Ersin Yurtsever

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/2034007/publications.pdf

Version: 2024-02-01

168 papers	2,282 citations	304368 22 h-index	288905 40 g-index
170 all docs	170 docs citations	170 times ranked	1978 citing authors

#	Article	IF	Citations
1	HeH⁺ Collisions with H₂: Rotationally Inelastic Cross Sections and Rate Coefficients from Quantum Dynamics at Interstellar Temperatures. Journal of Physical Chemistry A, 2022, 126, 2244-2261.	1.1	11
2	Dimerization dynamics of carboxylic acids in helium nanodroplets. Journal of Chemical Physics, 2022, 156, 174304.	1.2	2
3	Collision-driven state-changing efficiency of different buffer gases in cold traps: He(¹S), Ar(¹S) and p-H₂(¹Î£) on trapped CN^{â¯}(¹Î£). Physical Chemistry Chemical Physics, 2021, 23, 7703-7713.	1.3	8
4	The metastable structures of anthracene-argon clusters inside helium nanodroplets. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	2
5	Vibrational quenching of CNâ¯ in collisions with He and Ar. Journal of Chemical Physics, 2021, 154, 084305.	1.2	5
6	Energy-transfer quantum dynamics of HeH+ with He atoms: Rotationally inelastic cross sections and rate coefficients. Journal of Chemical Physics, 2021, 154, 054311.	1.2	10
7	The structure of 1,3-butadiene clusters. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	0
8	Dynamics of HeHHe⁺ Rotational State Changes Induced by Collision with He: A Possible New Path in Early Universe Chemistry. Journal of Physical Chemistry A, 2021, 125, 3748-3759.	1.1	4
9	Efficiency of rovibrational cooling of HeH+ by collisions with He: Cross sections and rate coefficients from quantum dynamics. Journal of Chemical Physics, 2021, 155, 154301.	1.2	2
10	Rotationally inelastic processes of ${{m{C}}}_{2}^{-}$ (${}^{2}{{m{Sigma }}}_{g}^{+}$) colliding with He (1 S) at low temperatures: ab initio interaction potential, state changing rates and kinetic modelling. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 025201.	0.6	7
11	Solvation of coronene oligomers by para-H₂ molecules: the effects of size and shape. Physical Chemistry Chemical Physics, 2020, 22, 12465-12475.	1.3	3
12	Rovibrational quenching of C2â¯ anions in collisions with He, Ne, and Ar atoms. Physical Review A, 2020, 102, .	1.0	10
13	Thermalisation of C2â¯ with noble gases in cold ion traps. International Journal of Mass Spectrometry, 2020, 457, 116426.	0.7	6
14	On the Formation of Interstellar CH^{â€“} Anions: Exploring Mechanism and Rates for CH₂ Reacting with H^{â€“}. Journal of Physical Chemistry A, 2020, 124, 5098-5108.	1.1	7
15	Rotational-state-changing collisions between <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msubsup><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:msubsup></mml:math> and Rb at low energies. Physical Review A, 2020, 101, .	1.0	7
16	Modeling Ionic Reactions at Interstellar Temperatures: The Case of NH₂^{â€“} + H₂ â‡” NH₃ + H^{â€“}. Journal of Physical Chemistry A, 2019, 123, 9905-9918.	1.1	9
17	Energy Landscapes in Photochemical Dissociation of Small Peroxides. Journal of Physical Chemistry A, 2019, 123, 1353-1362.	1.1	5
18	N2+(2Î£g) and Rb(2S) in a hybrid trap: modeling ion losses from radiative association paths. Physical Chemistry Chemical Physics, 2019, 21, 8342-8351.	1.3	3

