radical Crystals. <i>Journal of Chemical Physics</i> , 1967, 46, 4284-4288.	1.2	71
22	Ionicity and paramagnetism of strong organic charge-transfer complexes. <i>Journal of Chemical Physics</i> , 1981, 74, 5287-5294.	1.2	69
23	Fluorescence and excited-state structure of conjugated polymers. <i>Advanced Materials</i> , 1994, 6, 280-287.	11.1	67
24	Ground-state alternation and excitation energy of $S=(1/2)$ linear Heisenberg antiferromagnets. <i>Physical Review B</i> , 1985, 32, 3124-3128.	1.1	64
25	Magnetic Excitations in Charge-Transfer Complexes. I. β -Phenylenediamine-Chloranil. <i>Journal of Chemical Physics</i> , 1968, 48, 1066-1076.	1.2	58
26	Charge redistribution and electronic polarization in organic molecular crystals. <i>Chemical Physics Letters</i> , 2001, 342, 652-658.	1.2	53
27	Site representation for charge transfer excitations in molecular crystals. <i>Molecular Physics</i> , 1971, 20, 1013-1024.	0.8	51
28	Second hyperpolarizability of Hückel rings: Analytical results for size and alternation dependencies. <i>Journal of Chemical Physics</i> , 1993, 99, 9265-9271.	1.2	51
29	Dielectric response of modified Hubbard models with neutral-ionic and Peierls transitions. <i>Journal of Chemical Physics</i> , 2004, 120, 6712-6720.	1.2	50
30	Giant Infrared Intensity of the Peierls Mode at the Neutral-Ionic Phase Transition. <i>Physical Review Letters</i> , 2002, 89, 027402.	2.9	49
31	Theory of charge-transfer excitations at the neutral-ionic interface. <i>Journal of Chemical Physics</i> , 1986, 85, 601-610.	1.2	48
32	Symmetry crossover and excitation thresholds at the neutral-ionic transition of the modified Hubbard model. <i>Physical Review B</i> , 2001, 63, .	1.1	47
33	Charge fluctuations and electron-phonon coupling in organic charge-transfer salts with neutral-ionic and Peierls transitions. <i>Synthetic Metals</i> , 2004, 141, 129-138.	2.1	47
34	Electron-phonon coupling in conjugated polymers: Reference force field and transferable coupling constants for polyacetylene. <i>Journal of Chemical Physics</i> , 1993, 98, 7459-7465.	1.2	46
35	Ionization in organic thin films: Electrostatic potential, electronic polarization, and dopants in pentacene films. <i>Physical Review B</i> , 2011, 84, .	1.1	45
36	Modified Hubbard Model for Complex TCNQ Salts. <i>Journal of Chemical Physics</i> , 1971, 55, 3284-3290.	1.2	44

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37	Electronic correlations and midgap absorption in polyacetylene. Journal of Chemical Physics, 1983, 78, 4092-4095.	1.2	41
38	PHENAZINE CATION RADICAL SALTS: CHARGE-TRANSFER COMPLEXES WITH TCNQ. Annals of the New York Academy of Sciences, 1978, 313, 442-458.	1.8	39
39	Cation radical salts of phenazine. Journal of the American Chemical Society, 1977, 99, 5040-5044.	6.6	37
40	Interchain dispersion and second hyperpolarizability of conjugated polymers. Journal of Chemical Physics, 1991, 95, 2127-2134.	1.2	35
41	Metastable domains and potential energy surfaces in organic charge-transfer salts with neutral-ionic phase transitions. Physical Review B, 2007, 75, .	1.1	35
