Michael A Collins

List of Publications by Year
in descending order

81	4,531	117453	98622
papers	citations	34 h-index	67 g-index

83	83	83	1647
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accelerating the Calculation of Soluteâ€“Solvent Interaction Energies through Systematic Molecular Fragmentation. Journal of Physical Chemistry A, 2019, 123, 8476-8484.	1.1	3
2	The SMFA program for quantum chemistry calculations on large molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1413.	6.2	6
3	Application of the Systematic Molecular Fragmentation by Annihilation Method to ab Initio NMR Chemical Shift Calculations. Journal of Physical Chemistry A, 2018, 122, 9135-9141.	1.1	12
4	Microsolvation within the Systematic Molecular Fragmentation by Annihilation Approach. Journal of Physical Chemistry A, 2017, 121, 334-341.	1.1	16
5	Can Systematic Molecular Fragmentation Be Applied to Direct Ab Initio Molecular Dynamics?. Journal of Physical Chemistry A, 2016, 120, 9281-9291.	1.1	15
6	Energy-Based Molecular Fragmentation Methods. Chemical Reviews, 2015, 115, 5607-5642.	23.0	240
7	Approximating CCSD(T) Nuclear Magnetic Shielding Calculations Using Composite Methods. Journal of Chemical Theory and Computation, 2015, 11, 5177-5181.	2.3	17
8	Calculating nuclear magnetic resonance shieldings using systematic molecular fragmentation by annihilation. Physical Chemistry Chemical Physics, 2015, 17, 5314-5320.	1.3	17
9	H₂ Adsorption in a Porous Crystal: Accurate First-Principles Quantum Simulation. Journal of Physical Chemistry A, 2015, 119, 12166-12181.	1.1	5
10	Molecular forces, geometries, and frequencies by systematic molecular fragmentation including embedded charges. Journal of Chemical Physics, 2014, 141, 094108.	1.2	43
11	Systematic Study of Locally Dense Basis Sets for NMR Shielding Constants. Journal of Chemical Theory and Computation, 2014, 10, 146-152.	2.3	44
12	The Combined Fragmentation and Systematic Molecular Fragmentation Methods. Accounts of Chemical Research, 2014, 47, 2776-2785.	7.6	69
13	Molecular electrostatic potentials by systematic molecular fragmentation. Journal of Chemical Physics, 2013, 139, 184117.	1.2	13
14	Growing Fragmented Potentials for Gasâ€“Surface Reactions: The Reaction between Hydrogen Atoms and Hydrogen-Terminated Silicon (111). Journal of Physical Chemistry C, 2012, 116, 7793-7802.	1.5	14
15	The fragment molecular orbital and systematic molecular fragmentation methods applied to water clusters. Physical Chemistry Chemical Physics, 2012, 14, 7752.	1.3	61
16	Systematic fragmentation of large molecules by annihilation. Physical Chemistry Chemical Physics, 2012, 14, 7744.	1.3	82
17	Potential energy surfaces for gas-surface reactions. Physical Chemistry Chemical Physics, 2011, 13, 8379.	1.3	29
18	Ab initio lattice dynamics of nonconducting crystals by systematic fragmentation. Journal of Chemical Physics, 2011, 134, 164110.	1.2	20

