Oktay Sinanoglu

List of Publications by Year
in descending order

111 papers	4,153 citations	126907 33 h-index	123424 61 g-index
114 all docs	114 docs citations	114 times ranked	752 citing authors

#	Article	IF	Citations
1	Comparison of doubly-excited helium energy levels, isoelectronic series, autoionization lifetimes, and group-theoretical configuration-mixing predictions with large-configuration-interaction calculations and experimental spectra. Physical Review A, 1975, 11, 97-110.	2.5	433
2	Theory of Atomic Structure Including Electron Correlation. I. Three Kinds of Correlation in Ground and Excited Configurations. Physical Review, 1969, 181, 42-53.	2.7	209
3	Many-Electron Theory of Atoms, Molecules and Their Interactions. Advances in Chemical Physics, 2007, , 315-412.	0.3	208
4	Interactions between Molecules Adsorbed on a Surface. Journal of Chemical Physics, 1960, 32, 1279-1288.	3.0	204
5	Manyâ€Electron Theory of Nonclosedâ€Shell Atoms and Molecules. I. Orbital Wavefunction and Perturbation Theory. Journal of Chemical Physics, 1966, 44, 1899-1907.	3.0	199
6	Manyâ€Electron Theory of Atoms and Molecules. II. Journal of Chemical Physics, 1962, 36, 3198-3208.	3.0	194
7	Group theoretic prediction of configuration mixing effects due to Coulomb repulsions in atoms with applications to doublyâ€excited spectra. Journal of Chemical Physics, 1975, 62, 886-892.	3.0	152
8	Theory of Atomic Structure Including Electron Correlation. III. Calculations of Multiplet Oscillator Strengths and Comparisons with Experiments for CII, NI, NII, NIII, OII, OIII, OIV, FII, NeII, and NaIII. Physical Review, 1969, 183, 56-68.	2.7	121
9	Theory of Atomic Structure Including Electron Correlation. II. All-External Pair Correlations in the Various States and Ions of B, C, N, O, F, Ne, and Na, and Prediction of Electron Affinities and Atomic Excitation Energies. Physical Review, 1969, 181, 54-65.	2.7	112
10	Manyâ€Electron Theory of Nonclosedâ€Shell Atoms and Molecules. II. Variational Theory. Journal of Chemical Physics, 1966, 44, 3608-3617.	3.0	100
11	Semiempirical Method for the Determination of Localized Orbitals in Molecules. Journal of Chemical Physics, 1968, 49, 65-71.	3.0	91
12	Microscopic surface tension down to molecular dimensions and microthermodynamic surface areas of molecules or clusters. Journal of Chemical Physics, 1981, 75, 463-468.	3.0	91
13	Theory of Atomic Structure Including Electron Correlation. IV. Method for Forbidden-Transition Probabilities with Results for [O I], [O II], [O III], [N I], [N II], and [C I].. Physical Review A, 1971, 4, 1400-1410.	2.5	85
14	Interâ€•and Intraâ€Atomic Correlation Energies and Theory of Coreâ€Polarization. Journal of Chemical Physics, 1960, 33, 1212-1226.	3.0	81
15	Perturbation Theory of Many-Electron Atoms and Molecules. Physical Review, 1961, 122, 493-499.	2.7	75
16	Theory of Atomic Structure Including Electron Correlation. Physical Review Letters, 1968, 21, 507-511.	7.8	73
17	Manyâ€Electron Theory of Atoms and Molecules. III. Effect of Correlation on Orbitals. Journal of Chemical Physics, 1963, 38, 1740-1748.	3.0	71
18	Effective Intermolecular Pair Potentials in Nonpolar Media. Journal of Chemical Physics, 1963, 38, 1730-1739.	3.0	71

