Josep M Bofill

List of Publications by Year
in descending order

167 papers	4,547 citations	117625 34 h-index	123424 61 g-index
173 all docs	173 docs citations	173 times ranked	3638 citing authors

#	Article	IF	Citations
1	Use of Onium Salt-Based Coupling Reagents in Peptide Synthesis1. Journal of Organic Chemistry, 1998, 63, 9678-9683.	3.2	245
2	Shape and Symmetry of Heptacoordinate Transition-Metal Complexes: Structural Trends. Chemistry - A European Journal, 2003, 9, 1281-1295.	3.3	225
3	Updated Hessian matrix and the restricted step method for locating transition structures. Journal of Computational Chemistry, 1994, 15, 1-11.	3.3	212
4	The unrestricted natural orbitalâ€“complete active space (UNOâ€“CAS) method: An inexpensive alternative to the complete active spaceâ€“selfâ€consistentâ€field (CASâ€“SCF) method. Journal of Chemical Physics, 1989, 90, 3637-3646.	3.0	195
5	Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â˜9). Journal of Organic Chemistry, 2005, 70, 2509-2521.	3.2	195
6	Unimolecular Isomerizations and Oxygen Atom Loss in Formaldehyde and Acetaldehyde Carbonyl Oxides. A Theoretical Investigation. Journal of the American Chemical Society, 1996, 118, 4636-4647.	13.7	137
7	The Ozonolysis of Ethylene: A Theoretical Study of the Gas-Phase Reaction Mechanism. Chemistry - A European Journal, 1999, 5, 1809-1822.	3.3	134
8	Extent and limitations of density-functional theory in describing magnetic systems. Physical Review B, 2004, 70, .	3.2	122
9	Atmospheric Formation of OH Radicals and H2O2 from Alkene Ozonolysis under Humid Conditions. ChemPhysChem, 2002, 3, 215-221.	2.1	100
10	Tropospheric Formation of Hydroxymethyl Hydroperoxide, Formic Acid, H2O2, and OH from Carbonyl Oxide in the Presence of Water Vapor: A Theoretical Study of the Reaction Mechanism. Chemistry - A European Journal, 2001, 7, 2227-2235.	3.3	92
11	A reduced-restricted-quasi-Newton-Raphson method for locating and optimizing energy crossing points between two potential energy surfaces. Journal of Computational Chemistry, 1997, 18, 992-1003.	3.3	91
12	Finding transition states using reduced potential-energy surfaces. Theoretical Chemistry Accounts, 2001, 105, 463-472.	1.4	81
13	The Mechanism of Methoxy Radical Oxidation by O2in the Gas Phase. Computational Evidence for Direct H Atom Transfer Assisted by an Intermolecular Noncovalent OÂ·Â·Â·O Bonding Interaction. Journal of the American Chemical Society, 1999, 121, 1337-1347.	13.7	77
14	Spin Symmetry Requirements in Density Functional Theory: The Proper Way to Predict Magnetic Coupling Constants in Molecules and Solids. Theoretical Chemistry Accounts, 2006, 116, 587-597.	1.4	77
15	Point-Dipole Approximation of the Exciton Coupling Model Versus Type of Bonding and of Excitons in Porphyrin Supramolecular Structures. Chemistry - A European Journal, 2001, 7, 2733-2737.	3.3	76
16	Inductive Effects in Neutral Pentacoordinated Silicon Compounds Containing a Si â†•N Dative Bond. A Theoretical Study. Organometallics, 1999, 18, 5584-5593.	2.3	69
17	Local Aromaticity of the Lowest-Lying Singlet States of [n]Acenes (n = 6â˜9). Journal of Physical Chemistry A, 2005, 109, 10629-10632.	2.5	68
18	A new look at the reduced-gradient-following path. Theoretical Chemistry Accounts, 2002, 107, 130-139.	1.4	63

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19	Mechanism of the Hydrogen Transfer from the OH Group to Oxygen-Centered Radicals: Proton-Coupled Electron-Transfer versus Radical Hydrogen Abstraction. Chemistry - A European Journal, 2004, 10, 3404-3410.	3.3	63
