Hai Lin

List of Publications by Year
in descending order

96 papers	3,993 citations	136950 32 h-index	118850 62 g-index
98 all docs	98 docs citations	98 times ranked	3129 citing authors

#	Article	IF	Citations
1	QM/MM: what have we learned, where are we, and where do we go from here?. Theoretical Chemistry Accounts, 2007, 117, 185-199.	1.4	1,053
2	The Elusive Oxidant Species of Cytochrome P450 Enzymes:â€‰ Characterization by Combined Quantum Mechanical/Molecular Mechanical (QM/MM) Calculations. Journal of the American Chemical Society, 2002, 124, 8142-8151.	13.7	290
3	Quantum Mechanical/Molecular Mechanical Investigation of the Mechanism of Câˆ’H Hydroxylation of Camphor by Cytochrome P450cam:Â Theory Supports a Two-State Rebound Mechanism. Journal of the American Chemical Society, 2004, 126, 4017-4034.	13.7	269
4	Adaptive Partitioning in Combined Quantum Mechanical and Molecular Mechanical Calculations of Potential Energy Functions for Multiscale Simulations. Journal of Physical Chemistry B, 2007, 111, 2231-2241.	2.6	172
5	Identifying Molecular Orientation of IndividualC60on aSi(111)âˆ’(7Ã—7)Surface. Physical Review Letters, 1999, 83, 3001-3004.	7.8	135
6	Redistributed Charge and Dipole Schemes for Combined Quantum Mechanical and Molecular Mechanical Calculations. Journal of Physical Chemistry A, 2005, 109, 3991-4004.	2.5	123
7	Green Fluorescent Proteins:Â Empirical Force Field for the Neutral and Deprotonated Forms of the Chromophore. Molecular Dynamics Simulations of the Wild Type and S65T Mutant. Journal of Physical Chemistry B, 2002, 106, 6310-6321.	2.6	110
8	Vibrational energies for NH3 based on high level ab initio potential energy surfaces. Journal of Chemical Physics, 2002, 117, 11265-11276.	3.0	68
9	Potential-energy surface for the electronic ground state of NH3 up to 20000cmâˆ’1 above equilibrium. Journal of Chemical Physics, 2005, 123, 134308.	3.0	68
10	Self-Consistent Polarization of the Boundary in the Redistributed Charge and Dipole Scheme for Combined Quantum-Mechanical and Molecular-Mechanical Calculations. Journal of Chemical Theory and Computation, 2007, 3, 1378-1398.	5.3	65
11	High-Resolution Study of Strongly Interacting Vibrational Bands of HDO in the Region 7600â€“8100 cmâˆ’1. Journal of Molecular Spectroscopy, 2000, 203, 228-234.	1.2	62
12	Adaptive quantum/molecular mechanics: what have we learned, where are we, and where do we go from here?. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1310.	14.6	60
13	High-Resolution Fourier Transform Spectrum of the D2O Molecule in the Region of the Second Triad of Interacting Vibrational States. Journal of Molecular Spectroscopy, 2000, 200, 34-39.	1.2	55
14	Rotationâ€“vibration motion of pyramidal XY3molecules described in the Eckart frame: Theory and application to NH3. Molecular Physics, 2005, 103, 359-378.	1.7	55
15	Recent developments in QM/MM methods towards open-boundary multi-scale simulations. Molecular Simulation, 2015, 41, 168-189.	2.0	55
16	High-Resolution Study of the First Hexad of D2O. Journal of Molecular Spectroscopy, 2000, 200, 25-33.	1.2	52
17	High-Resolution Study of the (v1 + 12v2 + v3 = 3) Polyad of Strongly Interacting Vibrational Bands of D2O. Journal of Molecular Spectroscopy, 2000, 204, 216-225.	1.2	52
18	High-Resolution Fourier-Transform Intracavity Laser Absorption Spectroscopy of D2O in the Region of the 4Î½1+Î½3 Band. Journal of Molecular Spectroscopy, 2002, 212, 89-95.	1.2	52

