

Zoltan G Soos

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Density matrix renormalization group approach to the low temperature thermodynamics of correlated 1D fermionic models. Journal of Magnetism and Magnetic Materials, 2022, 552, 169150. Spin-Peierls transition of J_1 and extended models with ferromagnetic J_2 : Sublattice dimerization and thermodynamics of zigzag chains in J_1 - J_2 spin-1/2 chains with spin-Peierls transitions and bond-order-wave phases. Journal of Magnetism and Magnetic Materials, 2021, 519, 167472.	1.0	2
2	Relaxor ferroelectricity in the polar M2P-TCNQ charge-transfer crystal at the neutral-ionic interface. Physical Review B, 2021, 103, .	1.1	3
3	Low-temperature thermodynamics of the antiferromagnetic J_1 - J_2 model: Entropy, critical points, and spin gap. Physical Review B, 2021, 103, . Modeling the spin-Peierls transition of spin-1/2 chains with correlated states: J_1 - J_2 model. Physical Review B, 2020, 101, .	1.1	1
4	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
5	Spin-specific heat determination of the ratio of competing first- and second-neighbor exchange interactions in frustrated spin-1/2 chains. Physical Review B, 2018, 97, .	1.1	7
6	Quantum phases of frustrated two-leg spin-1/2 ladders with skewed rungs. Physical Review B, 2017, 95, .	1.1	7
7	Modeling the Neutral-Ionic Transition with Correlated Electrons Coupled to Soft Lattices and Molecules. Crystals, 2017, 7, 144.	1.0	14
8	Dielectric properties of crystalline organic molecular films in the limit of zero overlap. Journal of Chemical Physics, 2016, 144, 034702.	1.2	11
9	Numerical study of incommensurate and decoupled phases of spin-1/2 chains with isotropic exchange J_1 and J_2 between first and second neighbors. Journal of Physics Condensed Matter, 2016, 28, 175603.	0.7	23
10	Electrostatic phenomena in organic semiconductors: fundamentals and implications for photovoltaics. Journal of Physics Condensed Matter, 2016, 28, 433002.	0.7	131
11	Efficient density matrix renormalization group algorithm to study Y junctions with integer and half-integer spin. Physical Review B, 2016, 93, .	1.1	8
12	Boundary-induced spin-density waves in linear Heisenberg antiferromagnetic spin chains with J_1 and J_2 . Physical Review B, 2016, 94, .	1.1	6
13	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
14	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
15	Electronic Polarization in Organic Crystals: A Comparative Study of Induced Dipoles and Intramolecular Charge Redistribution Schemes. Journal of Chemical Theory and Computation, 2014, 10, 4959-4971.	2.3	76

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19	Model for triplet state engineering in organic light emitting diodes. Journal of Chemical Physics, 2014, 140, 214313.	1.2	6
20	Spin-flop and antiferromagnetic phases of the ferromagnetic half-twist ladder compounds $Ba_3Cu_3In_4O_{12}$ and $Ba_3Cu_3Sc_4O_{12}$. Journal of Physics Condensed Matter, 2013, 25, 136004.	0.7	9
21	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
22	Quantum Spin Liquid in Frustrated One-Dimensional $LiCuSbO_4$. Physical Review Letters, 2012, 108, 187206.	2.9	76
23	Density matrix renormalization group algorithm for Bethe lattices of spin-1 sites with Heisenberg antiferromagnetic exchange. Physical Review B, 2012, 85, .	1.1	17
24	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
25	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
26	Profiles of Work Function Shifts and Collective Charge Transfer in Submonolayer Metal/Organic Films. Advanced Functional Materials, 2011, 21, 1931-1940.	7.8	27
27	Ionization in organic thin films: Electrostatic potential, electronic polarization, and dopants in pentacene films. Physical Review B, 2011, 84, .	1.1	45
28	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
29	Density matrix renormalization group algorithm for the zigzag spin- $\frac{1}{2}$ Heisenberg chain with frustrated antiferromagnetic exchange: Comparison with field theory at large bond-order wave phase, spin solitons, and thermodynamics of a frustrated linear spin- $\frac{1}{2}$ Heisenberg antiferromagnet. Physical Review B, 2010, 81, .		27
30	Bond-order wave phase of the extended Hubbard model: Electronic solitons, paramagnetism, and coupling to Peierls and Holstein phonons. Physical Review B, 2010, 82, .	1.1	27
31	Bond-order wave phase of the extended Hubbard model: Electronic solitons, paramagnetism, and coupling to Peierls and Holstein phonons. Physical Review B, 2010, 82, .	1.1	8
32	Tuning the bond-order wave phase in the half-filled extended Hubbard model. Physical Review B, 2009, 79, .	1.1	34
33	Dimerization transition of alkali-TCNQ salts: Charge degrees of freedom near the CDW boundary. Europhysics Letters, 2008, 83, 37001.	0.7	8
34	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
35	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
36	Metastable domains and potential energy surfaces in organic charge-transfer salts with neutral-ionic phase transitions. Physical Review B, 2007, 75, .	1.1	35