#	Article	IF	Citations
19	Quantum Chemical View on the Growth Mechanisms of Odd-Sized Nitrogen Cluster Anions. Journal of Physical Chemistry A, 2019, 123, 202-209.	1.1	6
20	Physisorption of H₂ on Fullerenes and the Solvation of C₆₀ by Hydrogen Clusters at Finite Temperature: A Theoretical Assessment. Journal of Physical Chemistry A, 2018, 122, 2792-2800.	1.1	7
21	Discovery of an Exceptionally Strong Luminescence of Polyethyleneimineâ€Superparamagnetic Iron Oxide Nanoparticles. Macromolecular Chemistry and Physics, 2018, 219, 1700563.	1.1	8
22	Isomeric Broadening of C₆₀⁺ Electronic Excitation in Helium Droplets: Experiments Meet Theory. Journal of Physical Chemistry Letters, 2018, 9, 1237-1242.	2.1	26
23	Evidence for reverse core-shell phase separation in mixed parahydrogen/orthodeuterium clusters with an ionic impurity. Chemical Physics Letters, 2018, 692, 416-420.	1.2	1
24	The quantum structure of anionic hydrogen clusters. Journal of Chemical Physics, 2018, 148, 102305.	1.2	12
25	NH2â^' in a cold ion trap with He buffer gas:Ab initioquantum modeling of the interaction potential and of state-changing multichannel dynamics. Journal of Chemical Physics, 2018, 148, 184305.	1.2	4
26	Collisional relaxation kinetics fororthoandparaNH2â^'under photodetachment in cold ion traps. Faraday Discussions, 2018, 212, 117-135.	1.6	11
27	Coating of $$hbox {C}_{60}$$ C 60 by para- $$hbox {H}_2$$ H 2. Journal of Mathematical Chemistry, 2017, 55, 1370-1375.	0.7	0
28	Formation of Anionic C, N-bearing Chains in the Interstellar Medium via Reactions of H^{â^'} with HC_xN for Odd-valued x from 1 to 7. Astrophysical Journal, 2017, 850, 42.	1.6	8
29	Possible Formation of Metastable PAH Dimers upon Pickup by Helium Droplets. Journal of Physical Chemistry A, 2016, 120, 1727-1736.	1.1	12
30	Solvation of carbonaceous molecules by para-H2 and ortho-D2 clusters. I. Polycyclic aromatic hydrocarbons. Journal of Chemical Physics, 2016, 144, 224302.	1.2	12
31	Solvation of carbonaceous molecules by para-H2 and ortho-D2 clusters. II. Fullerenes. Journal of Chemical Physics, 2016, 145, 084304.	1.2	4
32	A postâ€<scp>HF</scp> study on the halogen bonding interaction of pyrene with diatomic halogen molecules. International Journal of Quantum Chemistry, 2016, 116, 702-709.	1.0	2
33	Exploring a dynamical path for C2Hâ^' and NCOâ^' formation in dark molecular clouds. European Physical Journal D, 2016, 70, 1.	0.6	3
34	Forming NCO^{â€“} in Dense Molecular Clouds: Possible Gas-Phase Chemical Paths From Quantum Calculations. Journal of Physical Chemistry A, 2016, 120, 4693-4701.	1.1	3
35	A mixed basis with off-center Gaussian functions for the calculation of the potential energy surfaces for Ï€-stacking interactions: dimers of benzene and planar C6. Journal of Molecular Modeling, 2015, 21, 11.	0.8	4
36	Dimer formation of perylene: An ultracold spectroscopic and computational study. Journal of Molecular Structure, 2015, 1097, 29-36.	1.8	14