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19	Adaptive-Partitioning QM/MM for Molecular Dynamics Simulations: 4. Proton Hopping in Bulk Water. Journal of Chemical Theory and Computation, 2015, 11, 2398-2411.	5.3	49
20	Adaptive-Partitioning Redistributed Charge and Dipole Schemes for QM/MM Dynamics Simulations: On-the-fly Relocation of Boundaries that Pass through Covalent Bonds. Journal of Chemical Theory and Computation, 2011, 7, 3625-3634.	5.3	48
21	The high-affinity calcium sensor synaptotagmin-7 serves multiple roles in regulated exocytosis. Journal of General Physiology, 2018, 150, 783-807.	1.9	48
22	Combined valence bond-molecular mechanics potential-energy surface and direct dynamics study of rate constants and kinetic isotope effects for the H+C2H6 reaction. Journal of Chemical Physics, 2006, 124, 044315.	3.0	47
23	High resolution vibration-rotation spectrum of the D2O molecule in the region near the 2Î½1+ Î½2+ Î½3absorption band. Molecular Physics, 2001, 99, 931-937.	1.7	45
24	Flexible-Boundary Quantum-Mechanical/Molecular-Mechanical Calculations:â€‰ Partial Charge Transfer between the Quantum-Mechanical and Molecular-Mechanical Subsystems. Journal of Chemical Theory and Computation, 2008, 4, 414-425.	5.3	45
25	Dipole moment and rovibrational intensities in the electronic ground state of NH3: Bridging the gap betweenab initiotheory and spectroscopic experiment. Journal of Chemical Physics, 2005, 122, 104317.	3.0	43
26	Specific Reaction Path Hamiltonian for Proton Transfer in Water: Reparameterized Semiempirical Models. Journal of Chemical Theory and Computation, 2013, 9, 2672-2686.	5.3	42
27	Multiconfiguration Molecular Mechanics Based on Combined Quantum Mechanical and Molecular Mechanical Calculations. Journal of Chemical Theory and Computation, 2006, 2, 1237-1254.	5.3	38
28	Rotationâ€“Vibration Motion of Pyramidal XY3 Molecules Described in the Eckart Frame: The Calculation of Intensities with Application to NH3. Advances in Quantum Chemistry, 2005, 48, 209-238.	0.8	37
29	Adaptive-Partitioning QM/MM Dynamics Simulations: 3. Solvent Molecules Entering and Leaving Protein Binding Sites. Journal of Chemical Theory and Computation, 2014, 10, 4765-4776.	5.3	36
30	Fourier-transform intra-cavity laser absorption spectroscopy of HOD Î½OD=5 overtone. Physical Chemistry Chemical Physics, 1999, 1, 3727-3730.	2.8	35
31	QM/MM Study of the Productâ^'Enzyme Complex in P450cam Catalysis. Journal of Physical Chemistry B, 2004, 108, 10083-10088.	2.6	34
32	Efficient Molecular Mechanics for Chemical Reactions:Â Multiconfiguration Molecular Mechanics Using Partial Electronic Structure Hessians. Journal of Physical Chemistry A, 2004, 108, 4112-4124.	2.5	32
33	Multicoefficient Gaussian-3 Calculation of the Rate Constant for the OH + CH4Reaction and Its12C/13C Kinetic Isotope Effect with Emphasis on the Effects of Coordinate System and Torsional Treatment. Journal of Physical Chemistry A, 2007, 111, 11706-11717.	2.5	30
34	The synaptotagmin C2B domain calcium-binding loops modulate the rate of fusion pore expansion. Molecular Biology of the Cell, 2018, 29, 834-845.	2.1	30
35	The stretching vibrational overtone spectra of PH3: Local mode vibrational analysis, dipole moment surfaces from density functional theory and band intensities. Journal of Chemical Physics, 2001, 114, 7018-7026.	3.0	28