42	Evidence for a soft mode in the temperature induced neutral-ionic transition of TTF-CA. Chemical Physics Letters, 2003, 369, 428-433.	1.2	34
43	Tuning the bond-order wave phase in the half-filled extended Hubbard model. Physical Review B, 2009, 79, .	1.1	34
44	Theory of exchange narrowing in low-dimensional correlated spin systems. Journal of Chemical Physics, 1978, 69, 3845-3853.	1.2	32
45	Triplet Spin Excitons in a Sigma-Bonded TCNQ Dimer Salt: N-Ethylphenazinium TCNQ, (NEP ⁺) ₂ (TCNQ ⁻) ₂ . Molecular Crystals and	0.9	32
46	Modified density matrix renormalization group algorithm for the zigzag spin-1/2 chain with frustrated antiferromagnetic exchange: Comparison with field theory at large	1.2	32
47	Polarization in organic molecular crystals and charge-transfer salts. Journal of Luminescence, 2004, 110, 332-341.	1.5	31
48	EPR of CO ₂ ^{•-} Defects in Calcite: Motional and Nonsecular Contributions. Journal of Chemical Physics, 1970, 52, 6302-6310.	1.2	29
49	The noncrossing rule and degeneracy in Hubbard models: Cyclobutadiene and benzene. Journal of Chemical Physics, 1979, 71, 3807-3812.	1.2	29
50	Electron Dipolar Linewidth of Single-Crystal TMPD Chloranil. Physical Review Letters, 1972, 28, 1054-1057.	2.9	28
51	Bond-order wave phase, spin solitons, and thermodynamics of a frustrated linear spin-1/2 chain. Physical Review B, 2010, 81, .	1.1	27
52	Profiles of Work Function Shifts and Collective Charge Transfer in Submonolayer Metal-Organic Films. Advanced Functional Materials, 2011, 21, 1931-1940.	7.8	27
53	Numerical study of incommensurate and decoupled phases of spin-1/2 chains with isotropic exchange between first and second neighbors. Journal of Physics Condensed Matter, 2016, 28, 175603.	0.7	23
54	Electron-transfer in molecular functional materials. Theoretical Chemistry Accounts, 2007, 117, 915-931.	0.5	22

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55	Comparison of Three Self-Consistent Ground States for the Linear Heisenberg Antiferromagnet. Journal of Chemical Physics, 1970, 53, 326-333.	1.2	21
56	Vibronic analysis of overlapping resonances and the third-harmonic-generation spectrum of β -carotene. Journal of Chemical Physics, 1994, 101, 5515-5522.	1.2	21
57	Nonlinear optical and electroabsorption spectra of polydiacetylene crystals and films. Journal of Chemical Physics, 1996, 104, 1600-1610.	1.2	20
58	Scaling exponents in spin-1/2 Heisenberg chains with dimerization and frustration studied with the density-matrix renormalization group. Physical Review B, 2007, 75, .	1.1	20
59	Symmetry adaptation of correlated states in the valence bond basis. Journal of Chemical Physics, 1993, 98, 4015-4022.	1.2	19
60	Anomalous Dispersion of Optical Phonons at the Neutral-Ionic Transition: Evidence from Diffuse X-Ray Scattering. Physical Review Letters, 2007, 99, 156407.	2.9	19
61	Yield of singlet and triplet excitons from x-ray and ruby laser excitation of anthracene single crystals. Journal of Chemical Physics, 1975, 63, 1122-1126.	1.2	18
62	Hopping transport in molecularly doped polymers: Joint modelling of positional and energetic disorder. Philosophical Magazine, 2003, 83, 901-928.	0.7	18