#	Article	IF	Citations
37	Evidence for broken ergodicity due to chemical alloying from the dissociation kinetics of binary clusters. Journal of Chemical Physics, 2014, 140, 214301.	1.2	2
38	A post-HF study on the interaction of iodine with small polyaromatic hydrocarbons. Journal of Molecular Modeling, 2014, 20, 2445.	0.8	7
39	Understanding the influence of hydrogen bonding and diisocyanate symmetry on the morphology and properties of segmented polyurethanes and polyureas: Computational and experimental study. Polymer, 2014, 55, 4563-4576.	1.8	120
40	Mapping the global minima of binary Morse clusters: The effects of range mismatch. Computational and Theoretical Chemistry, 2013, 1021, 7-15.	1.1	6
41	Mg+(2S) and Mg+(2P) in reaction with H2(): A description of the energy surfaces explaining the mechanisms. International Journal of Mass Spectrometry, 2013, 351, 47-55.	0.7	8
42	Weakly bound finite systems: (4He)Nâ€“Rb2(3Î£u), clustering structures from a quantum Monte Carlo approach. Journal of Physics Condensed Matter, 2012, 24, 104014.	0.7	4
43	Spin-Polarized Rb₂ Interacting with Bosonic He Atoms: Potential Energy Surface and Quantum Structures of Small Clusters. Journal of Physical Chemistry A, 2012, 116, 2394-2404.	1.1	19
44	Energy landscapes of ion clusters in isotropic quadrupolar and octupolar traps. Journal of Chemical Physics, 2012, 136, 024303.	1.2	1
45	Multiscale Modeling of the Morphology and Properties of Segmented Silicone-Urea Copolymers. Journal of Inorganic and Organometallic Polymers and Materials, 2012, 22, 604-616.	1.9	22
46	Quenching vibrations by collisions in cold traps: A quantum study for MgHâ€‰+â€‰ (X 1Î£â€‰+â€‰) with 4He(1S) #. Journal of Chemical Sciences, 2012, 124, 93-97.	0.7	6
47	Quantum Features of a Barely Bound Molecular Dopant: Cs₂(³Î£_u) in Bosonic Helium Droplets of Variable Size. Journal of Physical Chemistry A, 2011, 115, 6892-6902.	1.1	19
48	Quenching vibrations of cesium dimers by He at low and ultralow temperatures: quantum dynamical calculations. European Physical Journal D, 2011, 65, 167-175.	0.6	2
49	Cooling and quenching ofMg24H+(Xâ€‰1Î£+) byHe4(1S) in a Coulomb trap: A quantum study of the dynamics. Physical Review A, 2011, 84, .	1.0	6
50	Structure and dynamics of ion clusters in linear octupole traps: Phase diagrams, chirality, and melting mechanisms. Physical Review A, 2011, 83, .	1.0	5
51	Stacking of triphenylene: characterization of the potential energy surface. Theoretical Chemistry Accounts, 2010, 127, 133-139.	0.5	10
52	Reduction of Viscosity of Alumina Nanopowder Aqueous Suspensions by the Addition of Polyalcohols and Saccharides. Journal of the American Ceramic Society, 2010, 93, 2630-2636.	1.9	13
53	Quenching of internal rotations versus collisional cooling at ultralow energies for weakly interacting partners: Cs<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo		

#	Article	IF	Citations
55	Crystallization of ion clouds in octupole traps: Structural transitions, core melting, and scaling laws. Physical Review A, 2009, 80, .	1.0	17
56	Structuring a Quantum Solvent around a Weakly Bound Dopant: The Heâ‘Cs₂(³Î£_u) Complex. Journal of Physical Chemistry A, 2009, 113, 14718-14729.	1.1	23
57	Ï€-Stack Dimers of Small Polyaromatic Hydrocarbons: A Path to the Packing of Graphenes. Journal of Physical Chemistry A, 2009, 113, 924-930.	1.1	24
58	Emergence of 2MPA as an Effective Coating for Highly Stable and Luminescent Quantum Dots. Journal of Physical Chemistry C, 2009, 113, 10005-10012.	1.5	38
59	Shell Structure, Melting and Dynamics of Ion Clusters Confined in an Octupolar Trap. , 2009, , .		1
60	Energetics and Structures of Charged Helium Clusters: Comparing Stabilities of Dimer and Trimer Cationic Cores. ChemPhysChem, 2008, 9, 2618-2624.	1.0	11
61	Quenching efficiency of â€œhot" polar molecules by He buffer gas at ultralow energies: quantum results for MgH and LiH rotations. European Physical Journal D, 2008, 48, 75-82.	0.6	7
62	Effects of the range of the potential on the structure and dynamics of two-dimensional Coulomb clusters. Molecular Physics, 2008, 106, 289-298.	0.8	7
63	Vibrational cooling of spin-stretched dimer states by He buffer gas: Quantum calculations for Li2(aÎ£u+3) at ultralow energies. Journal of Chemical Physics, 2008, 128, 224312.	1.2	13
64	QUANTUM STRUCTURING OF 4He ATOMS AROUND IONIC DOPANTS: ENERGETICS OF Li+, Na+ AND K+ FROM STOCHASTIC CALCULATIONS. , 2008, , 227-240.		1
65	Bosonic helium droplets with cationic impurities: Onset of electrostriction and snowball effects from quantum calculations. Journal of Chemical Physics, 2007, 126, 124319.	1.2	51
66	Structural and thermodynamical studies of 2D Coulomb clusters with point defects. Physica Scripta, 2007, 76, C111-C114.	1.2	2
67	Solvation of K+ in helium droplets. European Physical Journal D, 2007, 43, 105-108.	0.6	6
68	Non-monotonic size effects on the structure and thermodynamics of Coulomb clusters in three-dimensional harmonic traps. European Physical Journal D, 2007, 44, 81-91.	0.6	17
69	Bosonic helium clusters doped by alkali metal cations: interaction forces and analysis of their most stable structures. Theoretical Chemistry Accounts, 2007, 118, 53-65.	0.5	30
70	Quantum Mechanical Calculations of Tryptophan and Comparison with Conformations in Native Proteins. Journal of Physical Chemistry A, 2006, 110, 13933-13938.	1.1	7
71	Invariant energy partitions in chemical reactions and cluster dynamics simulations. Computational Materials Science, 2006, 35, 187-191.	1.4	29
72	Fragmentation dynamics of <mml:math altimg="si2.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.com/x	1.4	2

