Ersin Yurtsever

List of Publications by Year in descending order

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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	Comparison of hydrogen bonding in polydimethylsiloxane and polyether based urethane and urea copolymers. Polymer, 2000, 41, 849-857.	1.8	226
2	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
3	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
4	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
5	A DFT study of polymerization mechanisms of indole. Polymer, 2002, 43, 6019-6025.	1.8	64
6	Global view of classical clusters: the hyperspherical approach to structure and dynamics. Physical Chemistry Chemical Physics, 2002, 4, 5040-5051.	1.3	56
7	Composition-induced structural transitions in mixed rare-gas clusters. Physical Review B, 2004, 70, .	1.1	54
8	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
9	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
10	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
11	Phase-Space Invariants as Indicators of the Critical Behavior of Nanoaggregates. Physical Review Letters, 2004, 93, 113402.	2.9	31
12	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
13	Invariant energy partitions in chemical reactions and cluster dynamics simulations. Computational Materials Science, 2006, 35, 187-191.	1.4	29
14	Structural studies of polythiophenes. Synthetic Metals, 1996, 78, 19-25.	2.1	26
15	Isomeric Broadening of C₆₀⁺ Electronic Excitation in Helium Droplets: Experiments Meet Theory. Journal of Physical Chemistry Letters, 2018, 9, 1237-1242.	2.1	26
16	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
17	Specific heats of clusters near a phase transition: Energy partitions among internal modes. Chemical Physics Letters, 2006, 430, 424-428.	1.2	25
18	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

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19	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
20	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
21	Hydrogen bonding in polyanilines. Synthetic Metals, 1994, 68, 57-60.	2.1	22
22	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
23	Computational Studies of Cyclobutadiene and Benzocyclobutene Fused top- ando-Quinoneâ€. Journal of Physical Chemistry A, 1998, 102, 2351-2356.	1.1	21
24	The synchronous 1,4-addition of methylene to cis-butadiene. Journal of the American Chemical Society, 1978, 100, 7548-7550.	6.6	20
25	Structural studies of polypyrroles. Synthetic Metals, 1999, 98, 229-236.	2.1	20
26	Vibrational quenching at ultralow energies: Calculations of theLi2(Î£g+1;Î½â=0)+Hesuperelastic scattering cross sections. Physical Review A, 2006, 73, .	1.0	20
27	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
28	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
29	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
30	An algorithm to solve open and closedâ€shell and restricted MCâ€"SCF equations. Journal of Chemical Physics, 1979, 70, 3188-3190.	1.2	18
31	Structural studies of polypyrroles. Synthetic Metals, 1999, 98, 221-227.	2.1	18
32	Chaotic behavior of triatomic clusters. Physical Review A, 1997, 55, 538-544.	1.0	17
33	Turkey's output in social science publications: 1970-1999. Scientometrics, 2002, 55, 103-121.	1.6	17
34	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
35	Crystallization of ion clouds in octupole traps: Structural transitions, core melting, and scaling laws. Physical Review A, 2009, 80, .	1.0	17
36	Sturmian basis matrix solution of vibrational potentials. Chemical Physics Letters, 1982, 85, 111-116.	1.2	16

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37	The increase in the rate of publications originating from Turkey. Scientometrics, 1999, 46, 321-336.	1.6	16
38	Influence of lithium chloride on the morphology of flexible slabstock polyurethane foams and their plaque counterparts. Polymer, 2003, 44, 757-768.	1.8	16
39	Chaos in rotating triatomic clusters. Europhysics Letters, 1997, 37, 91-96.	0.7	15
40	Neutral and ionic dopants in helium clusters: interaction forces for the and complexes. Molecular Physics, 2005, 103, 3223-3231.	0.8	14
41	Dimer formation of perylene: An ultracold spectroscopic and computational study. Journal of Molecular Structure, 2015, 1097, 29-36.	1.8	14
42	Angular-momentum-driven chaos in small clusters. Physical Review A, 1998, 58, 377-382.	1.0	13
43	A theoretical study of structural defects in conjugated polymers. Synthetic Metals, 1999, 101, 335-336.	2.1	13
44	Rotational cooling of Li2(1?g+) molecules by ultracold collisions with a helium gas buffer. Theoretical Chemistry Accounts, 2004, 112, 263.	0.5	13
45	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
46	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
47	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
48	Growth mechanisms of polypyrroles. Polymer, 1996, 37, 1151-1155.	1.8	12
49	Modelling ionic nucleation in small neon clusters. International Journal of Mass Spectrometry, 2002, 220, 193-209.	0.7	12
50	Possible Formation of Metastable PAH Dimers upon Pickup by Helium Droplets. Journal of Physical Chemistry A, 2016, 120, 1727-1736.	1.1	12
51	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
52	The quantum structure of anionic hydrogen clusters. Journal of Chemical Physics, 2018, 148, 102305.	1.2	12
53	Cusp conditions with Gauss type basis functions. Journal of Chemical Physics, 1978, 69, 3431-3432.	1.2	11
54	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