20	A theoretical investigation of the thermal ring opening of cyclopropyl radical into allyl radical. Evidence for a highly nonsymmetric transition state. Journal of the American Chemical Society, 1990, 112, 2160-2167.	13.7	61
21	Derivation of spin Hamiltonians from the exact Hamiltonian: Application to systems with two unpaired electrons per magnetic site. Physical Review B, 2002, 66, .	3.2	60
22	Reaction Modes of Carbonyl Oxide, Dioxirane, and Methylenebis(oxy) with Ethylene:â€‰ A New Reaction Mechanism. Journal of Physical Chemistry A, 2002, 106, 3917-3929.	2.5	57
23	Role of Electron Density and Magnetic Couplings on the Nucleus-Independent Chemical Shift (NICS) Profiles of [2.2]Paracyclophane and Related Species. Journal of Organic Chemistry, 2006, 71, 1700-1702.	3.2	57
24	On the quadratic reaction path evaluated in a reduced potential energy surface model and the problem to locate transition states. Journal of Computational Chemistry, 2001, 22, 387-406.	3.3	52
25	New strategies to incorporate the solvent polarization in selfâ€consistent reaction field and freeâ€energy perturbation simulations. Journal of Chemical Physics, 1995, 103, 10183-10191.	3.0	49
26	Unconventional Biradical Character of Titanium Enolates. Journal of the American Chemical Society, 2008, 130, 3242-3243.	13.7	46
27	Practical remarks on the selection of the active space in the CAS-SCF wavefunction. Chemical Physics Letters, 1995, 243, 151-157.	2.6	44
28	The reaction path intrinsic reaction coordinate method and the Hamiltonâ€“Jacobi theory. Journal of Chemical Physics, 2005, 122, 234105.	3.0	44
29	How good is a Broyden-Fletcher-Goldfarb-Shanno-like update Hessian formula to locate transition structures? Specific reformulation of Broyden-Fletcher-Goldfarb-Shanno for optimizing saddle points. Journal of Computational Chemistry, 1998, 19, 349-362.	3.3	43
30	On the automatic restricted-step rational-function-optimization method. Theoretical Chemistry Accounts, 1998, 100, 265-274.	1.4	41
31	Theoretical Mechanistic Study of the Oxidative Degradation of Benzene in the Troposphere: Reaction of Benzeneâ˙HO Radical Adduct with O₂. Journal of Chemical Theory and Computation, 2009, 5, 1607-1623.	5.3	41
32	The reaction between HO and (H2O) n (nÂ=Â1, 3) clusters: reaction mechanisms and tunneling effects. Theoretical Chemistry Accounts, 2011, 128, 579-592.	1.4	37
33	Theoretical Investigation of the Low-Lying Electronic States of Dioxirane:â€‰ Ring Opening to Dioxymethane and Dissociation into CO2 and H2. Journal of Physical Chemistry A, 1998, 102, 3398-3406.	2.5	36
34	Ab Initio Calculations on the Mechanism of the Oxidation of the Hydroxymethyl Radical by Molecular Oxygen in the Gas Phase: A Significant Reaction for Environmental Science. Chemistry - A European Journal, 2001, 7, 3377-3386.	3.3	35
35	Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in Ï€-stacked polyfluorenes?. Chemical Physics Letters, 2006, 428, 191-195.	2.6	33
36	Analysis of the updated Hessian matrices for locating transition structures. Journal of Computational Chemistry, 1995, 16, 1326-1338.	3.3	32

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37	Variational nature, integration, and properties of Newton reaction path. Journal of Chemical Physics, 2011, 134, 074101.	3.0	30
38	Prediction of approximate transition states by Bell-Evans-Polanyi principle: I. Journal of Computational Chemistry, 1999, 20, 1112-1129.	3.3	28