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19	An ab initio quasi-diabatic potential energy matrix for OH(2Î£) + H2. Journal of Chemical Physics, 2011, 135, 234307.	1.2	24
20	Converged quantum dynamics with modified Shepard interpolation and Gaussian wave packets. Chemical Physics Letters, 2010, 489, 242-247.	1.2	38
21	Accurate treatment of nonbonded interactions within systematic molecular fragmentation. Journal of Chemical Physics, 2009, 131, .	1.2	66
22	Systematic Fragmentation Method and the Effective Fragment Potential: An Efficient Method for Capturing Molecular Energies. Journal of Physical Chemistry A, 2009, 113, 10040-10049.	1.1	65
23	Locally Optimized Coordinates in Modified Shepard Interpolation. Journal of Physical Chemistry A, 2009, 113, 3979-3987.	1.1	11
24	Molecular potential energy surfaces constructed from interpolation of systematic fragment surfaces. Journal of Chemical Physics, 2007, 127, 024104.	1.2	61
25	Ab initio energies of nonconducting crystals by systematic fragmentation. Journal of Chemical Physics, 2007, 127, 134113.	1.2	66
26	The Interface Between Electronic Structure Theory and Reaction Dynamics by Reaction Path Methods. Advances in Chemical Physics, 2007, , 389-453.	0.3	21
27	Solitons in Chemical Physics. Advances in Chemical Physics, 2007, , 225-339.	0.3	46
28	Accuracy and efficiency of electronic energies from systematic molecular fragmentation. Journal of Chemical Physics, 2006, 125, 104104.	1.2	160
29	Interpolation of multidimensional diabatic potential energy matrices. Journal of Chemical Physics, 2006, 125, 104105.	1.2	85
30	Interpolated potential energy surface for abstraction and exchange reactions of NH3 + H and deuterated analogues. Theoretical Chemistry Accounts, 2005, 113, 225-232.	0.5	33
31	Interpolation of diabatic potential-energy surfaces: Quantum dynamics on ab initio surfaces. Journal of Chemical Physics, 2005, 123, 134110.	1.2	53
32	Approximateab initioenergies by systematic molecular fragmentation. Journal of Chemical Physics, 2005, 122, 154102.	1.2	255
33	Classical trajectory studies of the photodissociation reaction of sym-triazine. Physical Chemistry Chemical Physics, 2004, 6, 945.	1.3	14
34	Molecular potential energy surfaces by interpolation: Strategies for faster convergence. Journal of Chemical Physics, 2004, 121, 9769-9775.	1.2	24
35	Interpolation of diabatic potential energy surfaces. Journal of Chemical Physics, 2004, 121, 2515.	1.2	64
36	FIRST PRINCIPLES QUANTUM DYNAMICAL STUDY OF FOUR-ATOM REACTIONS. Advanced Series in Physical Chemistry, 2004, , 409-464.	1.5	4

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37	Calculation of accurate imaginary frequencies and tunnelling coefficients for hydrogen abstraction reactions using IRCmax. Molecular Physics, 2003, 101, 1329-1338.	0.8	37
38	Proton-transport catalysis, proton abstraction, and proton exchange in HF+HOC+ and H2O+HOC+ and analogous deuterated reactions. Journal of Chemical Physics, 2003, 118, 6222-6229.	1.2	23
39	The dynamics of the H+D2Oâ†'OD+HD reaction at 2.5 eV: Experiment and theory. Journal of Chemical Physics, 2003, 118, 1162-1174.	1.2	19
40	Interpolated potential energy surface and classical dynamics for H3++HD and H3++D2. Journal of Chemical Physics, 2003, 119, 5510-5517.	1.2	39
41	Probing the transition state via photoelectron and photodetachment spectroscopy of H3O-. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 11579-11582.	3.3	43
42	Molecular potential-energy surfaces for chemical reaction dynamics. Theoretical Chemistry Accounts, 2002, 108, 313-324.	0.5	370
43	A classical trajectory study of sym-triazine photodissociation on an interpolated potential energy surface. Chemical Physics Letters, 2001, 335, 481-488.	1.2	25
44	Capture rates for collisions of C (3Pj) and Ge (1S0) with unsaturated hydrocarbons. Journal of Chemical Physics, 2001, 114, 10342-10354.	1.2	3
45	Interpolated potential-energy surface and reaction dynamics for BH++H2. Journal of Chemical Physics, 2001, 114, 10711-10716.	1.2	14
46	Proton-transport catalysis and proton-abstraction reactions: Anab initiodynamical study of X+HOC+ and XH++CO (X=Ne, Ar, and Kr). Journal of Chemical Physics, 2000, 112, 6625-6634.	1.2	26
47	First-Principles Theory for the H + H2O, D2O Reactions. Science, 2000, 290, 961-963.	6.0	203
48	Learning to interpolate molecular potential energy surfaces with confidence: A Bayesian approach. Journal of Chemical Physics, 1999, 111, 816-826.	1.2	212
49	Interpolated potential energy surface and reaction dynamics for O(3P)+H3+(1A1â€²) and OH+(3Î£â˜)+H2(1Î£g+). Journal of Chemical Physics, 1999, 111, 6322-6332.	1.2	43
50	Construction of interpolated potential energy surfaces using constrained dynamics: Application to rotational inelastic scattering. Journal of Chemical Physics, 1999, 111, 1346-1353.	1.2	11
51	Molecular potential energy surfaces by interpolation in Cartesian coordinates. Journal of Chemical Physics, 1998, 108, 564-578.	1.2	83
52	Polyatomic molecular potential energy surfaces by interpolation in local internal coordinates. Journal of Chemical Physics, 1998, 108, 8302-8316.	1.2	226
53	Potential energy surfaces and dynamics for the reactions between C(3P) and H3+(1A1â€²). Journal of Chemical Physics, 1998, 108, 2424-2433.	1.2	42
54	Interpolated potential energy surface and dynamics for the reactions between N(4S) and H3+(1A1â€²). Journal of Chemical Physics, 1998, 109, 9728-9736.	1.2	41