36	Adaptive Partitioning QM/MM for Molecular Dynamics Simulations: 6. Proton Transport through a Biological Channel. Journal of Chemical Theory and Computation, 2019, 15, 892-905.	5.3	27

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37	Infrared intracavity laser absorption spectroscopy with a continuous-scan Fourier-transform interferometer. Applied Optics, 2000, 39, 2221.	2.1	24
38	Flexible-boundary QM/MM calculations: II. Partial charge transfer across the QM/MM boundary that passes through a covalent bond. Theoretical Chemistry Accounts, 2010, 126, 315-322.	1.4	22
39	Adaptive QM/MM for Molecular Dynamics Simulations: 5. On the Energy-Conserved Permuted Adaptive-Partitioning Schemes. Molecules, 2018, 23, 2170.	3.8	22
40	High-Resolution Spectroscopic Study of the (310) Local Mode Combination Band System of AsH3. Journal of Molecular Spectroscopy, 1998, 187, 89-96.	1.2	21
41	Temperature Dependence of Carbon-13 Kinetic Isotope Effects of Importance to Global Climate Change. Journal of the American Chemical Society, 2005, 127, 2830-2831.	13.7	21
42	Membrane Docking of the Synaptotagmin 7 C2A Domain: Computation Reveals Interplay between Electrostatic and Hydrophobic Contributions. Biochemistry, 2015, 54, 5696-5711.	2.5	21
43	Membrane Docking of the Synaptotagmin 7 C2A Domain: Electron Paramagnetic Resonance Measurements Show Contributions from Two Membrane Binding Loops. Biochemistry, 2015, 54, 5684-5695.	2.5	20
44	Molecular dynamics simulations of ion solvation by flexibleâ€boundary QM/MM: Onâ€theâ€fly partial charge transfer between QM and MM subsystems. Journal of Computational Chemistry, 2014, 35, 1778-1788.	3.3	19
45	Tracking Proton Transfer through Titratable Amino Acid Side Chains in Adaptive QM/MM Simulations. Journal of Chemical Theory and Computation, 2019, 15, 5794-5809.	5.3	18
46	Local mode overtone intensities of SiH4 and GeH4 from a bond dipole model with an ab initio calculated dipole moment surface. Chemical Physics Letters, 1999, 308, 137-141.	2.6	17
47	A theoretical study of temperature dependence of cluster formation from sulfuric acid and ammonia. Chemical Physics, 2014, 433, 60-66.	1.9	17
48	The Siâ€“H stretchingâ€“bending overtone polyads of SiHF3: Assignments, band intensities, internal coordinate force field, and ab initio dipole moment surfaces. Journal of Chemical Physics, 2001, 115, 1378-1391.	3.0	16
49	The vibrational overtones of SiH4 isotopomers: experimental wavenumbers, assignment, ab initio dipole moment surfaces and intensities. Physical Chemistry Chemical Physics, 2001, 3, 3506-3517.	2.8	14
50	High resolution spectroscopic study of CH₃D in the region 5900â€“6100 cm^{â^'1}. Molecular Physics, 1999, 97, 787-795.	1.7	13
51	Quantum Tunneling in Testosterone 6Î²-Hydroxylation by Cytochrome P450: Reaction Dynamics Calculations Employing Multiconfiguration Molecularâ^'Mechanical Potential Energy Surfaces. Journal of Physical Chemistry A, 2009, 113, 11501-11508.	2.5	13
52	Charge Transfer and Polarization for Chloride Ions Bound in ClC Transport Proteins: Natural Bond Orbital and Energy Decomposition Analyses. Journal of Physical Chemistry B, 2013, 117, 16029-16043.	2.6	13
53	Regioselectivity preference of testosterone hydroxylation by cytochrome P450 3A4. Theoretical Chemistry Accounts, 2008, 121, 313-319.	1.4	12