#	Article	IF	Citations
73	Specific heats of clusters near a phase transition: Energy partitions among internal modes. Chemical Physics Letters, 2006, 430, 424-428.	1.2	25
74	The entry of molecular species into the lattice of an electroactive polymer during its dissolution. Journal of Molecular Liquids, 2006, 124, 106-113.	2.3	5
75	Vibrational quenching at ultralow energies: Calculations of theLi2(Î£g+1;Î½â³¢0)+Hesuperelastic scattering cross sections. Physical Review A, 2006, 73, .	1.0	20
76	Ionic dimers in He droplets: Interaction potentials for Li2+â€“He,Na2+â€“He, and K2+â€“He and stability of the smaller clusters. Journal of Chemical Physics, 2006, 124, 074320.	1.2	20
77	The Weak Li2 ? He Interaction Revisited: a Combined Ab-initio and Empirical Modelling.. Journal of Low Temperature Physics, 2005, 138, 259-264.	0.6	23
78	Neutral and ionic dopants in helium clusters: interaction forces for the and complexes. Molecular Physics, 2005, 103, 3223-3231.	0.8	14
79	Finite-size effects in the dynamics and thermodynamics of two-dimensional Coulomb clusters. Physical Review E, 2005, 72, 026110.	0.8	11
80	Publisher's Note: Phase-Space Invariants as Indicators of the Critical Behavior of Nanoaggregates [Phys. Rev. Lett.93, 113402 (2004)]. Physical Review Letters, 2004, 93, .	2.9	0
81	Ab initio quantum dynamics with very weak van der Waals interactions: Structure and stability of small Li2(1Î£g+)â€“(He)n clusters. Journal of Chemical Physics, 2004, 120, 9160-9166.	1.2	25
82	Composition-induced structural transitions in mixed rare-gas clusters. Physical Review B, 2004, 70, .	1.1	54
83	Phase-Space Invariants as Indicators of the Critical Behavior of Nanoaggregates. Physical Review Letters, 2004, 93, 113402.	2.9	31
84	Density functional theory study of the electrochemical oligomerization of thiophene: transition states for radicalâ€“radical and radicalâ€“neutral pathways. Polymer, 2004, 45, 9039-9045.	1.8	5
85	Rotational cooling of Li2(1?g+) molecules by ultracold collisions with a helium gas buffer. Theoretical Chemistry Accounts, 2004, 112, 263.	0.5	13
86	Influence of lithium chloride on the morphology of flexible slabstock polyurethane foams and their plaque counterparts. Polymer, 2003, 44, 757-768.	1.8	16
87	Finding the global minima of clusters with non-empirical models: a comparison of results. Chemical Physics, 2003, 290, 279-295.	0.9	6
88	Vibrational spectroscopy of structural defects in oligothiophenes. Molecular Physics, 2003, 101, 2725-2729.	0.8	1
89	Conformational Similarities in Isomerization Dynamics of Clusters. Journal of Physical Chemistry A, 2003, 107, 6025-6031.	1.1	1
90	Rotational potential functions for oligomethylthiophenes. Synthetic Metals, 2003, 135-136, 427-428.	2.1	4

