

# Kin-Yiu Wong

## List of Publications by Year in descending order

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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	Theoretical Simulations of Heavy-Atom Kinetic Isotope Effects in Aliphatic Claisen Rearrangement. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10678-10686.	1.1	1
2	Practical approach for beryllium atomic clusters: TD-DFT potential energy surfaces from equilibrium to dissociation for excited states of $2s^2\ ^2P$ . <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	2
3	Pitfall in Free-Energy Simulations on Simplest Systems. <i>ChemistrySelect</i> , 2017, 2, 4398-4418.	0.7	0
4	17th Annual Conference of the Physical Society of Hong Kong. <i>Asia-Pacific Physics Newsletter</i> , 2015, 04, 47-47.	0.0	0
5	Review of computer simulations of isotope effects on biochemical reactions: From the Bigeleisen equation to Feynman's path integral. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2015, 1854, 1782-1794.	1.1	19
6	Mechanistic Insights into RNA Transphosphorylation from Kinetic Isotope Effects and Linear Free Energy Relationships of Model Reactions. <i>Chemistry - A European Journal</i> , 2014, 20, 14336-14343.	1.7	29
7	<i>Ab initio</i> path-integral calculations of kinetic and equilibrium isotope effects on base-catalyzed RNA transphosphorylation models. <i>Journal of Computational Chemistry</i> , 2014, 35, 1302-1316.	1.5	14
8	Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 24-34.	2.3	58
9	Review of Feynman's Path Integral in Quantum Statistics: from the Molecular Schrödinger Equation to Kleinert's Variational Perturbation Theory. <i>Communications in Computational Physics</i> , 2014, 15, 853-894.	0.7	11
10	Bridging the Gap Between Theory and Experiment to Derive a Detailed Understanding of Hammerhead Ribozyme Catalysis. <i>Progress in Molecular Biology and Translational Science</i> , 2013, 120, 25-91.	0.9	8
11	Experimental and computational analysis of the transition state for ribonuclease A-catalyzed RNA $2^{\circ}$ - $3^{\circ}$ transphosphorylation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 13002-13007.	3.3	62
12	Exact Relation between Potential of Mean Force and Free-Energy Profile. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3998-4003.	2.3	25
13	Innenrücktitelbild: Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment ( <i>Angew. Chem.</i> 3/2012). <i>Angewandte Chemie</i> , 2012, 124, 847-847.	1.6	0
14	Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 647-651.	7.2	49
15	Inside Back Cover: Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment ( <i>Angew. Chem. Int. Ed.</i> 3/2012). <i>Angewandte Chemie - International Edition</i> , 2012, 51, 823-823.	7.2	0
16	Active Participation of the $Mg^{2+}$ Ion in the Reaction Coordinate of RNA Self-Cleavage Catalyzed by the Hammerhead Ribozyme. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1-3.	2.3	50
17	Insight into the phosphodiesterase mechanism from combined QM/MM free energy simulations. <i>FEBS Journal</i> , 2011, 278, 2579-2595.	2.2	25
18	Determination of the Structure Form of the Fourth Ligand of Zinc in Acutolysin A Using Combined Quantum Mechanical and Molecular Mechanical Simulation. <i>Journal of Physical Chemistry B</i> , 2009, 113, 2477-2485.	1.2	28

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19	Theoretical Analysis of Kinetic Isotope Effects on Proton Transfer Reactions between Substituted $\hat{I}\pm$ -Methoxystyrenes and Substituted Acetic Acids. <i>Journal of the American Chemical Society</i> , 2009, 131, 13963-13971.	6.6	30
20	Kinetic Isotope Effects from Hybrid Classical and Quantum Path Integral Computations. <i>RSC Biomolecular Sciences</i> , 2009, , 105-131.	0.4	5
21	Quantum Mechanical Methods for Biomolecular Simulations. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2009, , 79-101.	0.6	0
22	Combined QM/MM and path integral simulations of kinetic isotope effects in the proton transfer reaction between nitroethane and acetate ion in water. <i>Journal of Computational Chemistry</i> , 2008, 29, 514-522.	1.5	45
23	Systematic Approach for Computing Zero-Point Energy, Quantum Partition Function, and Tunneling Effect Based on Kleinert's Variational Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1409-1422.	2.3	29
24	Hybrid Quantum and Classical Methods for Computing Kinetic Isotope Effects of Chemical Reactions in Solutions and in Enzymes. <i>Methods in Molecular Biology</i> , 2008, 443, 37-62.	0.4	5
25	An automated integration-free path-integral method based on Kleinert's variational perturbation theory. <i>Journal of Chemical Physics</i> , 2007, 127, 211103.	1.2	22
26	The Reaction Mechanism of Paraoxon Hydrolysis by Phosphotriesterase from Combined QM/MM Simulations. <i>Biochemistry</i> , 2007, 46, 13352-13369.	1.2	137
27	Theoretical investigation of a blue hydroxyquinaldine-based aluminum(III) complex. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2004, 321, 194-198.	0.9	6
28	Electronic State of Nitrogen Containing Polypyridine at the Interfaces with Model Sulfonic Acid Containing Polymer and Molecule. <i>Synthetic Metals</i> , 2003, 137, 1031-1032.	2.1	6
29	Developing a Systematic Approach for Ab Initio Path-Integral Simulations. , 0, , .		2