63	Quantum phases of frustrated two-leg spin-1/2 ladders with skewed rungs. Physical Review B, 2017, 95, .		
64	Disorder in organic charge-transfer single crystals: Dipolar disorder in ClMePD-DMeDCNQI. Journal of Chemical Physics, 2005, 122, 024710.	1.2	17
65	Ionization potentials of crystalline organic thin films: Position dependence due to molecular shape and charge redistribution. Chemical Physics Letters, 2010, 493, 251-254.	1.2	17
66	Density matrix renormalization group algorithm for Bethe lattices of spin-1/2 or spin-1 sites with Heisenberg antiferromagnetic exchange. Physical Review B, 2012, 85, .	1.1	17
67	Zeeman Populations of Optically Produced Triplet Excitons in Anthracene. Journal of Chemical Physics, 1969, 51, 2107-2112.	1.2	16
68	Valence Bond Theory of Organic Charge-Transfer Salts. Molecular Crystals and Liquid Crystals, 1979, 52, 93-102.	0.9	16
69	Electronic Structure of Ion-Radical Organic Solids and Polyenes. Israel Journal of Chemistry, 1983, 23, 37-48.	1.0	16
70	Dipole-Field Sums, Lorentz Factors, and Dielectric Properties of Organic Molecular Films Modeled as Crystalline Arrays of Polarizable Points. Advanced Functional Materials, 2015, 25, 2004-2012.	7.8	15
71	Level crossing, spin structure factor and quantum phases of the frustrated spin-1/2 chain with first and second neighbor exchange. Journal of Physics Condensed Matter, 2015, 27, 316001.	0.7	15
72	Modeling the Neutral-Ionic Transition with Correlated Electrons Coupled to Soft Lattices and Molecules. Crystals, 2017, 7, 144.	1.0	14

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73	Spin solitons in organic charge-transfer salts. Chemical Physics, 2006, 325, 60-70.	0.9	13
74	Theory of Temperature-Dependent g-Tensor Splittings in p-Phenylenediamine-Chloranil. Journal of Chemical Physics, 1968, 49, 2493-2498.	1.2	12
75	Resolution of the sign problem in quantum Monte Carlo simulations of annulenes. Molecular Physics, 1995, 84, 1127-1137.	0.8	12
76	Atomic multipolar contributions to electronic polarization in organic molecular crystals. Europhysics Letters, 2002, 60, 743-749.	0.7	12
77	Polarization and polarizability in extended one-dimensional organic materials. Chemical Physics, 2006, 325, 48-59.	0.9	12
78	Decoupled phase of frustrated spin- $\frac{1}{2}$ antiferromagnetic chains with and without long-range order in the ground state. Physical Review B, 2013, 88, .		12
79	Magnetic susceptibility of alkali-tetracyanoquinodimethane salts and extended Hubbard models with bond order and charge density wave phases. Journal of Chemical Physics, 2011, 134, 234304.	1.2	11
80	Spin-parity and broken symmetry in finite spin- $\frac{1}{2}$ chains with frustrated exchange: Quantum transition from high to low spin. Physical Review B, 2012, 85, .	1.1	11
81	Dielectric properties of crystalline organic molecular films in the limit of zero overlap. Journal of Chemical Physics, 2016, 144, 034702.	1.2	11
82	Electrostatic energy of aromatic ion radical crystals. Molecular Physics, 1972, 23, 775-785.	0.8	10
83	Correlated π -electronic states: Pyrene, 16-site polyene, and D2h symmetry adaptation. Journal of Chemical Physics, 1998, 108, 2486-2494.	1.2	10
84	Vibronic Structure of Frenkel and Charge-Transfer Excitons in PTCDA. Molecular Crystals and Liquid Crystals, 2001, 355, 41-63.	0.3	10
85	Peierls Transitions in Ionic Organic Charge-Transfer Crystals with Spin and Charge Degrees of Freedom. Journal of Physical Chemistry B, 2006, 110, 18748-18757.	1.2	10
86	Hybrid exact diagonalization and density matrix renormalization group approach to the thermodynamics of one-dimensional quantum models. Physical Review B, 2019, 99, .	1.1	10
87	Electron Transfer in Symmetric Complexes: Displaced Oscillators and [Fe(CN)6Pt(NH3)4Fe(CN)6]4-Spectra. Journal of Physical Chemistry A, 1998, 102, 8312-8319.	1.1	9