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19	Beam-foil spectroscopy and new atomic structure theory with a survey of results since 1970. Nuclear Instruments & Methods, 1973, 110, 193-209.	1.2	69
20	Electron Correlation in Atoms and Molecules. Advances in Chemical Physics, 2007, , 237-282.	0.3	63
21	Intermolecular Forces in Liquids. Advances in Chemical Physics, 2007, , 283-326.	0.3	62
22	Intermolecularâ€Potentialâ€Energy Curvesâ€”Theory and Calculations on the Heliumâ€”Helium Potential. Journal of Chemical Physics, 1966, 45, 194-207.	3.0	61
23	Sigma and Pi Changes in Valence States of Piâ€Electron Theory and Oneâ€Center Coulomb Repulsion Parameters. Journal of Chemical Physics, 1965, 43, 49-58.	3.0	60
24	Theory of chemical reaction networks. All possible mechanisms or synthetic pathways with given number of reaction steps or species. Journal of the American Chemical Society, 1975, 97, 2309-2320.	13.7	52
25	Variation-Perturbation Method for Excited States. Physical Review, 1961, 122, 491-492.	2.7	50
26	An intermolecular potential for use in liquids. Chemical Physics Letters, 1967, 1, 340-342.	2.6	50
27	The solvophobic theory for the prediction of molecular conformations and biopolymer bindings in solutions with recent direct experimental tests. International Journal of Quantum Chemistry, 1980, 18, 381-392.	2.0	50
28	Theoretical Transition Probabilities. Journal of Chemical Physics, 1966, 44, 1888-1898.	3.0	47
29	Resonance Transition Probabilities for Third-Row Atoms and Ions (Mgi, Siii-iii, Pii, Piv, Sii-iii, Cliii) Including the Important Correlation Effects. Physical Review Letters, 1972, 28, 945-948.	7.8	45
30	Estimation of binding energies of molecules by a semiempirical molecular orbital electron correlation method with applications to saturated and unsaturated hydrocarbons, aromatics, and heterocyclics. Journal of the American Chemical Society, 1973, 95, 5435-5442.	13.7	45
31	Ligandâ€Field Theory of Linear Gaseous Molecules Involving the First Transition Series Elements. Journal of Chemical Physics, 1960, 32, 1082-1087.	3.0	42
32	Relation of Perturbation Theory to Variation Method. Journal of Chemical Physics, 1961, 34, 1237-1240.	3.0	41
33	A Method for the Analysis of Many-Electron Wave Functions. Reviews of Modern Physics, 1963, 35, 517-519.	45.6	40
34	The C-potential surface for predicting conformations of molecules in solution. Theoretica Chimica Acta, 1974, 33, 279-284.	0.8	39
35	What size cluster is like a surface?. Chemical Physics Letters, 1981, 81, 188-190.	2.6	39
36	The GroupR4in Atomic-Structure Theory: The HydrogenicR4versus the MathematicalR4and the Coulomb Interaction in2sm2pnand3sm3pn3drConfigurations. Physical Review, 1969, 177, 77-85.	2.7	32