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37	Reply to "Comment on "Frequency response and origin of the spin-12 photoluminescence-detected magnetic resonance in a-conjugated polymer"â€œ. Physical Review B, 2007, 75, .	1.1	5
38	Identification of dimerization phase transitions driven by Peierls and other mechanisms. Chemical Physics Letters, 2007, 440, 87-91.	1.2	5
39	Polar organic films: Transport gap, chargeâ€“dipole interaction and electroluminescence of tritolyamine (TTA) derivatives. Chemical Physics Letters, 2007, 442, 285-288.	1.2	8
40	Electron-transfer in molecular functional materials. Theoretical Chemistry Accounts, 2007, 117, 915-931.	0.5	22
41	Peierls Transitions in Ionic Organic Charge-Transfer Crystals with Spin and Charge Degrees of Freedomâ€œ. Journal of Physical Chemistry B, 2006, 110, 18748-18757.	1.2	10
42	Polarization and polarizability in extended one-dimensional organic materials. Chemical Physics, 2006, 325, 48-59.	0.9	12
43	Spin solitons in organic charge-transfer salts. Chemical Physics, 2006, 325, 60-70.	0.9	13
44	Polarization in Organic Molecular Crystals and Charge-Transfer Salts. ChemInform, 2005, 36, no.	0.1	0
45	Disorder in organic charge-transfer single crystals: Dipolar disorder in ClMePD-DMeDCNQI. Journal of Chemical Physics, 2005, 122, 024710.	1.2	17
46	Electronic and structural instabilities of mixed-stack organic charge-transfer salts. Synthetic Metals, 2005, 155, 357-364.	2.1	4
47	Static polarizability of molecular materials: Environmental and vibrational contributions. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 703-720.	0.1	2
48	Dielectric response of modified Hubbard models with neutral-ionic and Peierls transitions. Journal of Chemical Physics, 2004, 120, 6712-6720.	1.2	50
49	Polarization in organic molecular crystals and charge-transfer salts. Journal of Luminescence, 2004, 110, 332-341.	1.5	31
50	Charge fluctuations and electronâ€“phonon coupling in organic charge-transfer salts with neutralâ€“ionic and Peierls transitions. Synthetic Metals, 2004, 141, 129-138.	2.1	47
51	Polarization energies, transport gap and charge transfer states of organic molecular crystals. Macromolecular Symposia, 2004, 212, 1-12.	0.4	2
52	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
53	Hopping transport in molecularly doped polymers: Joint modelling of positional and energetic disorder. Philosophical Magazine, 2003, 83, 901-928.	0.7	18
54	Electronic polarization in pentacene crystals and thin films. Physical Review B, 2003, 68, .	1.1	120

