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	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
2	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
3	A generalized Frenkelâ€“Kontorova model for a propagating austeniteâ€“martensite phase boundary: revisited numerically. European Physical Journal B, 2022, 95, .	1.5	0
4	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
5	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
6	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
7	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
8	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
9	Comment on â€œExploring Potential Energy Surface with External Forcesâ€• Journal of Chemical Theory and Computation, 2020, 16, 811-815.	5.3	1
10	Some Mathematical Reasoning on the Artificial Force Induced Reaction Method. Journal of Computational Chemistry, 2020, 41, 629-634.	3.3	8
11	Quantum equilibration of the double-proton transfer in a model system porphine. Physical Chemistry Chemical Physics, 2020, 22, 22332-22341.	2.8	0
12	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
13	Quantum Zermelo problem for general energy resource bounds. Physical Review Research, 2020, 2, .	3.6	2
14	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
15	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
16	Conformational analysis of enantiomerization coupled to internal rotation in triptycyl-n-helicenes. Physical Chemistry Chemical Physics, 2019, 21, 11395-11404.	2.8	1
17	A model for a driven Frenkelâ€“Kontorova chain. European Physical Journal B, 2019, 92, 1.	1.5	8
18	Newton trajectories for the tilted Frenkelâ€“Kontorova model. Molecular Physics, 2019, 117, 1541-1558.	1.7	14

#	Article	IF	Citations
19	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
20	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
21	Toward a theory of mechanochemistry: Simple models from the very beginnings. International Journal of Quantum Chemistry, 2018, 118, e25775.	2.0	18
22	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
23	The role of Li+ ions in the gas phase dehydrohalogenation and dehydration reactions of i-C3H7Br and i-C3H7OH molecules studied by radiofrequency-guided ion beam techniques and ab initio methods. Journal of Chemical Physics, 2017, 146, 134301.	3.0	0
24	Analysis of the Acting Forces in a Theory of Catalysis and Mechanochemistry. Journal of Physical Chemistry A, 2017, 121, 2820-2838.	2.5	24
25	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
26	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
27	A contribution to a theory of mechanochemical pathways by means of Newton trajectories. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	24
28	Reaction rates in a theory of mechanochemical pathways. Journal of Computational Chemistry, 2016, 37, 2467-2478.	3.3	20
29	Comment on â€œReaction Coordinates and Pathways of Mechanochemical Transformationsâ€• Journal of Physical Chemistry B, 2016, 120, 2644-2645.	2.6	8
30	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
31	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
32	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
33	Formylation of Electron-Rich Aromatic Rings Mediated by Dichloromethyl Methyl Ether and TiCl4: Scope and Limitations. Molecules, 2015, 20, 5409-5422.	3.8	20
34	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
35	Some remarks on the model of the extended gentlest ascent dynamics. Journal of Mathematical Chemistry, 2015, 53, 41-57.	1.5	6
36	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

#	Article	IF	Citations
37	Conditional Bornâ€“Oppenheimer Dynamics: Quantum Dynamics Simulations for the Model Porphine. Journal of Physical Chemistry Letters, 2015, 6, 1529-1535.	4.6	21
38	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
39	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
40	Remarks on the exact energy functional for fermions: an analysis using the LÃ¶wdin partitioningÂtechnique. Molecular Physics, 2014, 112, 809-817.	1.7	1
41	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
42	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
43	Locating transition states on potential energy surfaces by the gentlest ascent dynamics. Chemical Physics Letters, 2013, 583, 203-208.	2.6	16
44	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
45	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
46	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
47	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
48	The Variational Structure of Gradient Extremals. Journal of Chemical Theory and Computation, 2012, 8, 927-935.	5.3	20
49	Search for conical intersection points (CI) by Newton trajectories. Chemical Physics Letters, 2012, 541, 122-127.	2.6	10
50	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
51	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
52	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
53	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
54	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