39	Molecular and electronic structure of the low-lying electronic states of cycloalkenylidenes: cyclopropenylidene. Journal of the American Chemical Society, 1988, 110, 1694-1700.	13.7	26
40	Geometry optimization and transition state search in enzymes: Different options in the microiterative method. International Journal of Quantum Chemistry, 2004, 98, 367-377.	2.0	26
41	Use of 3,3'-Polymethylene-bridged Thiazolium Salts Plus Based as Catalysts of the Benzoin Condensation and Its Mechanistic Implications: Proposal of a New Mechanism in Aprotic Conditions. Heterocycles, 1994, 37, 1579.	0.7	25
42	A contribution to a theory of mechanochemical pathways by means of Newton trajectories. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	24
43	Analysis of the Acting Forces in a Theory of Catalysis and Mechanochemistry. Journal of Physical Chemistry A, 2017, 121, 2820-2838.	2.5	24
44	A theoretical study of benzoin condensation. Computational and Theoretical Chemistry, 1995, 339, 179-194.	1.5	23
45	A geometry optimization benchmark using highly correlated wavefunctions (FCI and MRD-CI). Theoretica Chimica Acta, 1995, 92, 369-381.	0.8	23
46	Analysis of the Valley-Ridge inflection points through the partitioning technique of the Hessian eigenvalue equation. Journal of Mathematical Chemistry, 2013, 51, 1099-1115.	1.5	23
47	Molecular and electronic structure of the low-lying electronic states of cycloalkenylidenes. Cyclopentadienylidene. Journal of the American Chemical Society, 1988, 110, 3740-3746.	13.7	22
48	An algorithm to locate optimal bond breaking points on a potential energy surface for applications in mechanochemistry and catalysis. Journal of Chemical Physics, 2017, 147, 152710.	3.0	22
49	Electronic Structure and Unimolecular Reactions of Cyclopropenone Carbonyl Oxide. A Theoretical Studyâ€. Journal of Organic Chemistry, 1997, 62, 2720-2726.	3.2	21
50	On the restricted step method coupled with the augmented Hessian for the search of stationary points of any continuous function. International Journal of Quantum Chemistry, 1997, 62, 153-165.	2.0	21
51	Conditional Bornâ€“Oppenheimer Dynamics: Quantum Dynamics Simulations for the Model Porphine. Journal of Physical Chemistry Letters, 2015, 6, 1529-1535.	4.6	21
52	Bipyridyl Derivatives as Photomemory Devices: A Comparative Electronicâ€Structure Study. Chemistry - A European Journal, 2010, 16, 6693-6703.	3.3	20
53	The Variational Structure of Gradient Extremals. Journal of Chemical Theory and Computation, 2012, 8, 927-935.	5.3	20
54	Formylation of Electron-Rich Aromatic Rings Mediated by Dichloromethyl Methyl Ether and TiCl4: Scope and Limitations. Molecules, 2015, 20, 5409-5422.	3.8	20

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55	Reaction rates in a theory of mechanochemical pathways. Journal of Computational Chemistry, 2016, 37, 2467-2478.	3.3	20
56	Theoretical Study of the Low-Lying Electronic States of 4-Oxo-2,5-cyclohexadienylidene and Their Formation from 1H-Bicyclo[3.1.0]hexa-3,5-dien-2-one. The Journal of Physical Chemistry, 1995, 99, 5934-5944.	2.9	19
57	A reaction pathâ€“Liouville approach to the rate constant for polyatomic chemical reactions. Physical Chemistry Chemical Physics, 2002, 4, 2921-2926.	2.8	19
58	A reaction path Hamiltonian defined on a Newton path. Journal of Chemical Physics, 2002, 116, 8713-8722.	3.0	19
59	Finding reaction paths using the potential energy as reaction coordinate. Journal of Chemical Physics, 2008, 128, 104102.	3.0	19
60	Exploration of cyclopropyl radical ring opening to allyl radical by Newton trajectories: importance of valley-ridge inflection points to understand the topography. Theoretical Chemistry Accounts, 2011, 129, 803-821.	1.4	19