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55	Atomic multipolar contributions to electronic polarization in organic molecular crystals. <i>Europhysics Letters</i> , 2002, 60, 743-749.	0.7	12
56	Giant Infrared Intensity of the Peierls Mode at the Neutral-Ionic Phase Transition. <i>Physical Review Letters</i> , 2002, 89, 027402.	2.9	49
57	Dilution and cluster contributions to hopping transport in a bias field. <i>Journal of Chemical Physics</i> , 2002, 116, 9475-9484.	1.2	7
58	Electronic polarization at surfaces and thin films of organic molecular crystals: PTCDA. <i>Chemical Physics Letters</i> , 2002, 360, 47-52.	1.2	261
59	Charge redistribution and electronic polarization in organic molecular crystals. <i>Chemical Physics Letters</i> , 2001, 342, 652-658.	1.2	53
60	Vibronic Structure of Frenkel and Charge-Transfer Excitons in PTCDA. <i>Molecular Crystals and Liquid Crystals</i> , 2001, 355, 41-63.	0.3	10
61	Zero-field mobility, exact mean dwell times, and disorder-induced steps in a Gaussian energy distribution. <i>Journal of Chemical Physics</i> , 2001, 114, 3330-3338.	1.2	4
62	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
63	Charge redistribution and polarization energy of organic molecular crystals. <i>Physical Review B</i> , 2001, 64, .	1.1	116
64	Raman Excitation Profiles with Self-Consistent Excited-State Displacements. <i>Journal of Physical Chemistry B</i> , 2000, 104, 10909-10914.	1.2	6
65	Vibronic Structure of PTCDA Stacks: Monomer-Dimer Equilibrium. <i>Materials Research Society Symposia Proceedings</i> , 1999, 598, 459.	0.1	0
66	Electron Transfer in Symmetric Complexes: Displaced Oscillators and $[\text{Fe}(\text{CN})_6\text{Pt}(\text{NH}_3)_4\text{Fe}(\text{CN})_6]^{4-}$ Spectra. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8312-8319.	1.1	9
67	Correlated π -electronic states: Pyrene, 16-site polyene, and D_{2h} symmetry adaptation. <i>Journal of Chemical Physics</i> , 1998, 108, 2486-2494.	1.2	10
68	THE ROLE OF EXCITONS IN CHARGE CARRIER PRODUCTION IN POLYSILANES. , 1998, , 363-383.		0
69	CORRELATIONS IN CONJUGATED POLYMERS. , 1998, , 1-19.		0
70	Exciton Bandwidth and Coupling to Intramolecular Phonons in PTCDA. <i>Materials Research Society Symposia Proceedings</i> , 1997, 488, 171.	0.1	4
71	Model Hamiltonians for Nonlinear Optical Properties of Conjugated Polymers. <i>ACS Symposium Series</i> , 1996, , 189-210.	0.5	1
72	Nonlinear optical and electroabsorption spectra of polydiacetylene crystals and films. <i>Journal of Chemical Physics</i> , 1996, 104, 1600-1610.	1.2	20

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73	Resolution of the sign problem in quantum Monte Carlo simulations of annulenes. <i>Molecular Physics</i> , 1995, 84, 1127-1137.	0.8	12
74	Electronic Properties of Polysilanes. <i>ACS Symposium Series</i> , 1995, , 387-397.	0.5	1
75	Herzbergâ€™Teller coupling and configuration interaction in a metalloporphyrin model: 1,3,5,7â€™tetramethylcycloâ€™octatetraene dianion. <i>Journal of Chemical Physics</i> , 1994, 101, 4644-4648.	1.2	3
76	Fluorescence and excited-state structure of conjugated polymers. <i>Advanced Materials</i> , 1994, 6, 280-287.	11.1	67
77	Charge-transfer states in dense hydrogenCharge-transfer states in dense hydrogen. <i>Nature</i> , 1994, 369, 384-387.	13.7	81
78	Vibronic analysis of overlapping resonances and the thirdâ€™harmonicâ€™generation spectrum of Î²â€™carotene. <i>Journal of Chemical Physics</i> , 1994, 101, 5515-5522.	1.2	21
79	Delocalization Contributions to Polyacetylene Force Fields. <i>Molecular Crystals and Liquid Crystals</i> , 1994, 256, 711-719.	0.3	5
80	Temperature Dependence of the Two-Photon Absorption Spectrum of Poly(di-n-Hexylsilane). <i>Molecular Crystals and Liquid Crystals</i> , 1994, 256, 143-148.	0.3	0
81	Molecular Correlations and Neutral Excitations of Conjugated Polymers. <i>Molecular Crystals and Liquid Crystals</i> , 1994, 256, 35-44.	0.3	6
82	Second hyperpolarizability of HÄ¼ckel rings: Analytical results for size and alternation dependencies. <i>Journal of Chemical Physics</i> , 1993, 99, 9265-9271.	1.2	51
83	Electronâ€™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
84	Symmetry adaptation of correlated states in the valence bond basis. <i>Journal of Chemical Physics</i> , 1993, 98, 4015-4022.	1.2	19
85	Excitation and relaxation energies oftrans-stilbene: Confined singlet, triplet, and charged bipolarons. <i>Physical Review B</i> , 1993, 47, 1742-1753.	1.1	101
86	Temperature Dependence of the Exciton-Exciton Annihilation Rate Constant in Poly (Di-N-Hexylsilane). <i>Materials Research Society Symposia Proceedings</i> , 1993, 328, 679.	0.1	0
87	ELECTRONIC PROPERTIES OF POLYSILANES: EXCITATIONS OF Î¶f-CONJUGATED CHAINS. , 1993, , 100-133.		5
88	Charge Carrier Generation by Exciton-Exciton Annihilation in Poly(Di-N-Hexylsilane). <i>Materials Research Society Symposia Proceedings</i> , 1992, 247, 655.	0.1	0
89	Multiphoton Spectra of Conjugated Polymers. <i>Materials Research Society Symposia Proceedings</i> , 1992, 247, 79.	0.1	0
90	Exact nonlinear optical coefficients of quantum cell models with interacting electrons. <i>International Journal of Quantum Chemistry</i> , 1992, 43, 37-60.	1.0	4