88	Spin-flop and antiferromagnetic phases of the ferromagnetic half-twist ladder compounds Ba ₃ Cu ₃ In ₄ O ₁₂ and Ba ₃ Cu ₃ Sc ₄ O ₁₂ . Journal of Physics Condensed Matter, 2013, 25, 136004.	0.7	9
89	Peierls transition of spin- $\frac{1}{2}$ chains with correlated states: model. Physical Review B, 2020, 101, .		9
90	Spin Dynamics in Disordered TCNQ Salts. Molecular Crystals and Liquid Crystals, 1982, 85, 19-31.	0.9	8

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91	Structure and Paramagnetism of Strong Charge-Transfer Complexes: 5.10-Dihydro-2.3.5.7.8.10-hexamethylphenazine-tetracyanoethylene (M_{6P}) (TCNE). <i>Molecular Crystals and Liquid Crystals</i> , 1983, 95, 149-164.	0.9	8
92	Polar organic films: Transport gap, charge dipole interaction and electroluminescence of tritolylamine (TTA) derivatives. <i>Chemical Physics Letters</i> , 2007, 442, 285-288.	1.2	8
93	Dimerization transition of alkali-TCNQ salts: Charge degrees of freedom near the CDW boundary. <i>Europhysics Letters</i> , 2008, 83, 37001.	0.7	8
94	Bond-order wave phase of the extended Hubbard model: Electronic solitons, paramagnetism, and coupling to Peierls and Holstein phonons. <i>Physical Review B</i> , 2010, 82, .	1.1	8
95	Efficient density matrix renormalization group algorithm to study Y junctions with integer and half-integer spin. <i>Physical Review B</i> , 2016, 93, .	1.1	8
96	Exchange Mechanisms in Ferrocinium Complexes. <i>Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics</i> , 1989, 176, 369-379.	0.3	7
97	Dilution and cluster contributions to hopping transport in a bias field. <i>Journal of Chemical Physics</i> , 2002, 116, 9475-9484.	1.2	7
98	Spin-specific heat determination of the ratio of competing first- and second-neighbor exchange interactions in frustrated spin-1/2 chains. <i>Physical Review B</i> , 2018, 97, .	1.1	7
99	Observation of the dynamic behavior of the antiferromagnetic ferromagnetic phase transition in the one-dimensional spin-1/2 antiferromagnet CuNSal . <i>Journal of Applied Physics</i> , 1979, 50, 1859-1861.	1.1	6
100	Charge-Transfer Excitations In Partly-Ionic Complexes. <i>Molecular Crystals and Liquid Crystals</i> , 1985, 125, 59-70.	0.9	6
101	Molecular Correlations and Neutral Excitations of Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , 1994, 256, 35-44.	0.3	6
102	Raman Excitation Profiles with Self-Consistent Excited-State Displacements. <i>Journal of Physical Chemistry B</i> , 2000, 104, 10909-10914.	1.2	6
103	Model for triplet state engineering in organic light emitting diodes. <i>Journal of Chemical Physics</i> , 2014, 140, 214313.	1.2	6
104	Boundary-induced spin-density waves in linear Heisenberg antiferromagnetic spin chains with $S=1$. <i>Physical Review B</i> , 2016, 94, .	1.1	6
105	Theory of Dipolar Lineshifts in Free Radical Crystals. <i>Journal of Chemical Physics</i> , 1969, 50, 2911-2916.	1.2	5
106	Delocalization Contributions to Polyacetylene Force Fields. <i>Molecular Crystals and Liquid Crystals</i> , 1994, 256, 711-719.	0.3	5
107	Reply to Comment on Frequency response and origin of the spin-1/2 photoluminescence-detected magnetic resonance in α -conjugated polymer. <i>Physical Review B</i> , 2007, 75, .	1.1	5
108	Identification of dimerization phase transitions driven by Peierls and other mechanisms. <i>Chemical Physics Letters</i> , 2007, 440, 87-91.	1.2	5

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109	ELECTRONIC PROPERTIES OF POLYSILANES: EXCITATIONS OF π -CONJUGATED CHAINS. , 1993, , 100-133.		5
110	Dimerization and Peierls Instability in Polyacetylene. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1988, 160, 421-432.	0.3	4
