Wolfgang Quapp

List of Publications by Year
in descending order

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100	2,535	201385	223531
papers	citations	27 h-index	46 g-index

101	101	101	1099
all docs	docs citations	times ranked	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.	0.9	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.	2.3	6
3	A generalized Frenkelâ€“Kontorova model for a propagating austeniteâ€“martensite phase boundary: revisited numerically. European Physical Journal B, 2022, 95, .	0.6	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.	2.3	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.	0.6	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.	0.6	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.	0.6	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.	0.8	8
9	Comment on â€œExploring Potential Energy Surface with External Forcesâ€. Journal of Chemical Theory and Computation, 2020, 16, 811-815.	2.3	1
10	Some Mathematical Reasoning on the Artificial Force Induced Reaction Method. Journal of Computational Chemistry, 2020, 41, 629-634.	1.5	8
11	The movement of a one-dimensional Wigner solid explained by a modified Frenkel-Kontorova model. European Physical Journal B, 2020, 93, 1.	0.6	4
12	Quantum Zermelo problem for general energy resource bounds. Physical Review Research, 2020, 2, .	1.3	2
13	Interplay between the Gentlest Ascent Dynamics Method and Conjugate Directions to Locate Transition States. Journal of Chemical Theory and Computation, 2019, 15, 5426-5439.	2.3	3
14	Sliding paths for series of Frenkel-Kontorova models â€“ a contribution to the concept of 1D-superlubricity. European Physical Journal B, 2019, 92, 1.	0.6	11
15	Conformational analysis of enantiomerization coupled to internal rotation in triptycyl-n-helicenes. Physical Chemistry Chemical Physics, 2019, 21, 11395-11404.	1.3	1
16	A model for a driven Frenkelâ€“Kontorova chain. European Physical Journal B, 2019, 92, 1.	0.6	8
17	Newton trajectories for the tilted Frenkelâ€“Kontorova model. Molecular Physics, 2019, 117, 1541-1558.	0.8	14
18	A minimal 2D model of the free energy surface for a unidirectional natural molecular motor. Journal of Mathematical Chemistry, 2018, 56, 1339-1347.	0.7	4

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19	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.	1.0	13
20	Toward a theory of mechanochemistry: Simple models from the very beginnings. International Journal of Quantum Chemistry, 2018, 118, e25775.	1.0	18
21	Exploring potential energy surfaces with gentlest ascent dynamics in combination with the shrinking dimer method and Newtonian dynamics. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
22	Analysis of the Acting Forces in a Theory of Catalysis and Mechanochemistry. Journal of Physical Chemistry A, 2017, 121, 2820-2838.	1.1	24
23	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.	1.2	22
24	A contribution to a theory of mechanochemical pathways by means of Newton trajectories. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	24
25	Reaction rates in a theory of mechanochemical pathways. Journal of Computational Chemistry, 2016, 37, 2467-2478.	1.5	20
26	Comment on â€œReaction Coordinates and Pathways of Mechanochemical Transformationsâ€• Journal of Physical Chemistry B, 2016, 120, 2644-2645.	1.2	8
27	Can we understand the branching of reaction valleys for more than two degrees of freedom?. Journal of Mathematical Chemistry, 2016, 54, 137-148.	0.7	9
28	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.	0.5	9
29	Comment on â€œAnalyses of bifurcation of reaction pathways on a global reaction route map: A case study of gold cluster Au5â€•[J. Chem. Phys. 143, 014301 (2015)]. Journal of Chemical Physics, 2015, 143, 177101.	1.2	5
30	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.	1.0	13
31	Some remarks on the model of the extended gentlest ascent dynamics. Journal of Mathematical Chemistry, 2015, 53, 41-57.	0.7	6
32	Level sets as progressing waves: an example for wake-free waves in every dimension. Journal of Mathematical Chemistry, 2014, 52, 654-664.	0.7	1
33	Locating saddle points of any index on potential energy surfaces by the generalized gentlest ascent dynamics. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	12
34	Analysis of the Valley-Ridge inflection points through the partitioning technique of the Hessian eigenvalue equation. Journal of Mathematical Chemistry, 2013, 51, 1099-1115.	0.7	23
35	Search of manifolds of nonsymmetric Valley-Ridge inflection points on the potential energy surface of HCN. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	15
36	Unusual reaction paths of SN2 nucleophile substitution reactions CH4+Hâ¯â†'CH4+Hâ¯ and CH4+Fâ¯â†'CH3F+Hâ¯: Quantum chemical calculations. Chemical Physics, 2013, 425, 170-176.	0.9	13