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91	Interchain dispersion and second hyperpolarizability of conjugated polymers. Journal of Chemical Physics, 1991, 95, 2127-2134.	1.2	35
92	Valence bond approach to exact nonlinear optical properties of conjugated systems. Journal of Chemical Physics, 1989, 90, 1067-1076.	1.2	226
93	Exchange Mechanisms in Ferrocenium Complexes. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1989, 176, 369-379.	0.3	7
94	Dimerization and Peierls Instability in Polyacetylene. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1988, 160, 421-432.	0.3	4
95	Diamagnetic to Paramagnetic Transition in Trisdimethylaminocyclopropenium Tetracyanoquinodimethanide (TDAC-TCNQ). Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1987, 150, 473-492.	0.3	3
96	Extended Pariser-Parr-Pople Model for Polydiacetylene Excitations. ACS Symposium Series, 1987, , 190-201.	0.5	1
97	Theory of charge-transfer excitations at the neutral-ionic interface. Journal of Chemical Physics, 1986, 85, 601-610.	1.2	48
98	Ground-state alternation and excitation energy of $S=(1/2)$ linear Heisenberg antiferromagnets. Physical Review B, 1985, 32, 3124-3128.	1.1	64
99	Charge-Transfer Excitations In Partly-Ionic Complexes. Molecular Crystals and Liquid Crystals, 1985, 125, 59-70.	0.9	6
100	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
101	Diagrammatic valence-bond theory for finite model Hamiltonians. International Journal of Quantum Chemistry, 1984, 25, 1003-1021.	1.0	97
102	Valence-bond theory of linear Hubbard and Pariser-Parr-Pople models. Physical Review B, 1984, 29, 5410-5422.	1.1	261
103	Spin Densities and Correlations in Regular Polyene Radicals. Physical Review Letters, 1983, 51, 2374-2377.	2.9	122
104	Electronic correlations and midgap absorption in polyacetylene. Journal of Chemical Physics, 1983, 78, 4092-4095.	1.2	41
105	Structure and Paramagnetism of Strong Charge-Transfer Complexes: 5.10-Dihydro-2.3.5.7.8.10-hexamethylphenazine-tetracyanoethylene (M_{6P}) (TCNE). Molecular Crystals and Liquid Crystals, 1983, 95, 149-164.	0.9	8
106	Electronic Structure of Ion-Radical Organic Solids and Polyenes. Israel Journal of Chemistry, 1983, 23, 37-48.	1.0	16
107	Correlated states in finite polyenes: Exact PPP results. Journal of Chemical Physics, 1982, 76, 4094-4104.	1.2	75
108	Spin Dynamics in Disordered TCNQ Salts. Molecular Crystals and Liquid Crystals, 1982, 85, 19-31.	0.9	8

