Surjit Singh

List of Publications by Year
in descending order

87 papers	1,763 citations	304743 22 h-index	302126 39 g-index
88 all docs	88 docs citations	88 times ranked	960 citing authors

#	Article	IF	Citations
1	Pressure Effect on the Density of Water. Journal of Physical Chemistry A, 2002, 106, 7557-7561.	2.5	31
2	Water anomalies and the double-well Takahashi model. Chemical Physics, 1998, 232, 329-341.	1.9	9
3	Choet al.Reply:. Physical Review Letters, 1997, 79, 180-180.	7.8	9
4	Understanding all of waterâ€™s anomalies with a nonlocal potential. Journal of Chemical Physics, 1997, 107, 7979-7988.	3.0	109
5	Dipole function for the C-H oscillator. Journal of Chemical Sciences, 1997, 109, 181-188.	1.5	0
6	An Explanation of the Density Maximum in Water. Physical Review Letters, 1996, 76, 1651-1654.	7.8	99
7	Liquid water and biological systems: the most important problem in science that hardly anyone wants to see solved. Faraday Discussions, 1996, 103, 19.	3.2	76
8	Ab initio molecular orbital calculations on ion-molecule and ion-pair-molecule complexes of formamide with LiF and LiCl. Computational and Theoretical Chemistry, 1996, 361, 229-242.	1.5	5
9	An analytical study of the Berezhkovskii-Pollak-Zitserman theory of rate processes in the critical region. II. The critical coupling plane. Chemical Physics, 1996, 212, 125-135.	1.9	0
10	Universality in Isomerization Reactions in Polar Solvents. The Journal of Physical Chemistry, 1996, 100, 11907-11913.	2.9	9
11	Study of the Reaction Rate, in the Critical Regime, of a Solute Embedded in a Lennardâ€Jones Crystal. Journal of the Chinese Chemical Society, 1995, 42, 367-370.	1.4	1
12	Ab initio molecular orbital calculations on the associated complexes of lithium cyanide with ammonia. International Journal of Quantum Chemistry, 1995, 55, 477-484.	2.0	7
13	An analytical study of the Berezhkovskii-Pollak-Zitserman theory of rate processes in the memory-suppression region. Chemical Physics, 1995, 198, 257-268.	1.9	1
14	Critical scaling behavior in the activated barrier crossing problem. II. Powerâ€law potential. Journal of Chemical Physics, 1995, 103, 4920-4929.	3.0	3
15	A Study of the Quantum Activated Barrier Crossing Problem from the Viewpoint of Critical Phenomena. The Journal of Physical Chemistry, 1995, 99, 2764-2769.	2.9	5
16	Properties of Liquid Water. 4. The Isothermal Compressibility Minimum near 50 .degree.C. The Journal of Physical Chemistry, 1995, 99, 9263-9267.	2.9	42
17	Scaling in a Model of Chemical Reaction Rates with Space-Dependent Friction. The Journal of Physical Chemistry, 1994, 98, 7300-7306.	2.9	6
18	Accurate Mixture-Model Densities for D2O. The Journal of Physical Chemistry, 1994, 98, 8591-8593.	2.9	22

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19	Study of the van der Zwanâ€“Hynes model for dipole isomerization reaction rates from the viewpoint of critical phenomena. Journal of Chemical Physics, 1994, 100, 6640-6645.	3.0	7
20	Critical scaling behavior in the activated-barrier-crossing problem. Physical Review E, 1994, 49, 2540-2548.	2.1	5
21	Ab initio molecular orbital calculations on complexes of chloride ion with acetonitrile and vibrational spectroscopic studies. Journal of Molecular Structure, 1994, 327, 107-112.	3.6	3
22	Rate processes in dissipative systems: scaling in the canonical variational transition state theory. Chemical Physics, 1994, 183, 365-373.	1.9	6
23	Properties of Liquid Water: Origin of the Density Anomalies. The Journal of Physical Chemistry, 1994, 98, 2222-2230.	2.9	167
24	Ab initio molecular orbital calculations on ion pair-water complexes of metal halides and oxides. Journal of Chemical Sciences, 1994, 106, 339-351.	1.5	1
25	Anion-molecular interaction through CH3 groups: Modelab initio studies. Journal of Chemical Sciences, 1994, 106, 1315-1320.	1.5	0
26	Ab initio molecular orbital calculations on ion-molecule and ion pair-molecule complexes of the water-lithium cyanide system. Computational and Theoretical Chemistry, 1993, 284, 147-156.	1.5	5
27	Near infrared spectral studies on interactions of CH3 groups with halide ions. Journal of Chemical Sciences, 1993, 105, 71-78.	1.5	2
28	Critical phenomena and scaling behavior in theories of activated barrier crossing. Physical Review Letters, 1992, 68, 2608-2611.	7.8	14
29	Exact results for a finite-sized spherical model of ferromagnetism at the borderline dimensionality 4. Physical Review B, 1992, 45, 9759-9764.	3.2	11
30	Space-dependent friction in the theory of activated rate processes. Physical Review A, 1992, 45, 5408-5414.	2.5	21
31	Spaceâ€dependent friction in the theory of activated rate processes: The Hamiltonian approach. Journal of Chemical Physics, 1992, 97, 5516-5521.	3.0	21
32	Effect of hydrogen bonding and cooperativity on stretching force constants of formamide. International Journal of Quantum Chemistry, 1992, 44, 679-690.	2.0	24
33	Oî—¸H stretching force constants in complexes of water with Fâ^', Clâ^', Li+ ions and LiF, LiCl ion pairs by 6-31G ab initio MO calculations. Spectrochimica Acta Part A: Molecular Spectroscopy, 1992, 48, 1767-1772.	0.1	18
34	A new flexible/polarizable water model. Journal of Chemical Physics, 1991, 95, 2791-2799.	3.0	108
35	Velocity dependence of friction. Chemical Physics, 1991, 152, 221-228.	1.9	4
36	Aspects of modern condensed-phase chemistry. The Journal of Physical Chemistry, 1990, 94, 4-6.	2.9	22