61	Kinetic interpretation of aromaticity: a theoretical study. Journal of Organic Chemistry, 1988, 53, 5148-5149.	3.2	18
62	On the Reaction Path Hamiltonian for Polyatomic Molecules. Journal of Physical Chemistry A, 2001, 105, 5022-5029.	2.5	18
63	Toward a theory of mechanochemistry: Simple models from the very beginnings. International Journal of Quantum Chemistry, 2018, 118, e25775.	2.0	18
64	Response to â€œComment on â€˜New strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulationsâ€™â€‰â€•[J. Chem. Phys. 107, 1291 (1997)]. Journal of Chemical Physics, 1997, 107, 1293-1294.	3.0	17
65	Applications of analytic and geometry concepts of the theory of Calculus of Variations to the Intrinsic Reaction Coordinate model. Molecular Physics, 2007, 105, 2475-2492.	1.7	17
66	Cross-section energy dependence of the [C6H6â€“M]+ adduct formation between benzene molecules and alkali ions (M = Li, Na, K). Physical Chemistry Chemical Physics, 2011, 13, 15977.	2.8	17
67	Reinvestigation of some thermally â€œforbiddenâ€•pericyclic reactions and biradical processes in the semiempirical TCSCF approach. Computational and Theoretical Chemistry, 1988, 163, 285-304.	1.5	16
68	An updated Hessian formula for optimizing transition structures which explicitly contains the potential structure of the desired transition vector. Chemical Physics Letters, 1996, 260, 359-364.	2.6	16
69	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. Theoretical Chemistry Accounts, 2002, 107, 147-153.	1.4	16
70	Generalized reaction-path Hamiltonian dynamics. Theoretical Chemistry Accounts, 2004, 112, 75-83.	1.4	16
71	Theoretical Prediction of Benzyne-Like Species in Pyrene Diradicals. Journal of Physical Chemistry A, 2004, 108, 5111-5116.	2.5	16
72	Algorithm to evaluate rate constants for polyatomic chemical reactions. II. Applications. Journal of Computational Chemistry, 2007, 28, 2111-2121.	3.3	16

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73	Locating transition states on potential energy surfaces by the gentlest ascent dynamics. Chemical Physics Letters, 2013, 583, 203-208.	2.6	16
74	Title is missing!. Journal of Mathematical Chemistry, 1999, 25, 85-92.	1.5	15
75	Remarks on the updated Hessian matrix methods. International Journal of Quantum Chemistry, 2003, 94, 324-332.	2.0	15
76	Molecular and electronic structure of the low-lying electronic states of the 1-pyrazolyl and 1-imidazolyl radicals. Journal of the American Chemical Society, 1989, 111, 7740-7746.	13.7	14
77	Energy decomposition in molecular complexes: Implications for the treatment of polarization in molecular simulations. Journal of Computational Chemistry, 2003, 24, 1263-1275.	3.3	14
78	Studies on the Intramolecular Câ’HÂ·Â·Â·X (X = O, S) Interactions in (S)-N-Acyl-4-isopropyl-1,3-thiazolidine-2-thiones and Related 1,3-Oxazolidin-2-ones. Organic Letters, 2003, 5, 2809-2812.	4.6	14
79	Newton trajectories for the tilted Frenkelâ€“Kontorova model. Molecular Physics, 2019, 117, 1541-1558.	1.7	14
80	Understanding the structure/reactivity of aminium/uronium salts as coupling reagents in peptide synthesis. Tetrahedron Letters, 1999, 40, 2641-2644.	1.4	13
81	Conformational Analysis of Molecular Machines: Internal Rotation and Enantiomerization in Triptycyl[3]helicene. ChemPhysChem, 2008, 9, 1117-1119.	2.1	13
82	Topography of cyclopropyl radical ring opening to allyl radical on the CASSCF(3,3) surface: valley-ridge inflection points by Newton trajectories. Journal of Mathematical Chemistry, 2012, 50, 2061-2085.	1.5	13