#	Article	IF	Citations
91	Exploring Urea Phase Connectivity in Molded Flexible Polyurethane Foam Formulations Using LiBr as a Probe. Journal of Macromolecular Science - Physics, 2003, 42, 1125-1139.	0.4	9
92	Conformational Analysis of Model Poly(ether urethane) Chains in the Unperturbed State and under External Forces. Macromolecules, 2002, 35, 9825-9831.	2.2	5
93	Thermochromism in Oligothiophenes:â€‰ The Role of the Internal Rotation. Journal of Physical Chemistry A, 2002, 106, 11981-11986.	1.1	11
94	Global view of classical clusters: the hyperspherical approach to structure and dynamics. Physical Chemistry Chemical Physics, 2002, 4, 5040-5051.	1.3	56
95	Modelling ionic nucleation in small neon clusters. International Journal of Mass Spectrometry, 2002, 220, 193-209.	0.7	12
96	A DFT study of polymerization mechanisms of indole. Polymer, 2002, 43, 6019-6025.	1.8	64
97	Hydrogen bonding and polyurethane morphology. II. Spectroscopic, thermal and crystallization behavior of polyether blends with 1,3-dimethylurea and a model urethane compound. Polymer, 2002, 43, 6561-6568.	1.8	102
98	Hydrogen bonding and polyurethane morphology. I. Quantum mechanical calculations of hydrogen bond energies and vibrational spectroscopy of model compounds. Polymer, 2002, 43, 6551-6559.	1.8	223
99	Measuring chaos in rotating clusters. Computer Physics Communications, 2002, 145, 194-202.	3.0	3
100	Turkey's output in social science publications: 1970-1999. Scientometrics, 2002, 55, 103-121.	1.6	17
101	A quantum mechanical study of the electrochemical polymerization of pyrrole. Synthetic Metals, 2001, 119, 227-228.	2.1	5
102	Electronic excitations in stacked oligothiophenes. Synthetic Metals, 2001, 119, 247-248.	2.1	1
103	Comparison of hydrogen bonding in polydimethylsiloxane and polyether based urethane and urea copolymers. Polymer, 2000, 41, 849-857.	1.8	226
104	Lyapunov instability in rotating systems from ergodic molecular dynamics simulations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2000, 266, 387-393.	0.9	3
105	Many-body effects on the melting and dynamics of small clusters. Physical Review B, 2000, 62, 9977-9980.	1.1	11
106	Rotationally induced transitions in small clusters. Physical Review E, 2000, 63, 016202.	0.8	4
107	Structural Defects in Polythiophenes:Â Monte Carlo Simulations with Quantum Mechanical Growth Probabilities. Journal of Physical Chemistry A, 2000, 104, 362-369.	1.1	6
108	The increase in the rate of publications originating from Turkey. Scientometrics, 1999, 46, 321-336.	1.6	16