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109	Ionicity and paramagnetism of strong organic charge-transfer complexes. <i>Journal of Chemical Physics</i> , 1981, 74, 5287-5294.	1.2	69
110	Triplet Spin Excitons in a Sigma-Bonded TCNQ Dimer Salt: N-Ethylphenazinium TCNQ, (NEP ⁺) ₂ (TCNQ ⁻) ₂ . <i>Molecular Crystals and Liquid Crystals</i> , 1981, 65, 179-196.	0.9	32
111	Valence Bond Theory of Organic Charge-Transfer Salts. <i>Molecular Crystals and Liquid Crystals</i> , 1979, 52, 93-102.	0.9	16
112	The noncrossing rule and degeneracy in Hubbard models: Cyclobutadiene and benzene. <i>Journal of Chemical Physics</i> , 1979, 71, 3807-3812.	1.2	29
113	Observation of the dynamic behavior of the antiferromagnetic-ferromagnetic phase transition in the one-dimensional spin-1/2 antiferromagnet $\text{I}^{\pm}\text{CuNSal}$. <i>Journal of Applied Physics</i> , 1979, 50, 1859-1861.	1.1	6
114	PHENAZINE CATION RADICAL SALTS: CHARGE-TRANSFER COMPLEXES WITH TCNQ. <i>Annals of the New York Academy of Sciences</i> , 1978, 313, 442-458.	1.8	39
115	Neutral-ionic interface in organic charge-transfer salts. <i>Physical Review B</i> , 1978, 18, 1991-2003.	1.1	84
116	Theory of exchange narrowing in low-dimensional correlated spin systems. <i>Journal of Chemical Physics</i> , 1978, 69, 3845-3853.	1.2	32
117	Cation radical salts of phenazine. <i>Journal of the American Chemical Society</i> , 1977, 99, 5040-5044.	6.6	37
118	Dimensionality of spin fluctuations in highly anisotropic TCNQ salts. <i>Journal of Chemical Physics</i> , 1976, 64, 3592-3601.	1.2	83
119	Weak exchange in the Heisenberg linear chain: Structure and EPR of $[\text{N}(\text{n-Bu})_4]_2[\text{Cu}(\text{mnt})_2]$. <i>Journal of Chemical Physics</i> , 1975, 63, 1926-1942.	1.2	76
120	Yield of singlet and triplet excitons from x-ray and ruby laser excitation of anthracene single crystals. <i>Journal of Chemical Physics</i> , 1975, 63, 1122-1126.	1.2	18
121	Theory of π -Molecular Charge-Transfer Crystals. <i>Annual Review of Physical Chemistry</i> , 1974, 25, 121-153.	4.8	273
122	Electrostatic energy of aromatic ion radical crystals. <i>Molecular Physics</i> , 1972, 23, 775-785.	0.8	10
123	Electron Dipolar Linewidth of Single-Crystal TMPD Chloranil. <i>Physical Review Letters</i> , 1972, 28, 1054-1057.	2.9	28
124	Modified Hubbard Model for Complex TCNQ Salts. <i>Journal of Chemical Physics</i> , 1971, 55, 3284-3290.	1.2	44
125	Site representation for charge transfer excitations in molecular crystals. <i>Molecular Physics</i> , 1971, 20, 1013-1024.	0.8	51
126	A New Function for Dipole Orientation and Rubber Elasticity. <i>Rubber Chemistry and Technology</i> , 1970, 43, 878-882.	0.6	0

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127	Comparison of Three Self-Consistent Ground States for the Linear Heisenberg Antiferromagnet. Journal of Chemical Physics, 1970, 53, 326-333.	1.2	21
128	Theory of Charge Transfer in Aromatic Donor-Acceptor Crystals. Journal of Chemical Physics, 1970, 53, 4077-4090.	1.2	94
129	EPR of CO ₂ Defects in Calcite: Motional and Nonsecular Contributions. Journal of Chemical Physics, 1970, 52, 6302-6310.	1.2	29
130	Theory of Dipolar Lineshifts in Free Radical Crystals. Journal of Chemical Physics, 1969, 50, 2911-2916.	1.2	5
131	Zeeman Populations of Optically Produced Triplet Excitons in Anthracene. Journal of Chemical Physics, 1969, 51, 2107-2112.	1.2	16
132	Magnetic Excitations in Charge-Transfer Complexes. I. Phenylenediamine-Chloranil. Journal of Chemical Physics, 1968, 48, 1066-1076.	1.2	58
133	Theory of Temperature-Dependent g-Tensor Splittings in Phenylenediamine-Chloranil. Journal of Chemical Physics, 1968, 49, 2493-2498.	1.2	12
134	Frenkel and Wannier Spin Excitons in Organic Free Radical Crystals. Journal of Chemical Physics, 1967, 46, 4284-4288.	1.2	71
135	Spin Excitations in Ionic Molecular Crystals. Annual Review of Physical Chemistry, 1966, 17, 237-260.	4.8	168