83	Embedding of the saddle point of index two on the PES of the ring opening of cyclobutene. International Journal of Quantum Chemistry, 2015, 115, 1635-1649.	2.0	13
84	Mechanochemistry on the <scp>M</scp>Ã¼llerâ€“<scp>B</scp>rown surface by <scp>N</scp>ewton trajectories. International Journal of Quantum Chemistry, 2018, 118, e25522.	2.0	13
85	Remarks on large-scale matrix diagonalization using a Lagrange-Newton-Raphson minimization in a subspace. Theoretical Chemistry Accounts, 1999, 103, 163-166.	1.4	12
86	Electronic excitation and charge transfer processes in collisions between Mg(3â€Š1S0) atoms and Rb+(1S0) ions in the 0.07â€“4.00 keV energy range. Journal of Chemical Physics, 2004, 121, 5284-5292.	3.0	12
87	Crossed ionâ€“atom beam study of the inelastic collision processes between neutral Mg(31S0) atoms and Cs+(1S0) ions in the 0.05â€“4.20 keV energy range. Physical Chemistry Chemical Physics, 2005, 7, 310-317.	2.8	12
88	Narcissistic reaction pathways: an example of Maxwellâ€™s theorem of geometrical optics applied to the intrinsic reaction coordinate model. Theoretical Chemistry Accounts, 2008, 121, 279-288.	1.4	12
89	Locating saddle points of any index on potential energy surfaces by the generalized gentlest ascent dynamics. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	12
90	An experimental guided-ion-beam andab initiostudy of the ion-molecule gas-phase reactions between Li+ ions andiso-C3H7Cl in their ground electronic state. Journal of Chemical Physics, 2009, 131, 024306.	3.0	11

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91	Implementation of an algorithm based on the Rungeâ€Kuttaâ€Fehlberg technique and the potential energy as a reaction coordinate to locate intrinsic reaction paths. Journal of Computational Chemistry, 2010, 31, 2510-2525.	3.3	11
92	2,2,4,6,7â€Pentamethylâ€2,3â€dihydrobenzofuranâ€5â€methyl (Pbfm) as an Alternative to the Trityl Group for the Sideâ€Chain Protection of Cysteine and Asparagine/Glutamine. European Journal of Organic Chemistry, 2010, 2010, 3631-3640.	2.4	11
93	Sliding paths for series of Frenkel-Kontorova models â€“ a contribution to the concept of 1D-superlubricity. European Physical Journal B, 2019, 92, 1.	1.5	11
94	Inelastic electronic excitation and electron transfer processes in collisions between Mg(3S01) atoms and K+(S01) ions studied by crossed beams in the 0.10-3.80-keV energy range. Journal of Chemical Physics, 2005, 123, 124314.	3.0	10
95	On the implementation of the Rungeâ€“Kuttaâ€“Fehlberg algorithm to integrate intrinsic reaction coordinate paths. Chemical Physics Letters, 2006, 432, 375-382.	2.6	10
96	Quantum Trajectories from a Discreteâˆ’Variable Representation Method. Journal of Physical Chemistry A, 2007, 111, 10226-10233.	2.5	10
97	A restricted quantum reaction path Hamiltonian: Theory, discrete variable representation propagation algorithm, and applications. Journal of Chemical Physics, 2009, 131, 054108.	3.0	10
98	Search for conical intersection points (CI) by Newton trajectories. Chemical Physics Letters, 2012, 541, 122-127.	2.6	10
99	Experimental and Computational Evidence of the Biradical Structure and Reactivity of Titanium(IV) Enolates. Journal of Organic Chemistry, 2017, 82, 8909-8916.	3.2	10
100	Some remarks on the use of the three-term recurrence method in the configuration interaction eigenvalue problem. Chemical Physics, 1994, 183, 19-26.	1.9	9