#	Article	IF	Citations
55	Variational nature, integration, and properties of Newton reaction path. Journal of Chemical Physics, 2011, 134, 074101.	3.0	30
56	Differential Behavior of Aminoâ€“Imino Constitutional Isomers in Nonlinear Optical Processes. ChemPhysChem, 2010, 11, 912-919.	2.1	5
57	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
58	A comment to the nudged elastic band method. Journal of Computational Chemistry, 2010, 31, 2526-2531.	3.3	7
59	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
60	Bipyridyl Derivatives as Photomemory Devices: A Comparative Electronicâ€Structure Study. Chemistry - A European Journal, 2010, 16, 6693-6703.	3.3	20
61	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
62	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
63	The 65th birthday of Professor Santiago Olivella Nello. Theoretical Chemistry Accounts, 2009, 123, 1-2.	1.4	0
64	A Bohmian total potential view to quantum effects. II: decay of temporarily trapped states. Theoretical Chemistry Accounts, 2009, 123, 51-58.	1.4	3
65	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
66	Is the reduced gradient following path a curve with extremal properties?. Journal of Chemical Physics, 2009, 130, 176102.	3.0	5
67	A restricted quantum reaction path Hamiltonian: Theory, discrete variable representation propagation algorithm, and applications. Journal of Chemical Physics, 2009, 131, 054108.	3.0	10
68	Bohmian Total Potential View to Quantum Effects III. Tunnelling in Phase Space. Journal of Physical Chemistry A, 2009, 113, 15024-15030.	2.5	1
69	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
70	Effective potential, Bohmâ€™s potential plus classical potential, analysis of quantum transmission. Journal of Mathematical Chemistry, 2008, 43, 350-364.	1.5	6
71	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
72	Conformational Analysis of Molecular Machines: Internal Rotation and Enantiomerization in Triptycyl[3]helicene. ChemPhysChem, 2008, 9, 1117-1119.	2.1	13

#	Article	IF	Citations
73	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
74	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
75	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
76	Unconventional Biradical Character of Titanium Enolates. Journal of the American Chemical Society, 2008, 130, 3242-3243.	13.7	46
77	Finding reaction paths using the potential energy as reaction coordinate. Journal of Chemical Physics, 2008, 128, 104102.	3.0	19
78	Space and momentum representation analysis of Hartmanâ€™s effect in wave packet transmission. Physical Review A, 2008, 78, .	2.5	4
79	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
80	Quantum Trajectories from a Discreteâ^'Variable Representation Method. Journal of Physical Chemistry A, 2007, 111, 10226-10233.	2.5	10
81	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
82	Algorithm to evaluate rate constants for polyatomic chemical reactions. II. Applications. Journal of Computational Chemistry, 2007, 28, 2111-2121.	3.3	16
83	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
84	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
85	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
86	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
87	The Canonical Transformation Theory and its application to the Reaction Path Hamiltonian. Computational and Theoretical Chemistry, 2005, 727, 21-27.	1.5	2
88	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
89	Deterministic resonance formation and decay under bohmian mechanics. Computational and Theoretical Chemistry, 2005, 727, 205-212.	1.5	5
90	Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^'9). Journal of Organic Chemistry, 2005, 70, 2509-2521.	3.2	195

#	Article	IF	Citations
91	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
92	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
93	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
94	The reaction path intrinsic reaction coordinate method and the Hamiltonâ€“Jacobi theory. Journal of Chemical Physics, 2005, 122, 234105.	3.0	44
95	Extent and limitations of density-functional theory in describing magnetic systems. Physical Review B, 2004, 70, .	3.2	122
96	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
97	Generalized reaction-path Hamiltonian dynamics. Theoretical Chemistry Accounts, 2004, 112, 75-83.	1.4	16
98	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
99	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
100	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
101	Theoretical Prediction of Benzyne-Like Species in Pyrene Diradicals. Journal of Physical Chemistry A, 2004, 108, 5111-5116.	2.5	16
102	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
103	Shape and Symmetry of Heptacoordinate Transition-Metal Complexes: Structural Trends. Chemistry - A European Journal, 2003, 9, 1281-1295.	3.3	225
104	Remarks on the updated Hessian matrix methods. International Journal of Quantum Chemistry, 2003, 94, 324-332.	2.0	15
105	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
106	On the evaluation of selected eigenpairs of large matrices based on function optimization algorithms. Molecular Physics, 2003, 101, 45-51.	1.7	1
107	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
108	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