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55	Multiple bipolaron formation in oligothiophenes. Synthetic Metals, 1999, 105, 179-183.	2.1	11
56	Many-body effects on the melting and dynamics of small clusters. Physical Review B, 2000, 62, 9977-9980.	1.1	11
57	Thermochromism in Oligothiophenes:â€‰ The Role of the Internal Rotation. Journal of Physical Chemistry A, 2002, 106, 11981-11986.	1.1	11
58	Finite-size effects in the dynamics and thermodynamics of two-dimensional Coulomb clusters. Physical Review E, 2005, 72, 026110.	0.8	11
59	Energetics and Structures of Charged Helium Clusters: Comparing Stabilities of Dimer and Trimer Cationic Cores. ChemPhysChem, 2008, 9, 2618-2624.	1.0	11
60	Collisional relaxation kinetics fororthoandparaNH2â^'under photodetachment in cold ion traps. Faraday Discussions, 2018, 212, 117-135.	1.6	11
61	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
62	Stacking of triphenylene: characterization of the potential energy surface. Theoretical Chemistry Accounts, 2010, 127, 133-139.	0.5	10
63	Rovibrational quenching of C2â^' anions in collisions with He, Ne, and Ar atoms. Physical Review A, 2020, 102, .	1.0	10
64	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
65	Regularity in nonlinearly coupled quantum oscillators far from the semiclassical limit. Physical Review A, 1990, 41, 6688-6691.	1.0	9
66	On the possibility of grafting conducting polymers into insulating ones. Synthetic Metals, 1996, 81, 5-8.	2.1	9
67	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
68	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
69	Configurational properties of polypyrrole chains. Polymer, 1993, 34, 3887-3892.	1.8	8
70	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
71	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
72	Discovery of an Exceptionally Strong Luminescence of Polyethyleneimineâ€Superparamagnetic Iron Oxide Nanoparticles. Macromolecular Chemistry and Physics, 2018, 219, 1700563.	1.1	8

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73	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
74	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
75	Structural studies of polypyrroles: oligomerization mechanism of N-methacryloyl pyrrole. Computational and Theoretical Chemistry, 1993, 280, 1-4.	1.5	7
76	Quantum Mechanical Calculations of Tryptophan and Comparison with Conformations in Native Proteins. Journal of Physical Chemistry A, 2006, 110, 13933-13938.	1.1	7
77	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
78	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
79	A post-HF study on the interaction of iodine with small polyaromatic hydrocarbons. Journal of Molecular Modeling, 2014, 20, 2445.	0.8	7
80	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
81	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
82	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
83	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
84	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
85	A slater-transform-preuss (STP) wavefunction for the ground state of Be. Chemical Physics Letters, 1976, 40, 447-450.	1.2	6
86	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
87	Improved convergence modification of the orthogonal gradient multiconfiguration SCF method. Chemical Physics Letters, 1983, 94, 316-320.	1.2	6
88	Computationally induced â€˜â€˜irregularityâ€™â€™ in the spectra of integrable quantum systems. Physical Review A, 1988, 38, 1027-1035.	1.0	6
89	Quantal-classical mixed-mode dynamics and chaotic behavior. Physical Review E, 1994, 50, 3422-3430.	0.8	6
90	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

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91	A New Antiaromatic Compound:Â 1,4-Biphenylenequinone Synthesis and Trapping Reactions. Journal of Organic Chemistry, 1997, 62, 3434-3435.	1.7	6
92	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
93	Finding the global minima of clusters with non-empirical models: a comparison of results. Chemical Physics, 2003, 290, 279-295.	0.9	6
94	Solvation of K+ in helium droplets. European Physical Journal D, 2007, 43, 105-108.	0.6	6
95	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
96	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
97	Mapping the global minima of binary Morse clusters: The effects of range mismatch. Computational and Theoretical Chemistry, 2013, 1021, 7-15.	1.1	6
98	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
99	Thermalisation of C2â^’ with noble gases in cold ion traps. International Journal of Mass Spectrometry, 2020, 457, 116426.	0.7	6
100	The Hellmannâ€“Feynman theorem for openâ€shell and multiconfiguration SCF wave functions. Journal of Chemical Physics, 1979, 71, 1511-1511.	1.2	5
101	A quantum mechanical study of the electrochemical polymerization of pyrrole. Synthetic Metals, 2001, 119, 227-228.	2.1	5
102	Conformational Analysis of Model Poly(ether urethane) Chains in the Unperturbed State and under External Forces. Macromolecules, 2002, 35, 9825-9831.	2.2	5
103	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
104	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
105	Structure and dynamics of ion clusters in linear octupole traps: Phase diagrams, chirality, and melting mechanisms. Physical Review A, 2011, 83, .	1.0	5
106	Energy Landscapes in Photochemical Dissociation of Small Peroxides. Journal of Physical Chemistry A, 2019, 123, 1353-1362.	1.1	5
107	Vibrational quenching of CNâ^’ in collisions with He and Ar. Journal of Chemical Physics, 2021, 154, 084305.	1.2	5
108	Careful neglect of small two-electron integrals applied to borazane and diazirine. Chemical Physics Letters, 1974, 25, 605-607.	1.2	4