101	Accurate and efficient determination of higher roots in diagonalization of large matrices based in function restricted optimization algorithms. Journal of Computational Chemistry, 2000, 21, 1375-1386.	3.3	9
102	Experimental cross-sections energy dependence and an ab initio electronic structure survey of the ground singlet potential surface for reactive Li+ + n-C3H7Cl collisions at low energies. Physical Chemistry Chemical Physics, 2010, 12, 13646.	2.8	9
103	The variational nature of the gentlest ascent dynamics and the relation of a variational minimum of a curve and the minimum energy path. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	9
104	Dynamical study of the Cs+(1S0)+Mg(3Â1S0) non adiabatic collision system in the few keV energy range. European Physical Journal D, 2008, 47, 63-70.	1.3	8
105	Comment on â€œReaction Coordinates and Pathways of Mechanochemical Transformationsâ€• Journal of Physical Chemistry B, 2016, 120, 2644-2645.	2.6	8
106	A model for a driven Frenkelâ€“Kontorova chain. European Physical Journal B, 2019, 92, 1.	1.5	8
107	Calculus of variations as a basic tool for modelling of reaction paths and localisation of stationary points on potential energy surfaces. Molecular Physics, 2020, 118, e1667035.	1.7	8
108	Some Mathematical Reasoning on the Artificial Force Induced Reaction Method. Journal of Computational Chemistry, 2020, 41, 629-634.	3.3	8

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109	Calculation of clustered eigenvalues of large matrices using variance minimization method. Journal of Computational Chemistry, 1998, 19, 1777-1785.	3.3	7
110	A Bohmian total potential view to quantum effects. I. Methodology and simple model systems. Journal of Chemical Physics, 2004, 120, 10961-10971.	3.0	7
111	A computational study and valence bond approach to the intramolecular electrophilic aromatic substitution mechanism of ortho-allyl-N-benzylanilines. Tetrahedron, 2008, 64, 7407-7418.	1.9	7
112	Guided-Ion-Beam and ab Initio Study of the Li⁺, K⁺, and Rb⁺ Association Reactions with Gas-Phase Butanone and Cyclohexanone in Their Ground Electronic States. Journal of Physical Chemistry A, 2009, 113, 14766-14773.	2.5	7
113	A comment to the nudged elastic band method. Journal of Computational Chemistry, 2010, 31, 2526-2531.	3.3	7
114	A Conjugate Gradient Algorithm with a Trust Region for Molecular Geometry Optimization. Journal of Molecular Modeling, 1995, 1, 11-17.	1.8	6
115	Effective potential, Bohmâ€™s potential plus classical potential, analysis of quantum transmission. Journal of Mathematical Chemistry, 2008, 43, 350-364.	1.5	6
116	Azomethane Decomposition Catalyzed by Pt(111):â€‰ An Example of Anti-BrÃ¶nstedâ^'Evansâ^'Polanyi Behavior. Journal of Physical Chemistry C, 2008, 112, 1072-1080.	3.1	6
117	Some remarks on the model of the extended gentlest ascent dynamics. Journal of Mathematical Chemistry, 2015, 53, 41-57.	1.5	6
118	Barnes Update Applied in the Gaussâ€“Newton Method: An Improved Algorithm to Locate Bond Breaking Points. Journal of Chemical Theory and Computation, 2021, 17, 996-1007.	5.3	6
119	Controlling Chemical Reactivity with Optimally Oriented Electric Fields: A Generalization of the Newton Trajectory Method. Journal of Chemical Theory and Computation, 2022, 18, 935-952.	5.3	6
120	Energy partitioning using two-electron average matrices. Chemical Physics Letters, 1994, 222, 51-57.	2.6	5
121	Analysis of the convergence of the general coupling operator method for one-configuration-type wave functions. Journal of Computational Chemistry, 1998, 19, 368-376.	3.3	5