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37	Bonds and Intramolecular Forces. Journal of Chemical Physics, 1962, 37, 191-192.	3.0	27
38	Oscillator strengths for transitions involving excited states not lowest of their symmetry oxygen I and oxygen II transitions. Journal of Chemical Physics, 1976, 64, 1495-1497.	3.0	26
39	The denaturation maxima of proteins and of drug-biomolecule complex formation in a wide range of methanol/water mixtures. Biophysical Chemistry, 1985, 21, 157-162.	2.8	24
40	Theory of atomic structures including electron correlation. V. Excited states not lowest of their symmetry and oscillator strengths in neutral and singly ionized atoms. Physical Review A, 1976, 13, 1293-1306.	2.5	22
41	Algebra of the Noncompact GroupO(3,Â2)and the Hydrogen-Atom Radial Functions. Physical Review A, 1972, 5, 2309-2313.	2.5	21
42	Correlations between tetrahedrally localized orbitals. Chemical Physics Letters, 1968, 1, 699-702.	2.6	20
43	Denaturation of proteins in methanol/water mixtures. Biophysical Chemistry, 1985, 21, 163-166.	2.8	20
44	A theorem for qualitative deductions in organic or inorganic chemistry regarding the relative stabilities, distortions and reactions of molecules. Chemical Physics Letters, 1984, 103, 315-322.	2.6	19
45	Structural covariance of graphs. Theoretica Chimica Acta, 1984, 65, 255-265.	0.8	19
46	1â€•and 2â€topology of reaction networks. Journal of Mathematical Physics, 1981, 22, 1504-1512.	1.1	18
47	HFS constants of Be I 1s22s2p 3p0, B I 1s22s2p24P and B I 1s22s2p22D obtained from the non-closed shell many-electron theory for excited states. Chemical Physics Letters, 1973, 20, 221-224.	2.6	17
48	Non-closed-shell many-electron-theory atomic charge wavefunctions. Atomic Data and Nuclear Data Tables, 1976, 18, 525-585.	2.4	17
49	SOME ASPECTS OF THE QUANTUM THEORY OF ATOMS, MOLECULES, AND THEIR INTERACTIONS. The Journal of Physical Chemistry, 1962, 66, 2283-2287.	2.9	16
50	Correlation effects in the neutral and ionized ground states of acetylene. Theoretica Chimica Acta, 1973, 30, 177-190.	0.8	16
51	Prediction of molecular excited state properties, potential energy curves, and the non-closed shell many-electron theory. Journal of Molecular Structure, 1973, 19, 81-91.	3.6	16
52	New theoretical transition probabilities for the Si I 3s23p23pP â€" 3s3p33D0 isoelectronic sequence including the important correlation effects. Chemical Physics Letters, 1974, 24, 20-21.	2.6	16
53	Multiplet generalized oscillator strengths and inelastic scattering cross sections calculated including the electron correlation effects: Transitions of neutral atoms: Be, B, C, N, and O. Journal of Chemical Physics, 1975, 62, 3664.	3.0	16
54	Nontransferable Correlation Effects and Multiplet Oscillator Strengths for Electric Dipole Transitions in Atoms with Results on C ii, N i, N ii, N III, O ii, O III, O iv, F ii, and NE II. Astrophysical Journal, 1969, 157, 997.	4.5	16

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55	New method for qualitative quantum chemical deductions on organic or inorganic molecules or clusters directly from structural formulas or ORTEP diagrams. Theoretica Chimica Acta, 1985, 68, 251-270.	0.8	15
56	Core Polarization in Li2. Journal of Chemical Physics, 1961, 34, 1078-1079.	3.0	14
57	Electron correlation in excited states and term splittings in the carbonâ€‹ isoelectronic sequence. Journal of Chemical Physics, 1974, 61, 3670-3675.	3.0	14
58	The large effects of electron correlation on the multiplet generalized oscillator strengths of non-closed shell systems: Be 1s22s21S â†' 1s22s2p 1P0 and B 1s22s22p 2p0 â†' 1s22s2p22D. Chemical Physics Letters, 1975, 32, 449-454.	2.6	14
59	Finding all possiblea priori mechanisms for a given type of overall reaction. Theoretica Chimica Acta, 1978, 48, 287-299.	0.8	14
60	Symmetry-breaking instabilities under nonclassical bifurcation conditions. Physical Review A, 1984, 29, 2029-2032.	2.5	14
61	Symmetry Properties of Oneâ€•and Twoâ€Electron Correlation Functions in the Manyâ€Electron Theory of Atoms and Molecules. Journal of Chemical Physics, 1967, 46, 854-859.	3.0	13
62	A principle of linear covariance for quantum mechanics and the electronic structure theory of molecules and other atom clusters. Theoretica Chimica Acta, 1984, 65, 233-242.	0.8	13
63	Electronic quadrupole moments of excited states and the charge wavefunction of the many-electron theory. Chemical Physics Letters, 1973, 21, 247-250.	2.6	12
64	Locally attractive normal modes for chemical process. Journal of Mathematical Physics, 1984, 25, 2576-2581.	1.1	12
65	Solvophobic forces and molecular surface area changes in drug-biomolecule associations as with actinomycin-deoxyguanosine in a wide range of methanol/water mixtures. Biophysical Chemistry, 1985, 21, 167-171.	2.8	12
66	Theoretical Preâ€Exponential Rate Factors for Abstraction Reactions. Journal of Chemical Physics, 1959, 30, 422-427.	3.0	11
67	Mediumâ€Dependent Intermolecular Potential for Liquids and Its Use in Obtaining Free Energy and Entropy. Journal of Chemical Physics, 1968, 49, 996-1000.	3.0	11
68	Relativistic effects in transitions of highly ionized heavy atoms. Chemical Physics Letters, 1973, 20, 407-410.	2.6	11
69	Directed graphs of structurally stable potential energy surfaces representing a-priori reaction pathways. Theoretica Chimica Acta, 1984, 65, 179-190.	0.8	11
70	Ten classes of bicyclo[p.q.0]pi-hydrocarbons, and their anions and cations. Electronic rules directly from structural formulas. Tetrahedron Letters, 1988, 29, 889-892.	1.4	11
71	Predicted lifetimes, oscillator strengths, and wavelengths of highly ionized manyâ€electron heavy atoms (P XI to Sn XLVI), with both relativistic and correlation effects. Journal of Chemical Physics, 1976, 64, 4197-4204.	3.0	10
72	Conditions for the validity of Ginzburg-Landau equations in far-from-equilibrium kinetics. Physical Review A, 1984, 30, 1522-1524.	2.5	10