#	Article	IF	Citations
109	Structural studies of polypyrroles. Synthetic Metals, 1999, 98, 221-227.	2.1	18
110	Structural studies of polypyrroles. Synthetic Metals, 1999, 98, 229-236.	2.1	20
111	A theoretical study of structural defects in conjugated polymers. Synthetic Metals, 1999, 101, 335-336.	2.1	13
112	Multiple bipolaron formation in oligothiophenes. Synthetic Metals, 1999, 105, 179-183.	2.1	11
113	Computational Studies of Cyclobutadiene and Benzocyclobutene Fused top- ando-Quinoneâ€. Journal of Physical Chemistry A, 1998, 102, 2351-2356.	1.1	21
114	Angular-momentum-driven chaos in small clusters. Physical Review A, 1998, 58, 377-382.	1.0	13
115	Chaos in rotating triatomic clusters. Europhysics Letters, 1997, 37, 91-96.	0.7	15
116	Chaotic behavior of triatomic clusters. Physical Review A, 1997, 55, 538-544.	1.0	17
117	A New Antiaromatic Compound:Â 1,4-Biphenylenequinone Synthesis and Trapping Reactions. Journal of Organic Chemistry, 1997, 62, 3434-3435.	1.7	6
118	Phase-space reconstruction in Hamiltonian systems through multiple time series. Chemical Physics Letters, 1997, 276, 282-288.	1.2	2
119	Structural studies of polythiophenes. Synthetic Metals, 1996, 78, 19-25.	2.1	26
120	On the possibility of grafting conducting polymers into insulating ones. Synthetic Metals, 1996, 81, 5-8.	2.1	9
121	Growth mechanisms of polypyrroles. Polymer, 1996, 37, 1151-1155.	1.8	12
122	Lyapunov exponents for classical-quantum mixed-mode dynamics. Physical Review E, 1996, 54, 4701-4707.	0.8	2
123	Mixed Mode Dynamics within the TDSCF Approximation. , 1995, , 393-406.		1
124	Quantal-classical mixed-mode dynamics and chaotic behavior. Physical Review E, 1994, 50, 3422-3430.	0.8	6
125	Hydrogen bonding in polyanilines. Synthetic Metals, 1994, 68, 57-60.	2.1	22
126	Hamiltonâ€Jacobi dynamics for the solution of time dependent quantum problems II. Wave packet propagation in two dimensional, nonlinearly coupled oscillators â€“ exact and timeâ€dependent SCFâ€solutionsâ€“. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 1552-1562.	0.9	6

#	Article	IF	Citations
127	Monte Carlo simulation studies of binary mixtures: A measure of the mixing. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 47-52.	0.9	2
128	Hamiltonâ€jacobi dynamics for the solution of time dependent quantum problems I. Formalism and wave packet propagation in one dimension. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 554-559.	0.9	3
129	Quantal-Classical Mixed mode Dynamics of Coupled Oscillators. NATO ASI Series Series B: Physics, 1994, , 315-320.	0.2	0
130	Structural studies of polypyrroles: oligomerization mechanism of N-methacryloyl pyrrole. Computational and Theoretical Chemistry, 1993, 280, 1-4.	1.5	7
131	Configurational properties of polypyrrole chains. Polymer, 1993, 34, 3887-3892.	1.8	8
132	Unimolecular dissociation in the regular regime. Journal of Chemical Physics, 1993, 99, 1135-1144.	1.2	1
133	Quantumâ€Classical Mixed Mode Analysis of Nonlinearly Coupled Oscillators: A Timeâ€Dependent Selfâ€Consistentâ€Field Approach. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1992, 96, 142-146.	0.9	7
134	The dynamics of a quantal reservoir coupled to classical modes: A mixedâ€mode approach to dissociating molecules. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1992, 96, 906-913.	0.9	4
135	Lattice polymers: behaviour far from Î¸-conditions. Polymer, 1992, 33, 2725-2728.	1.8	0
136	On the Stability of Microclusters with Threeâ€Body Forces. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1991, 95, 467-473.	0.9	1
137	Monte Carlo studies of binary mixtures: A fast algorithm for equilibration. Chemical Physics Letters, 1991, 187, 8-12.	1.2	4
138	Does Quantum Mechanics Select Out Regularity and Local Mode Behaviour in Nonlinearly Coupled Vibrational Systems?. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1990, 94, 804-827.	0.9	11
139	Multipoint Wronskian Method Applied on Model Potentials and Numerical Potential of Triplet H₂. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1990, 45, 889-892.	0.7	1
140	Regularity in nonlinearly coupled quantum oscillators far from the semiclassical limit. Physical Review A, 1990, 41, 6688-6691.	1.0	9
141	A New Equilibration Algorithm for Monte Carlo Simulations. Molecular Simulation, 1989, 2, 189-199.	0.9	2
142	Correlation of anodic peak potentials with the semi-empirical orbital and HOMO energies of various vinyl compounds. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1989, 261, 105-112.	0.3	12
143	Computationally induced â€˜â€˜irregularityâ€™â€™ in the spectra of integrable quantum systems. Physical Review A, 1988, 38, 1027-1035.	1.0	6
144	A Comparative Study of Variational Techniques for SchrÃ¶dinger Equations. Pointwise Quality Criteria. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1988, 43, 745-750.	0.7	0