54	Charge delocalization upon chloride ion binding in ClC chloride ion channels/transporters. Chemical Physics Letters, 2011, 502, 112-117.	2.6	12

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55	Absorption Intensity of Stretching Overtone States of Silane and Germane. Journal of Molecular Spectroscopy, 1998, 192, 249-256.	1.2	11
56	The ab initio calculated dipole moment surface and overtone relative intensities of CH chromophore in CHCl3. Journal of Chemical Physics, 2000, 112, 7484-7489.	3.0	11
57	Recent Progress in Adaptive-Partitioning QM/MM Methods for Born-Oppenheimer Molecular Dynamics. Challenges and Advances in Computational Chemistry and Physics, 2015, , 93-113.	0.6	11
58	Chloride Ion Transport by the E. coli CLC Clâ^'/H+ Antiporter: A Combined Quantum-Mechanical and Molecular-Mechanical Study. Frontiers in Chemistry, 2018, 6, 62.	3.6	10
59	Band strengths for Câ€“H stretching polyads of CHBr3 calculated by use of a two-dimensional electric dipole moment surface from density functional theory. Journal of Chemical Physics, 2001, 114, 8905-8912.	3.0	9
60	Overtones of the Siâ^'H Stretchingâ^'Bending Polyad in SiHD3: Internal Coordinate Force Field, ab initio Dipole Moment Surfaces, and Band Intensities. Journal of Physical Chemistry A, 2001, 105, 6065-6072.	2.5	9
61	Calculating relative intensities for CH stretching polyads of CHI3 with ab initio dipole moment surface. Chemical Physics Letters, 2000, 332, 569-575.	2.6	8
62	Adaptive Partitioning QM/MM Dynamics Simulations for Substrate Uptake, Product Release, and Solvent Exchange. Methods in Enzymology, 2016, 577, 341-357.	1.0	8
63	Multivalent lipid targeting by the calcium-independent C2A domain of synaptotagmin-like protein 4/granuphilin. Journal of Biological Chemistry, 2021, 296, 100159.	3.4	8
64	The high resolution spectrum of AsH3 (400) local mode state: symmetry reduction and rotational re-quantization. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 54, 1947-1960.	3.9	7
65	High-resolution spectroscopic study of H₂⁸⁰Se in the Î½(stretch) = 5 and 6 local-mode pairs states. Molecular Physics, 1999, 97, 503-510.	1.7	7
66	Nonlinearity of the Dipole Moment Surface and Intensities Anomaly of CHCl ₃. Chinese Physics Letters, 2000, 17, 13-15.	3.3	7
67	Restrained Proton Indicator in Combined Quantum-Mechanics/Molecular-Mechanics Dynamics Simulations of Proton Transfer through a Carbon Nanotube. Journal of Physical Chemistry B, 2017, 121, 8585-8592.	2.6	7
68	Anion pathways in CLCF fluoride/proton antiporters. Chemical Physics Letters, 2021, 762, 138123.	2.6	7
69	Adaptive-Partitioning Multilayer Dynamics Simulations: 1. On-the-Fly Switch between Two Quantum Levels of Theory. Journal of Chemical Theory and Computation, 2021, 17, 5456-5465.	5.3	7
70	High resolution spectroscopic study of arsine in the region 6000â€“6500 cmâ^'1. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 55, 109-119.	3.9	6
71	Alcohol Binding to the Odorant Binding Protein LUSH: Multiple Factors Affecting Binding Affinities. Biochemistry, 2010, 49, 6136-6142.	2.5	6
72	Title is missing!. , 0, , .		6

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73	High resolution vibrationâ€“rotation spectra of the arsine local mode (110 A1/E) band. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1397-1401.	1.7	5
74	Four-dimensional dipole moment surfaces and local mode vibrational band intensities of GeH4. Chemical Physics Letters, 2001, 349, 131-136.	2.6	5
