Hui Li

List of Publications by Year in descending order

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32 papers	1,311 citations	394421 19 h-index	414414 32 g-index
32 all docs	32 docs citations	32 times ranked	1429 citing authors

#	Article	IF	Citations
1	The polarizable continuum model (PCM) interfaced with the fragment molecular orbital method (FMO). Journal of Computational Chemistry, 2006, 27, 976-985.	3.3	161
2	Improving the efficiency and convergence of geometry optimization with the polarizable continuum model: New energy gradients and molecular surface tessellation. Journal of Computational Chemistry, 2004, 25, 1449-1462.	3.3	144
3	Determinants of the Relative Reduction Potentials of Type-1 Copper Sites in Proteins. Journal of the American Chemical Society, 2004, 126, 8010-8019.	13.7	134
4	Partial Hessian vibrational analysis: the localization of the molecular vibrational energy and entropy. Theoretical Chemistry Accounts, 2002, 107, 211-219.	1.4	109
5	Continuum solvation of large molecules described by QM/MM: a semi-iterative implementation of the PCM/EFP interface. Theoretical Chemistry Accounts, 2003, 109, 71-84.	1.4	91
6	Continuous and smooth potential energy surface for conductorlike screening solvation model using fixed points with variable areas. Journal of Chemical Physics, 2009, 130, 074109.	3.0	75
7	Charge transfer interaction in the effective fragment potential method. Journal of Chemical Physics, 2006, 124, 214108.	3.0	74
8	Excited state geometry of photoactive yellow protein chromophore: A combined conductorlike polarizable continuum model and time-dependent density functional study. Journal of Chemical Physics, 2010, 133, 034108.	3.0	60
9	Gradients of the polarization energy in the effective fragment potential method. Journal of Chemical Physics, 2006, 125, 194103.	3.0	55
10	Energy gradients in combined fragment molecular orbital and polarizable continuum model (FMO/PCM) calculation. Journal of Computational Chemistry, 2010, 31, 778-790.	3.3	37
11	QuanPol: A full spectrum and seamless QM/MM program. Journal of Computational Chemistry, 2013, 34, 2816-2833.	3.3	37
12	The 8-Silyloxyquinoline Scaffold as a Versatile Platform for the Sensitive Detection of Aqueous Fluoride. Analytical Chemistry, 2015, 87, 4081-4086.	6.5	36
13	Quantum mechanical/molecular mechanical/continuum style solvation model: Linear response theory, variational treatment, and nuclear gradients. Journal of Chemical Physics, 2009, 131, 184103.	3.0	35
14	Polarization energy gradients in combined quantum mechanics, effective fragment potential, and polarizable continuum model calculations. Journal of Chemical Physics, 2007, 126, 124112.	3.0	30
15	Analytic energy gradient in combined time-dependent density functional theory and polarizable force field calculation. Journal of Chemical Physics, 2010, 133, 144112.	3.0	26
16	Computational Approach for Studying Optical Properties of DNA Systems in Solution. Journal of Chemical Theory and Computation, 2016, 12, 5050-5057.	5.3	26
17	Improved Photoinduced Fluorogenic Alkeneâ€“Tetrazole Reaction for Protein Labeling. Bioconjugate Chemistry, 2017, 28, 2859-2864.	3.6	23
18	Gradients of the Exchange-repulsion Energy in the General Effective Fragment Potential Method. Theoretical Chemistry Accounts, 2006, 115, 385-390.	1.4	22

#	Article	IF	Citations
19	Heterogeneous conductorlike solvation model. Journal of Chemical Physics, 2009, 131, 044123.	3.0	21
20	Note: FixSol solvation model and FIXPVA2 tessellation scheme. Journal of Chemical Physics, 2012, 137, 246101.	3.0	18
21	Composition and charge state influence on the ion-neutral collision cross sections of protonated N-linked glycopeptides: an experimental and theoretical deconstruction of coulombic repulsion vs. charge solvation effects. Analyst, The, 2019, 144, 5738-5747.	3.5	15
22	Molecular dynamics simulation of ion mobility in gases. Journal of Chemical Physics, 2018, 148, 064109.	3.0	14
23	Hydrogen Abstraction of Camphor Catalyzed by Cytochrome P450_{cam}: A QM/MM Study. Journal of Physical Chemistry B, 2016, 120, 12312-12320.	2.6	11
24	Analytic Energy Gradient in Combined Second-Order MÃ¸llerâ€“Plesset Perturbation Theory and Polarizable Force Field Calculation. Journal of Physical Chemistry A, 2011, 115, 11824-11831.	2.5	10
25	Analytic energy gradients in combined second order MÃ¸ller-Plesset perturbation theory and conductorlike polarizable continuum model calculation. Journal of Chemical Physics, 2011, 135, 144107.	3.0	9
26	Catalytic Mechanism of Amyloid-Î² Peptide Degradation by Insulin Degrading Enzyme: Insights from Quantum Mechanics and Molecular Mechanics Style MÃ¸llerâ€“Plesset Second Order Perturbation Theory Calculation. Journal of Chemical Information and Modeling, 2018, 58, 1926-1934.	5.4	9
27	An Antifungal Polycyclic Tetramate Macrolactam, Heat-Stable Antifungal Factor (HSAF), Is a Novel Oxidative Stress Modulator in Lysobacter enzymogenes. Applied and Environmental Microbiology, 2021, 87, .	3.1	8
28	Computational Methods for Biochemical Simulations Implemented in GAMESS. Methods in Molecular Biology, 2020, 2114, 123-142.	0.9	7
29	Quantum mechanical/molecular mechanical/continuum style solvation model: Time-dependent density functional theory. Journal of Chemical Physics, 2013, 139, 084106.	3.0	6
30	Mean field QM/MM method: Average position approximation. Journal of Chemical Physics, 2013, 138, 174114.	3.0	6
31	Quantum mechanical/molecular mechanical/continuum style solvation model: Second order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2014, 140, 174115.	3.0	1
32	Quantum Chemical Study of the Redox Potential of the Co(OH2)62+/3+ Couple and the Singletâ€“Quintet Gibbs Energy Difference of the Co(OH2)63+ Ion. Inorganic Chemistry, 2018, 57, 10122-10127.	4.0	1