Kin-Yiu Wong

List of Publications by Year
in descending order

29 papers	672 citations	623574 14 h-index	610775 24 g-index
30 all docs	30 docs citations	30 times ranked	715 citing authors

#	Article	IF	Citations
1	The Reaction Mechanism of Paraoxon Hydrolysis by Phosphotriesterase from Combined QM/MM Simulations. Biochemistry, 2007, 46, 13352-13369.	1.2	137
2	Experimental and computational analysis of the transition state for ribonuclease A-catalyzed RNA 2â€²-O -transphosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13002-13007.	3.3	62
3	Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach. Journal of Chemical Theory and Computation, 2014, 10, 24-34.	2.3	58
4	Active Participation of the Mg²⁺ Ion in the Reaction Coordinate of RNA Self-Cleavage Catalyzed by the Hammerhead Ribozyme. Journal of Chemical Theory and Computation, 2011, 7, 1-3.	2.3	50
5	Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment. Angewandte Chemie - International Edition, 2012, 51, 647-651.	7.2	49
6	Combined QM/MM and path integral simulations of kinetic isotope effects in the proton transfer reaction between nitroethane and acetate ion in water. Journal of Computational Chemistry, 2008, 29, 514-522.	1.5	45
7	Theoretical Analysis of Kinetic Isotope Effects on Proton Transfer Reactions between Substituted Î±-Methoxystyrenes and Substituted Acetic Acids. Journal of the American Chemical Society, 2009, 131, 13963-13971.	6.6	30
8	Systematic Approach for Computing Zero-Point Energy, Quantum Partition Function, and Tunneling Effect Based on Kleinertâ€™s Variational Perturbation Theory. Journal of Chemical Theory and Computation, 2008, 4, 1409-1422.	2.3	29
9	Mechanistic Insights into RNA Transphosphorylation from Kinetic Isotope Effects and Linear Free Energy Relationships of Model Reactions. Chemistry - A European Journal, 2014, 20, 14336-14343.	1.7	29
10	Determination of the Structure Form of the Fourth Ligand of Zinc in Acutolysin A Using Combined Quantum Mechanical and Molecular Mechanical Simulation. Journal of Physical Chemistry B, 2009, 113, 2477-2485.	1.2	28
11	Insight into the phosphodiesterase mechanism from combined QM/MM free energy simulations. FEBS Journal, 2011, 278, 2579-2595.	2.2	25
12	Exact Relation between Potential of Mean Force and Free-Energy Profile. Journal of Chemical Theory and Computation, 2012, 8, 3998-4003.	2.3	25
13	An automated integration-free path-integral method based on Kleinertâ€™s variational perturbation theory. Journal of Chemical Physics, 2007, 127, 211103.	1.2	22
14	Review of computer simulations of isotope effects on biochemical reactions: From the Bigeleisen equation to Feynman's path integral. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1782-1794.	1.1	19
15	Ab initio pathâ€integral calculations of kinetic and equilibrium isotope effects on baseâ€catalyzed RNA transphosphorylation models. Journal of Computational Chemistry, 2014, 35, 1302-1316.	1.5	14
16	Review of Feynmanâ€™s Path Integral in Quantum Statistics: from the Molecular SchrÃ¶dinger Equation to Kleinertâ€™s Variational Perturbation Theory. Communications in Computational Physics, 2014, 15, 853-894.	0.7	11
17	Bridging the Gap Between Theory and Experiment to Derive a Detailed Understanding of Hammerhead Ribozyme Catalysis. Progress in Molecular Biology and Translational Science, 2013, 120, 25-91.	0.9	8
18	Electronic State of Nitrogen Containing Polypyridine at the Interfaces with Model Sulfonic Acid Containing Polymer and Molecule. Synthetic Metals, 2003, 137, 1031-1032.	2.1	6

#	Article	IF	Citations
19	Theoretical investigation of a blue hydroxyquinaldine-based aluminum(III) complex. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 321, 194-198.	0.9	6
20	Hybrid Quantum and Classical Methods for Computing Kinetic Isotope Effects of Chemical Reactions in Solutions and in Enzymes. Methods in Molecular Biology, 2008, 443, 37-62.	0.4	5
21	Kinetic Isotope Effects from Hybrid Classical and Quantum Path Integral Computations. RSC Biomolecular Sciences, 2009, , 105-131.	0.4	5
22	Developing a Systematic Approach for Ab Initio Path-Integral Simulations. , 0, , .		2
23	Practical approach for beryllium atomic clusters: TD-DFT potential energy surfaces from equilibrium to dissociation for excited states of 2sÂâ†'Â2p. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	2
24	Theoretical Simulations of Heavy-Atom Kinetic Isotope Effects in Aliphatic Claisen Rearrangement. Journal of Physical Chemistry A, 2020, 124, 10678-10686.	1.1	1
25	InnenrÃ¼cktitelbild: Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment (Angew. Chem. 3/2012). Angewandte Chemie, 2012, 124, 847-847.	1.6	0
26	Inside Back Cover: Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment (Angew. Chem. Int. Ed. 3/2012). Angewandte Chemie - International Edition, 2012, 51, 823-823.	7.2	0
27	17th Annual Conference of the Physical Society of Hong Kong. Asia-Pacific Physics Newsletter, 2015, 04, 47-47.	0.0	0
28	Pitfall in Freeâ€Energy Simulations on Simplest Systems. ChemistrySelect, 2017, 2, 4398-4418.	0.7	0
29	Quantum Mechanical Methods for Biomolecular Simulations. Challenges and Advances in Computational Chemistry and Physics, 2009, , 79-101.	0.6	0