#	Article	IF	Citations
109	A reaction pathâ€“Liouville approach to the rate constant for polyatomic chemical reactions. Physical Chemistry Chemical Physics, 2002, 4, 2921-2926.	2.8	19
110	A reaction path Hamiltonian defined on a Newton path. Journal of Chemical Physics, 2002, 116, 8713-8722.	3.0	19
111	Atmospheric Formation of OH Radicals and H2O2 from Alkene Ozonolysis under Humid Conditions. ChemPhysChem, 2002, 3, 215-221.	2.1	100
112	A new look at the reduced-gradient-following path. Theoretical Chemistry Accounts, 2002, 107, 130-139.	1.4	63
113	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. Theoretical Chemistry Accounts, 2002, 107, 147-153.	1.4	16
114	On the Reaction Path Hamiltonian for Polyatomic Molecules. Journal of Physical Chemistry A, 2001, 105, 5022-5029.	2.5	18
115	Finding transition states using reduced potential-energy surfaces. Theoretical Chemistry Accounts, 2001, 105, 463-472.	1.4	81
116	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
117	Reply on the comment ?On the quadratic reaction path evaluated in a reduced potential energy surface model and the problem to locate transition states? [by J. M. Anglada, E. Besalï¿½, J. M. Bofill, and R. Crehuet, J Comput Chem 2001, 22, 4, 387-406]. Journal of Computational Chemistry, 2001, 22, 541-544.	3.3	0
118	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
119	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
120	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
121	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
122	Quantum Chemical Reactivity: Beyond the Study of Small Molecules. Mathematical and Computational Chemistry, 2001, , 125-141.	0.3	1
123	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
124	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
125	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
126	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

#	Article	IF	Citations
127	Understanding the structure/reactivity of aminium/uronium salts as coupling reagents in peptide synthesis. Tetrahedron Letters, 1999, 40, 2641-2644.	1.4	13
128	Title is missing!. Journal of Mathematical Chemistry, 1999, 25, 85-92.	1.5	15
129	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
130	Prediction of approximate transition states by Bell-Evans-Polanyi principle: I. Journal of Computational Chemistry, 1999, 20, 1112-1129.	3.3	28
131	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
132	The Ozonolysis of Ethylene: A Theoretical Study of the Gas-Phase Reaction Mechanism. Chemistry - A European Journal, 1999, 5, 1809-1822.	3.3	134
133	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
134	Use of Onium Salt-Based Coupling Reagents in Peptide Synthesis1. Journal of Organic Chemistry, 1998, 63, 9678-9683.	3.2	245
135	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
136	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
137	Calculation of clustered eigenvalues of large matrices using variance minimization method. Journal of Computational Chemistry, 1998, 19, 1777-1785.	3.3	7
138	On the automatic restricted-step rational-function-optimization method. Theoretical Chemistry Accounts, 1998, 100, 265-274.	1.4	41
139	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
140	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
141	Electronic Structure and Unimolecular Reactions of Cyclopropenone Carbonyl Oxide. A Theoretical Studyâ€. Journal of Organic Chemistry, 1997, 62, 2720-2726.	3.2	21
142	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
143	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
144	A symmetric orthogonal transformation applied to molecular geometry optimizations constrained on a hypersphere. Chemical Physics Letters, 1997, 269, 469-474.	2.6	1

#	Article	IF	Citations
145	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
146	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
147	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
148	Practical remarks on the selection of the active space in the CAS-SCF wavefunction. Chemical Physics Letters, 1995, 243, 151-157.	2.6	44
149	Analysis of the updated Hessian matrices for locating transition structures. Journal of Computational Chemistry, 1995, 16, 1326-1338.	3.3	32
150	A theoretical study of benzoin condensation. Computational and Theoretical Chemistry, 1995, 339, 179-194.	1.5	23
151	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
152	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
153	A geometry optimization benchmark using highly correlated wavefunctions (FCI and MRD-CI). Theoretica Chimica Acta, 1995, 92, 369-381.	0.8	23
154	A Conjugate Gradient Algorithm with a Trust Region for Molecular Geometry Optimization. Journal of Molecular Modeling, 1995, 1, 11-17.	1.8	6
155	A geometry optimization benchmark using highly correlated wavefunctions (FCI and MRD-CI). Theoretica Chimica Acta, 1995, 92, 369.	0.8	0
156	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
157	Energy partitioning using two-electron average matrices. Chemical Physics Letters, 1994, 222, 51-57.	2.6	5
158	Updated Hessian matrix and the restricted step method for locating transition structures. Journal of Computational Chemistry, 1994, 15, 1-11.	3.3	212
159	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
160	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
161	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
162	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

#	Article	IF	Citations
163	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
164	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
165	Kinetic interpretation of aromaticity: a theoretical study. Journal of Organic Chemistry, 1988, 53, 5148-5149.	3.2	18
166	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
167	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