#	Article	IF	Citations
145	Monte Carlo Simulation of Model Threeâ€€Component Liquid Systems. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1987, 91, 600-603.	0.9	4
146	Pair-excitationMCSCF treatment of small molecules in an optimized Slater-Transform-Preuss basis set. International Journal of Quantum Chemistry, 1987, 32, 551-562.	1.0	3
147	The least-squares stabilization method for resonance eigenvalues. Chemical Physics Letters, 1987, 137, 569-572.	1.2	0
148	Algebraic approaches to eigenvalue equations: The Wronskian method. Chemical Physics Letters, 1987, 141, 386-390.	1.2	0
149	Correlation of the anodic peak potentials with the quantum mechanical properties of various vinyl compounds. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1987, 237, 187-190.	0.3	1
150	One-dimensional vibrational eigenvalue problem with numerical potentials. Computer Physics Communications, 1986, 39, 431-437.	3.0	3
151	A CNDO/S study of core hole satellites in the photoelectron spectra of para-, meta- and ortho-nitroanilines. Chemical Physics Letters, 1985, 115, 154-157.	1.2	1
152	Improved convergence modification of the orthogonal gradient multiconfiguration SCF method. Chemical Physics Letters, 1983, 94, 316-320.	1.2	6
153	Sturmian basis matrix solution of vibrational potentials. Chemical Physics Letters, 1982, 85, 111-116.	1.2	16
154	Franckâ€"Condon integrals over a sturmian basis. An application to photoelectron spectra of H2 and N2. Chemical Physics Letters, 1982, 91, 21-26.	1.2	6
155	An algorithm to solve open and closedâ€shell and restricted MCâ€"SCF equations. Journal of Chemical Physics, 1979, 70, 3188-3190.	1.2	18
156	The orthogonal gradient method. A simple method to solve the closedâ€shell, openâ€shell, and multiconfiguration SCF equations. Journal of Chemical Physics, 1979, 70, 1101-1106.	1.2	31
157	The Hellmannâ€"Feynman theorem for openâ€shell and multiconfiguration SCF wave functions. Journal of Chemical Physics, 1979, 71, 1511-1511.	1.2	5
158	Minimum basis sets of slater-transformâ€"preuss functions for the first row atoms. Chemical Physics Letters, 1979, 63, 318-321.	1.2	1
159	On ab-initio calculations of singly excited states of atoms with augmented fuess-type basis functions. Chemical Physics Letters, 1979, 66, 104-107.	1.2	2
160	On the applications of slater-transform-preuss (STP) functions. Chemical Physics, 1978, 28, 243-251.	0.9	3
161	An integral package for one-center integrals over Slater-Transform-Preuss functions. Computer Physics Communications, 1978, 16, 65-71.	3.0	1
162	The synchronous 1,4-addition of methylene to cis-butadiene. Journal of the American Chemical Society, 1978, 100, 7548-7550.	6.6	20

#	Article	IF	Citations
163	Cusp conditions with Gauss type basis functions. Journal of Chemical Physics, 1978, 69, 3431-3432.	1.2	11
164	Slater-transforms-preuss basis sets for He TO Ne and energies for H2, LiH and HF. Chemical Physics Letters, 1976, 43, 20-22.	1.2	6
165	A slater-transform-preuss (STP) wavefunction for the ground state of Be. Chemical Physics Letters, 1976, 40, 447-450.	1.2	6
166	Semi-empirical natural orbital analysis of the bonding and rotational energy barrier in cyclopropylmethyl cation. Chemical Physics Letters, 1975, 36, 365-368.	1.2	3
167	Careful neglect of small two-electron integrals applied to borazane and diazirine. Chemical Physics Letters, 1974, 25, 605-607.	1.2	4
168	Competitive hydrogen bonding in aspirin-aspirin and aspirin-leucine interactions. Turkish Journal of Chemistry, 0, , .	0.5	2