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73	Quantum Numbers and Masses of Mesons as Quark-Antiquark Systems. Physical Review Letters, 1966, 16, 207-210.	7.8	9
74	Meson Spectrum, Mass Formula, and the Quark-Antiquark Interaction. Physical Review, 1966, 145, 1205-1211.	2.7	9
75	Global attractors and global stability for closed chemical systems. Journal of Mathematical Physics, 1984, 25, 406-409.	1.1	9
76	Upper and lower bounds and the generalized variation-perturbation approach of many-electron theory. International Journal of Quantum Chemistry, 1968, 2, 397-403.	2.0	7
77	Finding the possible mechanisms for a given type of overall reaction. Theoretica Chimica Acta, 1979, 51, 1-9.	0.8	7
78	Reaction Mechanisms and Chemical Networks â€" Types of Elementary Steps and Generation of Laminar Mechanisms*. Zeitschrift Fur Physikalische Chemie, 1981, 125, 129-160.	2.8	7
79	On the algebraic construction of chemistry from quantum mechanics. A fundamental valency vector field defined on the euclidean 3-space and its relation to the Hilbert space. Theoretica Chimica Acta, 1984, 65, 243-248.	0.8	7
80	Theoretical Oscillator Strengths of Neutral, Singly-Ionized, and Multiply-Ionized Atoms. Topics in Current Physics, 1976, , 111-146.	0.5	7
81	Theory of Intravalency and Rydberg Transitions in Molecules. , 1974, , 337-384.		7
82	The structural stability restriction rules out certain frontside S N 2 pathways. Theoretica Chimica Acta, 1984, 66, 147-149.	0.8	6
83	Crucial role of electron correlation in both the upper and lower states in optical transitions. Theoretica Chimica Acta, 1974, 34, 183-187.	0.8	5
84	Non-unitary classification of molecular electronic structures and other atom clusters. Theoretica Chimica Acta, 1984, 65, 249-254.	0.8	5
85	Subordination of the fast-relaxing degree of freedom in the center manifold of the Belousov-Zhabotinsky system. Physical Review A, 1985, 31, 2736-2737.	2.5	5
86	Expansion of the Density Matrix of an Nâ€Fermion System in Terms of the Correlation Densities of Fermion Clusters. Journal of Mathematical Physics, 1969, 10, 1032-1037.	1.1	4
87	A proposed correction to the solar abundances of carbon and oxygen utilizing new and accurate theoretical forbidden transition probabilities. Solar Physics, 1973, 29, 17-22.	2.5	4
88	Autocatalytic and other general networks for chemical mechanisms, pathways, and cycles: Their systematic and topological generation. Journal of Mathematical Chemistry, 1993, 12, 319-363.	1.5	4
89	Spin-free wave functions in many-electron perturbation theory. I. Closed-shell systems. International Journal of Quantum Chemistry, 1973, 7, 1145-1158.	2.0	3
90	Deformational covariance of graphs. Theoretica Chimica Acta, 1984, 65, 267-270.	0.8	3