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37	Theory of activated rate processes with space-dependent friction. Chemical Physics Letters, 1990, 175, 338-342.	2.6	11
38	Breakdown of the Brownian motion model in ultrafast dynamics. Physical Review A, 1989, 40, 1109-1115.	2.5	9
39	Finite-size scaling of O(n) models with long-range interactions. Physical Review B, 1989, 40, 9238-9248.	3.2	12
40	Raman spectral studies on interactions of Brâ^' ions with CD3 group of acetonitrile, nitromethane and dimethyl sulfoxide. Journal of Molecular Structure, 1989, 194, 73-82.	3.6	18
41	Raman spectral studies of ion-molecular interactions of lithium bromide and lithium iodide with dimethyl sulphoxide. Journal of Raman Spectroscopy, 1989, 20, 169-179.	2.5	15
42	The cooperativity effect and the effect of self-association on the stretching force constants of acetonitrile. Chemical Physics Letters, 1989, 164, 63-67.	2.6	14
43	O?H stretching force constant in associated methanol species and the cooperativity effect. International Journal of Quantum Chemistry, 1989, 36, 105-118.	2.0	28
44	Raman spectral studies on solutions of lithium bromide in binary mixtures of water and acetonitrile in the Cî—¸H and Cî—¼N stretching regions. Spectrochimica Acta Part A: Molecular Spectroscopy, 1988, 44, 277-282.	0.1	12
45	Finite-size scaling of O(n) models in higher dimensions. Physical Review B, 1988, 38, 2740-2748.	3.2	16
46	Phase transitions in finite systems with O(n) symmetry: Magnetization and susceptibility in the presence of an external field. Physical Review B, 1988, 37, 7806-7814.	3.2	9
47	Effect of cooperativity on the O-H stretching force constant in associated water species. Proceedings of the Indian Academy of Sciences - Section A, 1988, 100, 413-424.	0.2	10
48	Spin-spin correlations in finite systems with O(n) symmetry: Scaling hypothesis and corrections to bulk behavior. Physical Review B, 1987, 36, 3769-3781.	3.2	31
49	Finite-size scaling for a relativistic Bose gas with pair production. Physical Review A, 1987, 35, 4814-4825.	2.5	4
50	Effect of molecular interactions on the O-H stretching force constants for associated water species. Chemical Physics Letters, 1986, 131, 394-397.	2.6	26
51	Finite-size scaling of O(n) models in higher dimensions. Physics Letters, Section A: General, Atomic and Solid State Physics, 1986, 118, 131-135.	2.1	7
52	Spin-spin correlations in finite systems: Scaling hypothesis and corrections to bulk behavior. Physical Review B, 1986, 33, 672-674.	3.2	16
53	Role of fluctuations in determining finite-size effects in a system undergoing a phase transition. Physical Review B, 1986, 34, 2045-2048.	3.2	16
54	Singh and Pathria Respond. Physical Review Letters, 1986, 56, 2226-2226.	7.8	14