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37	Locating transition states on potential energy surfaces by the gentlest ascent dynamics. Chemical Physics Letters, 2013, 583, 203-208.	1.2	16
38	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.	0.7	13
39	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.	2.3	3
40	The Variational Structure of Gradient Extremals. Journal of Chemical Theory and Computation, 2012, 8, 927-935.	2.3	20
41	Search for conical intersection points (CI) by Newton trajectories. Chemical Physics Letters, 2012, 541, 122-127.	1.2	10
42	An empirical, variational method of approach to unsymmetric valley-ridge inflection points. Theoretical Chemistry Accounts, 2011, 128, 47-61.	0.5	30
43	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.	0.5	19
44	Reply to the comment by Sheppard and Henkelman on the nudged elastic band method. Journal of Computational Chemistry, 2011, 32, 1772-1773.	1.5	1
45	Variational nature, integration, and properties of Newton reaction path. Journal of Chemical Physics, 2011, 134, 074101.	1.2	30
46	Transition state theory with Tsallis statistics. Journal of Computational Chemistry, 2010, 31, 573-585.	1.5	17
47	A comment to the nudged elastic band method. Journal of Computational Chemistry, 2010, 31, 2526-2531.	1.5	7
48	THE GROWING STRING METHOD FOR FLOWS OF NEWTON TRAJECTORIES BY A SECOND-ORDER METHOD. Journal of Theoretical and Computational Chemistry, 2009, 08, 101-117.	1.8	15
49	Chemical reaction paths and calculus of variations. Theoretical Chemistry Accounts, 2008, 121, 227-237.	0.5	29
50	The mechanism of a barrierless reaction: hidden transition state and hidden intermediates in the reaction of methylene with ethene. Molecular Physics, 2007, 105, 2697-2717.	0.8	45
51	Finding the Transition State of Quasi-Barrierless Reactions by a Growing String Method for Newton Trajectories:â€‰ Application to the Dissociation of Methylenecyclopropene and Cyclopropane. Journal of Physical Chemistry A, 2007, 111, 11287-11293.	1.1	22
52	Finding the transition state without initial guess: The growing string method for Newton trajectory to isomerization and enantiomerization reaction of alanine dipeptide and poly(15)alanine. Journal of Computational Chemistry, 2007, 28, 1834-1847.	1.5	27
53	Test for non-linearity concerning linear calibrated chemical measurements. Accreditation and Quality Assurance, 2006, 11, 625-631.	0.4	48
54	Newton leaves on potential energy surfaces. Theoretical Chemistry Accounts, 2005, 113, 58-62.	0.5	2

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55	A growing string method for the reaction pathway defined by a Newton trajectory. Journal of Chemical Physics, 2005, 122, 174106.	1.2	54
56	Reaction Pathways and Convexity of the Potential Energy Surface: Application of Newton Trajectories. Journal of Mathematical Chemistry, 2004, 36, 307-340.	0.7	40
57	Newton Trajectories in the Curvilinear Metric of Internal Coordinates. Journal of Mathematical Chemistry, 2004, 36, 365-379.	0.7	19
58	An approach to reaction path branching using valley?ridge inflection points of potential-energy surfaces. Theoretical Chemistry Accounts, 2004, 112, 40-51.	0.5	64
59	Reaction pathways and projection operators: Application to string methods. Journal of Computational Chemistry, 2004, 25, 1277-1285.	1.5	26
60	Reaction channels of the potential energy surface: application of Newton trajectories. Computational and Theoretical Chemistry, 2004, 683, 1-13.	1.5	48
61	How does a reaction path branching take place? A classification of bifurcation events. Journal of Molecular Structure, 2004, 695-696, 95-101.	1.8	70
62	The reaction pathway of a potential energy surface as curve with induced tangent. Chemical Physics Letters, 2004, 395, 150-156.	1.2	38
63	REDUCED GRADIENT METHODS AND THEIR RELATION TO REACTION PATHS. Journal of Theoretical and Computational Chemistry, 2003, 02, 385-417.	1.8	69
64	A Valley Following Method. Optimization, 2003, 52, 317-331.	1.0	10
65	The Bending Vibrational Ladder of H13C15N by Hot Gas Emission Spectroscopy. Journal of Molecular Spectroscopy, 2002, 211, 189-197.	0.4	10
66	High-Temperature Infrared Emission Spectra of D12C14N and D13C14N. Journal of Molecular Spectroscopy, 2002, 212, 22-31.	0.4	12
67	Determination of energy minima and saddle points using multireference configuration interaction methods in combination with reduced gradient following: The S0 surface of H2CO and the T1 and T2 surfaces of acetylene. Journal of Computational Chemistry, 2002, 23, 576-583.	1.5	41
68	Improved RGF method to find saddle points. Journal of Computational Chemistry, 2002, 23, 887-894.	1.5	45
69	Exploring the potential energy surface of the ethyl cation by new procedures. Computational and Theoretical Chemistry, 2002, 585, 105-117.	1.5	24
70	Comment on â€œCritical points and reaction paths characterization on a potential energy hypersurfaceâ€• [J. Chem. Phys. 112, 4923 (2000)]. Journal of Chemical Physics, 2001, 114, 609.	1.2	8
71	Valley ridge inflection points on the potential energy surfaces of H2S, H2Se and H2CO. Physical Chemistry Chemical Physics, 2001, 3, 2735-2741.	1.3	25
72	Searching minima of an N-dimensional surface: A robust valley following method. Computers and Mathematics With Applications, 2001, 41, 407-414.	1.4	12