122	Prediction of approximate transition states by Bell-Evans-Polanyi principle: II. Gas phase unimolecular decomposition of methyldioxirane. Journal of Computational Chemistry, 1999, 20, 1130-1137.	3.3	5
123	Deterministic resonance formation and decay under bohmian mechanics. Computational and Theoretical Chemistry, 2005, 727, 205-212.	1.5	5
124	Is the reduced gradient following path a curve with extremal properties?. Journal of Chemical Physics, 2009, 130, 176102.	3.0	5
125	Differential Behavior of Aminoâ€“Imino Constitutional Isomers in Nonlinear Optical Processes. ChemPhysChem, 2010, 11, 912-919.	2.1	5
126	A comparison model between density functional and wave function theories by means of the LÃ¶wdin partitioning technique. Journal of Chemical Physics, 2013, 138, 174107.	3.0	5

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127	Algorithm to evaluate rate constants for polyatomic chemical reactions. I. Theory and computational details. Journal of Computational Chemistry, 2007, 28, 2102-2110.	3.3	4
128	Space and momentum representation analysis of Hartmanâ€™s effect in wave packet transmission. Physical Review A, 2008, 78, .	2.5	4
129	An ab initio theoretical approach to the gas phase decomposition of C₃H₇⁺ produced in ground state Li⁺ + iâ€C₃H₇Cl collisions. International Journal of Quantum Chemistry, 2011, 111, 493-504.	2.0	4
130	Experimental and ab initio studies of the reactive processes in gas phase i-C3H7Br and i-C3H7OH collisions with potassium ions. Journal of Chemical Physics, 2014, 141, 164310.	3.0	4
131	On the Mechanism of Phenolic Formylation Mediated by TiCl₄ Complexes: Existence of Diradical Intermediates Induced by Valence Tautomerism. European Journal of Organic Chemistry, 2015, 2015, 2111-2118.	2.4	4
132	The movement of a one-dimensional Wigner solid explained by a modified Frenkel-Kontorova model. European Physical Journal B, 2020, 93, 1.	1.5	4
133	A Bohmian total potential view to quantum effects. II: decay of temporarily trapped states. Theoretical Chemistry Accounts, 2009, 123, 51-58.	1.4	3
134	Crossed molecular beams study of inelastic non-adiabatic processes in gas phase collisions between sodium ions and ZnBr2 molecules in the 0.10â€“3.50 keV energy range. Journal of Chemical Physics, 2012, 137, 154202.	3.0	3
135	A Relation Between the Eikonal Equation Associated to a Potential Energy Surface and a Hyperbolic Wave Equation. Journal of Chemical Theory and Computation, 2012, 8, 4856-4862.	5.3	3
136	Comment on â€œExploring the potential energy landscape of the Thomson problem via Newton homotopiesâ€•[J. Chem. Phys. 142, 194113 (2015)]. Journal of Chemical Physics, 2015, 143, 247101.	3.0	3
137	Exploring potential energy surfaces with gentlest ascent dynamics in combination with the shrinking dimer method and Newtonian dynamics. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	3
138	Interplay between the Gentlest Ascent Dynamics Method and Conjugate Directions to Locate Transition States. Journal of Chemical Theory and Computation, 2019, 15, 5426-5439.	5.3	3
139	Description of Shapiro steps on the potential energy surface of a Frenkelâ€“Kontorova model Part I: The chain in a variable box. European Physical Journal B, 2021, 94, 1.	1.5	3
140	Description of Shapiro steps on the potential energy surface of a Frenkelâ€“Kontorova model, Part II: free boundaries of the chain. European Physical Journal B, 2021, 94, 1.	1.5	3
141	On the quadratic reaction path evaluated in a reduced potential energy surface model and the problem to locate transition states. Journal of Computational Chemistry, 2001, 22, 387-406.	3.3	3