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55	Phase transition in a supersymmetric theory. Physical Review D, 1986, 34, 1859-1862.	4.7	1
56	Finite-size effects in the spherical model of ferromagnetism: Zero-field susceptibility under antiperiodic boundary conditions. Physical Review B, 1986, 33, 6415-6422.	3.2	10
57	Random-Field Critical Behavior: Finite-Size Effects. Physical Review Letters, 1985, 55, 2220-2222.	7.8	4
58	Privman-Fisher hypothesis on finite systems: Verification in the case of the spherical model of ferromagnetism. Physical Review B, 1985, 31, 4483-4490.	3.2	65
59	Phase transitions in finite systems: Influence of geometry on approach towards bulk critical behavior. Physical Review Letters, 1985, 55, 347-350.	7.8	34
60	Privman-Fisher hypothesis on finite systems: Verification in the case of a relativistic Bose gas with pair production. Physical Review A, 1985, 31, 1816-1824.	2.5	10
61	Finite-size effects in the spherical model of ferromagnetism: Antiperiodic boundary conditions. Physical Review B, 1985, 32, 4618-4627.	3.2	20
62	Presentation of Molecular Force Fields in Terms of Dimensionless Coordinates. Spectroscopy Letters, 1985, 18, 229-238.	1.0	3
63	Variation of Dipole Moment Function of O-H Bond of t-Butanol with the Nature of Solvent and Its Temperature. Spectroscopy Letters, 1985, 18, 283-299.	1.0	24
64	Response to "Comment on `Supersymmetric Phase Transition' ". Physical Review Letters, 1984, 52, 2006-2006.	7.8	0
65	Bose-Einstein condensation in finite noninteracting systems: A relativistic gas with pair production. II. Physical Review A, 1984, 30, 3198-3204.	2.5	11
66	Self-association of dimethyl sulphoxide and its dipolar interactions with water: Raman spectral studies. Journal of Raman Spectroscopy, 1984, 15, 80-85.	2.5	71
67	Bose-Einstein condensation in finite noninteracting systems: A relativistic gas with pair production. Physical Review A, 1984, 30, 442-449.	2.5	23
68	Crossover scaling behaviour of the quasi-one-dimensional n-vector models. Physics Letters, Section A: General, Atomic and Solid State Physics, 1983, 96, 225-227.	2.1	0
69	Supersymmetric Phase Transition. Physical Review Letters, 1983, 50, 1550-1552.	7.8	3
70	Scaling and universality of thermodynamics and correlations of an ideal relativistic Bose gas with pair production. Physical Review A, 1983, 28, 1752-1761.	2.5	26
71	Force field calculations for formamide, acetamide, and urea using the CNDO/force method. Journal of Chemical Physics, 1982, 77, 860-869.	3.0	26
72	Surface properties of an ideal relativistic Bose gas with pair production. Physics Letters, Section A: General, Atomic and Solid State Physics, 1982, 93, 70-72.	2.1	0

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73	Critical behaviour of a relativistic ideal Bose gas with pair production. Physics Letters, Section A: General, Atomic and Solid State Physics, 1982, 92, 65-67.	2.1	4
74	Raman spectral studies of aqueous solutions of non-electrolytes: Dimethylsulfoxide, acetone and acetonitrile. Journal of Raman Spectroscopy, 1982, 13, 178-188.	2.5	34
75	Crossover behaviour of the susceptibility of the quasi-two-dimensional Ising model: g = 0 behaviour. Physics Letters, Section A: General, Atomic and Solid State Physics, 1982, 88, 251-253.	2.1	3
76	Scale factor universality in the anisotropic crossover behaviour of the quasi-two-dimensional ising model. Physics Letters, Section A: General, Atomic and Solid State Physics, 1982, 89, 313-315.	2.1	2
77	Infrared band intensities: a comparative study of the transition moment matrix elements for fundamentals and overtones. Journal of Molecular Structure, 1981, 74, 49-64.	3.6	19
78	INTRAMOLECULAR OHÂ·Â·Â·S HYDROGEN BONDS AND MOLECULAR CONFORMATIONS IN 2-METHYLMERCAPTOETHANOL. Phosphorous and Sulfur and the Related Elements, 1979, 6, 177-178.	0.2	0
79	Infrared band intensities and polar tensors: Properties of effective charge Î¾Î± and its relation to the sign of dipole moment derivatives. Journal of Chemical Physics, 1977, 66, 1621-1630.	3.0	19
80	Infrared intensities: A comprehensive quantitative analysis for transition metal carbonyls M(CO)6 (M=Cr, Mo, and W) and Ni(CO)4. Journal of Chemical Physics, 1977, 67, 4384-4397.	3.0	12
81	Calculation of electro-optical parameters: A new approach. Chemical Physics Letters, 1975, 31, 535-538.	2.6	6
82	Crossover scaling function for exchange anisotropy: Heisenberg toXY-like crossover. Physical Review B, 1975, 12, 493-497.	3.2	21
83	Crossover scaling functions for exchange anisotropy:XÂYand planar models. Physical Review B, 1975, 11, 3445-3456.	3.2	30
84	Electronic and infrared spectral band shifts in binary solvent mixtures. Spectrochimica Acta Part A: Molecular Spectroscopy, 1974, 30, 285-293.	0.1	4
85	Electronic spectral intensities in binary solvent mixtures. Spectrochimica Acta Part A: Molecular Spectroscopy, 1973, 29, 981-996.	0.1	11
86	Spectroscopic studies of hydrogen bonding in donor-acceptor systems. Transactions of the Faraday Society, 1966, 62, 1056.	0.9	88
87	DEUTERIUM ISOTOPE EFFECTS ON HYDROGEN BONDING. Canadian Journal of Chemistry, 1966, 44, 2611-2615.	1.1	35