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109	Monte Carlo Simulation of Model Threeâ€Component Liquid Systems. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1987, 91, 600-603.	0.9	4
110	Monte Carlo studies of binary mixtures: A fast algorithm for equilibration. Chemical Physics Letters, 1991, 187, 8-12.	1.2	4
111	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
112	Rotationally induced transitions in small clusters. Physical Review E, 2000, 63, 016202.	0.8	4
113	Rotational potential functions for oligomethylthiophenes. Synthetic Metals, 2003, 135-136, 427-428.	2.1	4
114	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
115	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
116	Solvation of carbonaceous molecules by para-H2 and ortho-D2 clusters. II. Fullerenes. Journal of Chemical Physics, 2016, 145, 084304.	1.2	4
117	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
118	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
119	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
120	On the applications of slater-transform-preuss (STP) functions. Chemical Physics, 1978, 28, 243-251.	0.9	3
121	One-dimensional vibrational eigenvalue problem with numerical potentials. Computer Physics Communications, 1986, 39, 431-437.	3.0	3
122	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
123	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
124	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
125	Measuring chaos in rotating clusters. Computer Physics Communications, 2002, 145, 194-202.	3.0	3
126	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		

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127	HCHO in a Cold, Quantum Solvent: Size and Shape of Its â€œBubblesâ€•in ⁴He Droplets from Stochastic Simulations. Journal of Physical Chemistry A, 2010, 114, 9725-9732.	1.1	3
128	Exploring a dynamical path for C2Hâ^' and NCOâ^' formation in dark molecular clouds. European Physical Journal D, 2016, 70, 1.	0.6	3
129	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
130	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
131	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
132	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
133	A New Equilibration Algorithm for Monte Carlo Simulations. Molecular Simulation, 1989, 2, 189-199.	0.9	2
134	Monte Carlo simulation studies of binary mixtures: A measure of the mixing. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 47-52.	0.9	2
135	Lyapunov exponents for classical-quantum mixed-mode dynamics. Physical Review E, 1996, 54, 4701-4707.	0.8	2
136	Phase-space reconstruction in Hamiltonian systems through multiple time series. Chemical Physics Letters, 1997, 276, 282-288.	1.2	2
137	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/	1.4	2
138	Structural and thermodynamical studies of 2D Coulomb clusters with point defects. Physica Scripta, 2007, 76, C111-C114.	1.2	2
139	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
140	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
141	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
142	The metastable structures of anthracene-argon clusters inside helium nanodroplets. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	2
143	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
144	Competitive hydrogen bonding in aspirin-aspirin and aspirin-leucine interactions. Turkish Journal of Chemistry, 0, , .	0.5	2

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145	Dimerization dynamics of carboxylic acids in helium nanodroplets. Journal of Chemical Physics, 2022, 156, 174304.	1.2	2
146	An integral package for one-center integrals over Slater-Transform-Preuss functions. Computer Physics Communications, 1978, 16, 65-71.	3.0	1
147	Minimum basis sets of slater-transformâ€“preuss functions for the first row atoms. Chemical Physics Letters, 1979, 63, 318-321.	1.2	1
148	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
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	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
151	On the Stability of Microclusters with Threeâ€Body Forces. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1991, 95, 467-473.	0.9	1
152	Unimolecular dissociation in the regular regime. Journal of Chemical Physics, 1993, 99, 1135-1144.	1.2	1
153	Electronic excitations in stacked oligothiophenes. Synthetic Metals, 2001, 119, 247-248.	2.1	1
154	Vibrational spectroscopy of structural defects in oligothiophenes. Molecular Physics, 2003, 101, 2725-2729.	0.8	1
155	Conformational Similarities in Isomerization Dynamics of Clusters. Journal of Physical Chemistry A, 2003, 107, 6025-6031.	1.1	1
156	Shell Structure, Melting and Dynamics of Ion Clusters Confined in an Octupolar Trap. , 2009, , .		1
157	Energy landscapes of ion clusters in isotropic quadrupolar and octupolar traps. Journal of Chemical Physics, 2012, 136, 024303.	1.2	1
158	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
159	QUANTUM STRUCTURING OF 4He ATOMS AROUND IONIC DOPANTS: ENERGETICS OF Li+, Na+ AND K+ FROM STOCHASTIC CALCULATIONS. , 2008, , 227-240.		1
160	Mixed Mode Dynamics within the TDSCF Approximation. , 1995, , 393-406.		1
161	The least-squares stabilization method for resonance eigenvalues. Chemical Physics Letters, 1987, 137, 569-572.	1.2	0
162	Algebraic approaches to eigenvalue equations: The Wronskian method. Chemical Physics Letters, 1987, 141, 386-390.	1.2	0

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163	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
164	Lattice polymers: behaviour far from Î¸-conditions. Polymer, 1992, 33, 2725-2728.	1.8	0
165	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
166	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
167	The structure of 1,3-butadiene clusters. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	0
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