111	Exact nonlinear optical coefficients of quantum cell models with interacting electrons. International Journal of Quantum Chemistry, 1992, 43, 37-60.	1.0	4
112	Exciton Bandwidth and Coupling to Intramolecular Phonons in PTCDA. Materials Research Society Symposia Proceedings, 1997, 488, 171.	0.1	4
113	Zero-field mobility, exact mean dwell times, and disorder-induced steps in a Gaussian energy distribution. Journal of Chemical Physics, 2001, 114, 3330-3338.	1.2	4
114	Electronic and structural instabilities of mixed-stack organic charge-transfer salts. Synthetic Metals, 2005, 155, 357-364.	2.1	4
115	Diamagnetic to Paramagnetic Transition in Trisdimethylaminocyclopropenium Tetracyanoquinodimethanide (TDAC-TCNQ). Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1987, 150, 473-492.	0.3	3
116	Herzbergâ€™s Teller coupling and configuration interaction in a metalloporphyrin model: 1,3,5,7-tetramethylcycloâ€œoctatetraene dianion. Journal of Chemical Physics, 1994, 101, 4644-4648.	1.2	3
117	Relaxor ferroelectricity in the polar M2P-TCNQ charge-transfer crystal at the neutral-ionic interface. Physical Review B, 2021, 103, .	1.1	3
118	Static polarizability of molecular materials: Environmental and vibrational contributions. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 703-720.	0.1	2
119	Polarization energies, transport gap and charge transfer states of organic molecular crystals. Macromolecular Symposia, 2004, 212, 1-12.	0.4	2
120	Density matrix renormalization group approach to the low temperature thermodynamics of correlated 1D fermionic models. Journal of Magnetism and Magnetic Materials, 2022, 552, 169150.	1.0	2
121	Extended Pariser-Parr-Pople Model for Polydiacetylene Excitations. ACS Symposium Series, 1987, , 190-201.	0.5	1
122	Electronic Properties of Polysilanes. ACS Symposium Series, 1995, , 387-397.	0.5	1
123	Model Hamiltonians for Nonlinear Optical Properties of Conjugated Polymers. ACS Symposium Series, 1996, , 189-210.	0.5	1
124	Bond-bond correlations, gap relations and thermodynamics of spin-1/2 chains with spin-Peierls transitions and bond-order-wave phases. Journal of Magnetism and Magnetic Materials, 2021, 519, 167472.	1.0	1
125	Low-temperature thermodynamics of the antiferromagnetic $J_1\hat{\sim}J_2$ model: Entropy, critical points, and spin gap. Physical Review B, 2021, 103, .	1.1	1
126	Spin-Peierls transition of $J_1\hat{\sim}J_2$ and extended models with ferromagnetic J_1 and J_2 : Sublattice dimerization and thermodynamics of zigzag chains in $J_1\hat{\sim}J_2$ model. Physical Review B, 2022, 105, .	1.1	1

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127	A New Function for Dipole Orientation and Rubber Elasticity. Rubber Chemistry and Technology, 1970, 43, 878-882.	0.6	0
128	Charge Carrier Generation by Exciton-Exciton Annihilation in Poly(Di-N-Hexylsilane). Materials Research Society Symposia Proceedings, 1992, 247, 655.	0.1	0
129	Multiphoton Spectra of Conjugated Polymers. Materials Research Society Symposia Proceedings, 1992, 247, 79.	0.1	0
130	Temperature Dependence of the Exciton-Exciton Annihilation Rate Constant in Poly (Di-N-Hexylsilane). Materials Research Society Symposia Proceedings, 1993, 328, 679.	0.1	0
131	Temperature Dependence of the Two-Photon Absorption Spectrum of Poly(di-n-Hexylsilane). Molecular Crystals and Liquid Crystals, 1994, 256, 143-148.	0.3	0
132	THE ROLE OF EXCITONS IN CHARGE CARRIER PRODUCTION IN POLYSILANES. , 1998, , 363-383.		0
133	CORRELATIONS IN CONJUGATED POLYMERS. , 1998, , 1-19.		0
134	Vibronic Structure of PTCDA Stacks: Monomer-Dimer Equilibrium. Materials Research Society Symposia Proceedings, 1999, 598, 459.	0.1	0
135	Polarization in Organic Molecular Crystals and Charge-Transfer Salts. ChemInform, 2005, 36, no.	0.1	0