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55	Molecular potential-energy surfaces by interpolation: Further refinements. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 871-878.	1.7	122
56	An interpolated unrestricted Hartreeâ€“Fock potential energy surface for the OH+H2â†'H2O+H reaction. Journal of Chemical Physics, 1996, 104, 4600-4610.	1.2	69
57	Convergence of molecular potential energy surfaces by interpolation: Application to the OH+H2â†'H2O+H reaction. Journal of Chemical Physics, 1995, 102, 5647-5657.	1.2	213
58	The utility of higher order derivatives in constructing molecular potential energy surfaces by interpolation. Journal of Chemical Physics, 1995, 103, 9669-9675.	1.2	99
59	DYNAMICAL DISORDER IN A MODEL OF BASE PAIR MOTION IN DNA. , 1995, , .		0
60	SOLITARY WAVES IN POLYETHYLENE CRYSTALS. , 1995, , .		0
61	A model classical study of nonlinear resonance and torsional isomerization. Journal of Chemical Physics, 1994, 101, 307-321.	1.2	13
62	Quantum simulations of nonlinear resonance and torsional dynamics. Journal of Chemical Physics, 1994, 100, 2089-2103.	1.2	12
63	Molecular potential energy surfaces by interpolation. Journal of Chemical Physics, 1994, 100, 8080-8088.	1.2	438
64	Intramolecular vibrational energy redistribution and trapping in centroâ€symmetric chains by Fermi resonance. Journal of Chemical Physics, 1993, 98, 1817-1825.	1.2	10
65	Nonlinear resonance and torsional dynamics: Model simulations of HOOH and CH3OOCH3. Journal of Chemical Physics, 1993, 98, 1132-1148.	1.2	13
66	Implications of rotationâ€“inversionâ€“permutation invariance for analytic molecular potential energy surfaces. Journal of Chemical Physics, 1993, 99, 6756-6772.	1.2	67
67	Reaction path potentials in internal coordinates: Application to the dissociation of HCOH.+. Journal of Chemical Physics, 1992, 97, 4913-4920.	1.2	9
68	Potential energy surfaces describing ion complexes containing molecular hydrogen. Journal of Chemical Physics, 1992, 97, 1191-1210.	1.2	19
69	Classical trajectory study of the decomposition of HCOHâ‹…+ on a symmetryâ€invariant potentialâ€energy surface. Journal of Chemical Physics, 1992, 96, 1093-1104.	1.2	11
70	Symmetryâ€invariant reactionâ€path potentials. Journal of Chemical Physics, 1991, 94, 7084-7097.	1.2	31
71	Scaling the reaction path potential. Journal of Chemical Physics, 1990, 93, 4938-4945.	1.2	5
72	Simulation of coherent energy transfer in a hydrogen bonded amide chain by Fermi resonance. Journal of Chemical Physics, 1990, 93, 7894-7913.	1.2	12

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73	Simple model of coherent energy transfer by Fermi resonance. Journal of Chemical Physics, 1990, 92, 5602-5611.	1.2	23
74	Optical properties of poly-diacetylene monolayers. Journal of Polymer Science, Part B: Polymer Physics, 1988, 26, 367-387.	2.4	7
75	Determination of the intrinsic reaction coordinate: Comparison of gradient and local quadratic approximation methods. Journal of Chemical Physics, 1988, 89, 2881-2885.	1.2	43
76	The energy of the resonance soliton. Journal of Chemical Physics, 1988, 88, 399-404.	1.2	2
77	A classical trajectory study of the high CH and CD overtones in benzene and perdeuterobenzene. Journal of Chemical Physics, 1987, 86, 6871-6881.	1.2	23
78	CH and CD overtone decay times in partially deuterated benzenes. Journal of Chemical Physics, 1987, 87, 5312-5316.	1.2	19
79	Solitons in resonant energy transfer. International Reviews in Physical Chemistry, 1986, 5, 203-210.	0.9	2
80	Generalized Langer corrections. Journal of Chemical Physics, 1986, 85, 3902-3905.	1.2	3
81	Classical limit quantum mechanics for indistinguishable particles. Journal of Chemical Physics, 1984, 80, 279-288.	1.2	2