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73	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, 537-540.	1.5	23
74	High-Temperature Infrared Measurements in the Region of the Bending Fundamental of H12C14N, H12C15N, and H13C14N. Journal of Molecular Spectroscopy, 2000, 202, 67-82.	0.4	93
75	A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe. Chemical Physics, 2000, 253, 295-303.	0.9	26
76	Following the streambed reaction on potential-energy surfaces: a new robust method. Theoretical Chemistry Accounts, 2000, 105, 145-155.	0.5	30
77	Climbing the Bending Vibrational Ladder in D13C15N by Hot Gas Emission Spectroscopy. Journal of Molecular Spectroscopy, 1999, 195, 284-298.	0.4	25
78	The set of valleyâ€“ridge inflection points on the potential energy surface of water. Physical Chemistry Chemical Physics, 1999, 1, 5291-5299.	1.3	49
79	Infrared Spectrum of15N13C13C15N near 2100 cmâˆ’1. Journal of Molecular Spectroscopy, 1998, 187, 126-130.	0.4	6
80	Searching for saddle points of potential energy surfaces by following a reduced gradient. Journal of Computational Chemistry, 1998, 19, 1087-1100.	1.5	165
81	Bifurcation of reaction pathways: the set of valley ridge inflection points of a simple three-dimensional potential energy surface. Theoretical Chemistry Accounts, 1998, 100, 285-299.	0.5	129
82	Intensity Measurements of Î”l> 1 Transitions of Several Isotopomers of HCN. Journal of Molecular Spectroscopy, 1997, 185, 356-369.	0.4	23
83	A gradient-only algorithm for tracing a reaction path uphill to the saddle of a potential energy surface. Chemical Physics Letters, 1996, 253, 286-292.	1.2	42
84	Infrared Transitions of H12C14N and H12C15N between 500 and 10000 cmâˆ’1. Journal of Molecular Spectroscopy, 1996, 180, 323-336.	0.4	62
85	The CN Mode of HCN: A Comparative Study of the Variation of the Transition Dipole and Hermanâ€“Wallis Constants for Seven Isotopomers and the Influence of Vibrationâ€“Rotation Interaction. Journal of Molecular Spectroscopy, 1995, 174, 365-378.	0.4	40
86	Intensities of Hot-Band Transitions: HCN Hot Bands. Journal of Molecular Spectroscopy, 1995, 171, 420-434.	0.4	47
87	The Invariance of the Reaction Path Description in Any Coordinate System. , 1995, , 95-107.		5
88	Gradient Extremals and Their Relation to the Minimum Energy Path. , 1995, , 137-160.		15
89	Fourier Transform Spectra of Overtone Bands of HCN from 4800 to 9600 cmâˆ’1: Some New Transitions of Bending Combination Modes. Journal of Molecular Spectroscopy, 1994, 167, 375-382.	0.4	19
90	An approach to a realistic visualization of curvilinear molecular vibrations. Computational and Theoretical Chemistry, 1994, 315, 35-42.	1.5	4

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91	The FT-IR Spectrum of HC15NO: The Î½1, Î½2, 2Î½3, and Î½2 + Î½3 Band Systems. Journal of Molecular Spectroscopy, 1993, 160, 540-553.	0.4	15
92	What you thought you already knew about the bending motion of triatomic molecules. Journal of Mathematical Chemistry, 1993, 14, 259-285.	0.7	22
93	An analytical computation of Christoffel symbols for reaction coordinate and trajectory treatments under internal coordinates. Journal of Mathematical Chemistry, 1991, 6, 77-90.	0.7	5
94	The mass weighting problem of potential energy surfaces for chemical reactions: dissociation and isomerisation pathways of HCN. Computational and Theoretical Chemistry, 1990, 205, 245-259.	1.5	10
95	Internal vibrational energy redistribution and vibrationally induced nonlinearity of HCN. Journal of Molecular Structure, 1990, 218, 261-266.	1.8	3
96	Gradient extremals and valley floor bifurcations on potential energy surfaces. Theoretica Chimica Acta, 1989, 75, 447-460.	0.9	87
97	Interpretation of the IR spectral intensity anomaly of HCN by potential energy surface bifurcation along a normal mode. Infrared Physics, 1988, 28, 83-89.	0.5	6
98	A redefined anharmonic potential energy surface of HCN. Journal of Molecular Spectroscopy, 1987, 125, 122-127.	0.4	43
99	Saddle points of index 2 on potential energy surfaces and their role in theoretical reactivity investigations. Theoretica Chimica Acta, 1986, 70, 89-98.	0.9	49
100	Analysis of the concept of minimum energy path on the potential energy surface of chemically reacting systems. Theoretica Chimica Acta, 1984, 66, 245-260.	0.9	120