142	Large-scale matrix diagonalization methods by direct optimization of Taylor expansion of Rayleighâ€“Ritz quotient up to third order. Chemical Physics Letters, 2000, 329, 160-167.	2.6	2
143	The Canonical Transformation Theory and its application to the Reaction Path Hamiltonian. Computational and Theoretical Chemistry, 2005, 727, 21-27.	1.5	2
144	On the interplay between inner and outer Krylov spaces applied to large matrix diagonalization algorithms. Computational and Theoretical Chemistry, 2005, 727, 9-19.	1.5	2

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145	Dehydrohalogenation and Dehydration Reactions ofi-C3H7Br andi-C3H7OH by Sodium Ions Studied by Guided Ion Beam Techniques and Quantum Chemical Methods. Journal of Physical Chemistry A, 2016, 120, 4758-4769.	2.5	2
146	The reactivity of cyclopropyl cyanide in titan's atmosphere: a possible pre-biotic mechanism. Physical Chemistry Chemical Physics, 2018, 20, 6198-6210.	2.8	2
147	Description of zero field steps on the potential energy surface of a Frenkel-Kontorova model for annular Josephson junction arrays. European Physical Journal B, 2021, 94, 1.	1.5	2
148	Quantum Zermelo problem for general energy resource bounds. Physical Review Research, 2020, 2, .	3.6	2
149	Natural charge densities for the evaluation of MC-SCF energy derivatives without density matrix transformation. Chemical Physics Letters, 1989, 156, 501-504.	2.6	1
150	Generalized product functions: energy analytic derivatives. The variational theory of subsystems as a guide for solvation models. Computational and Theoretical Chemistry, 1996, 371, 45-50.	1.5	1
151	A symmetric orthogonal transformation applied to molecular geometry optimizations constrained on a hypersphere. Chemical Physics Letters, 1997, 269, 469-474.	2.6	1
152	On the evaluation of selected eigenpairs of large matrices based on function optimization algorithms. Molecular Physics, 2003, 101, 45-51.	1.7	1
153	Bohmian Total Potential View to Quantum Effects III. Tunnelling in Phase Space. Journal of Physical Chemistry A, 2009, 113, 15024-15030.	2.5	1
154	Reply to the comment by Sheppard and Henkelman on the nudged elastic band method. Journal of Computational Chemistry, 2011, 32, 1772-1773.	3.3	1
155	Level sets as progressing waves: an example for wake-free waves in every dimension. Journal of Mathematical Chemistry, 2014, 52, 654-664.	1.5	1
156	Remarks on the exact energy functional for fermions: an analysis using the LÃ¶wdin partitioningÂtechnique. Molecular Physics, 2014, 112, 809-817.	1.7	1
157	Conformational analysis of enantiomerization coupled to internal rotation in triptycyl-n-helicenes. Physical Chemistry Chemical Physics, 2019, 21, 11395-11404.	2.8	1
158	Comment on â€œExploring Potential Energy Surface with External Forcesâ€• Journal of Chemical Theory and Computation, 2020, 16, 811-815.	5.3	1
159	Quantum Chemical Reactivity: Beyond the Study of Small Molecules. Mathematical and Computational Chemistry, 2001, , 125-141.	0.3	1
160	Tropospheric Formation of Hydroxymethyl Hydroperoxide, Formic Acid, H2O2, and OH from Carbonyl Oxide in the Presence of Water Vapor: A Theoretical Study of the Reaction Mechanism. Chemistry - A European Journal, 2001, 7, 2227-2235.	3.3	1
161	Comment on â€˜Out-of-equilibrium Frenkelâ€“Kontorova modelâ€™ (Imparato A 2021 J. Stat. Mech. 013214). Journal of Statistical Mechanics: Theory and Experiment, 2022, 2022, 013204.	2.3	1
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