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91	The new pictorial structural covariance method for qualitative quantum chemistry. II: Arenes with or without polyene side chains and polyene bridges. Journal of Mathematical Chemistry, 1988, 2, 117-136.	1.5	3
92	Intermolecular Forces in Liquids: Comparison of the Analytic Effective Potential with Computer Calculations of the Many-Body Effects. Physical Review A, 1972, 5, 2223-2229.	2.5	2
93	Spin-free wave functions in many-electron perturbation theory. II. Systems with one nonclosed shell. International Journal of Quantum Chemistry, 1973, 7, 1159-1174.	2.0	2
94	The new pictorial structural covariance method for qualitative quantum chemistry. III: Fused polycyclics and their ions. Journal of Mathematical Chemistry, 1988, 2, 137-154.	1.5	2
95	Are oxygen rings (On) and their negative ions (On?) unstable?. International Journal of Quantum Chemistry, 1989, 36, 545-552.	2.0	2
96	Charge densities and transition densities from the theory of non-closed-shell states and their experimental tests. International Journal of Quantum Chemistry, 2009, 9, 155-164.	2.0	2
97	Reply to "Comment on `Theory of atomic structures including electron correlation. V.'". Physical Review A, 1978, 18, 1313-1317.	2.5	1
98	Spatial-temporal dissipative structures arising in open reactive systems with a negative feedback loop. BioSystems, 1984, 17, 3-9.	2.0	1
99	Hamiltonian as a Hessian on the Hibert space, eigenvectors as critical points, and their relation to topological invariants in the variation method. Theoretica Chimica Acta, 1984, 65, 271-278.	0.8	1
100	Topological electronic rules for polycyclic hydrocarbons?quantum chemical deductions directly from structural formulas. International Journal of Quantum Chemistry, 1988, 34, 143-147.	2.0	1
101	Dyad algebra and multiplication of graphs. I. Directed graphs. Journal of Mathematical Chemistry, 1993, 14, 185-194.	1.5	1
102	On the agreement between dipole length and dipole velocity calculated oscillator strengths. International Journal of Quantum Chemistry, 1973, 7, 65-67.	2.0	1
103	A Reactive System with Diffusive Transport Displaying Two Different Symmetry-Breaking Dissipative Structures. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1985, 40, 611-618.	1.5	1
104	The metric geometry of near equilibrium irreversible thermodynamics. Journal of Chemical Physics, 1980, 72, 3127-3129.	3.0	0
105	The lifting of an Ä°nÃ¶nÃ¼â€“Wigner contraction at the level of universal coverings. Journal of Mathematical Physics, 1982, 23, 2234-2235.	1.1	0
106	Nonorthogonality and theMO energy level patterns of molecules deduced directly from structural formulas by the newVIF method as compared with machine computations. International Journal of Quantum Chemistry, 1992, 44, 137-151.	2.0	0
107	Dyad algebra and multiplication of graphs. II. Undirected graphs. Journal of Mathematical Chemistry, 1993, 14, 195-205.	1.5	0
108	Interactions between Molecules Adsorbed on a Surface. World Scientific Series in 20th Century Chemistry, 1993, , 493-502.	0.0	0

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109	A Principal of Linear Covariance for Quantum Mechanics and Its Consequences Taking one Beyond Symmetry. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1997, 52, 46-48.	1.5	0
110	Remarks on dynamical and noncompact groups in physics and chemistry. International Journal of Quantum Chemistry, 1973, 7, 45-52.	2.0	0
111	Recent CI methods for the calculation of pair correlations and more-electron clusters in ground-state atoms. International Journal of Quantum Chemistry, 2009, 7, 57-63.	2.0	0