75	Computational Studies of Carbodiimide Rings. Journal of Organic Chemistry, 2014, 79, 3781-3788.	3.2	5
76	Study of the Perpendicular Band Intensities of the CH Chromophore in CHCl3, CHBr3, and CHI3 with Three-Dimensional Dipole Moment Surface from Density Functional Calculations. Journal of Physical Chemistry A, 2001, 105, 8428-8433.	2.5	4
77	Poreâ€scale modeling of vapor transport in partially saturated capillary tube with variable area using chemical potential. Water Resources Research, 2016, 52, 7023-7035.	4.2	4
78	Improved indicator algorithms for tracking a hydrated proton as a local structural defect in Grotthuss diffusion in aqueous solutions. Chemical Physics Letters, 2021, 784, 139121.	2.6	4
79	Calculation of the Siâ€“H stretchingâ€“bending overtones in SiHCl[sub 3] employing ab initio potential energy and dipole moment surfaces. Journal of Chemical Physics, 2002, 116, 105.	3.0	3
80	Study of the stretching vibrational band intensities of XH4 molecules employing four-dimensionalab initio(X=C and Sn) andeffective(X=C and Si) dipole moment surfaces. Journal of Chemical Physics, 2002, 117, 10073-10080.	3.0	3
81	Coriolis interaction in the local mode (n100;F2) combination states of GeH4. Molecular Physics, 2000, 98, 1409-1413.	1.7	2
82	Cover Image, Volume 7, Issue 5. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1339.	14.6	2
83	Theoretical Quantitative Spectroscopy: Computer Simulation of Molecular Spectra. , 2006, , 171-183.		1
84	Riding elevators into and out of cells. ELife, 2020, 9, .	6.0	1
85	Membrane Association of Synaptotagmin 7 C2A Domain by Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 248a.	0.5	0
86	Combined QM/MM Study of the Translocation of Chloride Ions through Escherichia Coli Chloride Ion Transporters. Biophysical Journal, 2015, 108, 466a-467a.	0.5	0
87	Multivalent Membrane Lipid Targeting by the Calcium-Independent C2 Domains of Granuphilin: Evidence from Computation and Experiment. Biophysical Journal, 2016, 110, 432a.	0.5	0
88	The Synaptotagmin Calcium-Binding Loops Modulate the Rate of Fusion Pore Expansion. Biophysical Journal, 2018, 114, 282a.	0.5	0
89	Multivalent Membrane Lipid Targeting by the Calcium-Independent C2A Domain of Slp-4/Granuphilin. Biophysical Journal, 2018, 114, 275a.	0.5	0
90	A Computational Study of the Essential Transmembrane Protein Nark as Nitrate/Nitrite Exchanger. Biophysical Journal, 2019, 116, 399a.	0.5	0

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91	Proton Transport in E. Coli CLC Transport Protein by Adaptive QM/MM Calculations. Biophysical Journal, 2019, 116, 432a.	0.5	0
92	Membrane Binding by Synaptotagmin-Like Protein 4: Site Directed Mutagenesis of the Lipid Interaction Surface. Biophysical Journal, 2019, 116, 518a.	0.5	0
93	Membrane Binding of Synaptotagmin-Like Protein 4: Insight from Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 372a.	0.5	0
94	Using High-Throughput Structure Prediction and Evolutionary Alignment to Map Electrostatic Protein-Membrane Interactions. Biophysical Journal, 2020, 118, 394a-395a.	0.5	0
95	Electrostatic Membrane Interaction of Synaptotagmin-Like Protein 4: Simulations of Mutant C2A Domains. Biophysical Journal, 2020, 118, 527a-528a.	0.5	0
96	Enabling Proton Transport Through Ion Channels with Adaptive QM/MM. Biophysical Journal, 2020, 118, 609a.	0.5	0