Nandini Ananth

List of Publications by Year
in descending order

28 papers	1,398 citations	471509 17 h-index	501196 28 g-index
28 all docs	28 docs citations	28 times ranked	1183 citing authors

#	Article	IF	Citations
1	Singlet fission and triplet pair recombination in bipentacenes with a twist. Materials Horizons, 2022, 9, 462-470.	12.2	14
2	Singularity-Free Internal Conversion Golden Rule Rate with Application to Correlated Triplet-Pair Recombination in Bipentacenes. Journal of Chemical Physics, 2022, 156, 044111.	3.0	4
3	Path Integrals for Nonadiabatic Dynamics: Multistate Ring Polymer Molecular Dynamics. Annual Review of Physical Chemistry, 2022, 73, 299-322.	10.8	12
4	Investigating the Stability and Accuracy of a Classical Mapping Variable Hamiltonian for Nonadiabatic Quantum Dynamics. Regular and Chaotic Dynamics, 2021, 26, 131-146.	0.8	2
5	Multistate ring polymer instantons and nonadiabatic reaction rates. Journal of Chemical Physics, 2020, 152, 114112.	3.0	8
6	Semiclassical dynamics in the mixed quantum-classical limit. Journal of Chemical Physics, 2019, 151, 134109.	3.0	13
7	Anticipating Acene-Based Chromophore Spectra with Molecular Orbital Arguments. Journal of Physical Chemistry A, 2019, 123, 2527-2536.	2.5	21
8	Nonadiabatic semiclassical dynamics in the mixed quantum-classical initial value representation. Journal of Chemical Physics, 2018, 148, 102326.	3.0	32
9	Tuning Singlet Fission in Ï€-Bridge-Ï€ Chromophores. Journal of the American Chemical Society, 2017, 139, 12488-12494.	13.7	147
10	Validating and implementing modified Filinov phase filtration in semiclassical dynamics. Journal of Chemical Physics, 2017, 146, 234104.	3.0	30
11	A mapping variable ring polymer molecular dynamics study of condensed phase proton-coupled electron transfer. Journal of Chemical Physics, 2017, 147, 234103.	3.0	25
12	Non-adiabatic reactions: general discussion. Faraday Discussions, 2016, 195, 311-344.	3.2	15
13	A Direct Mechanism of Ultrafast Intramolecular Singlet Fission in Pentacene Dimers. ACS Central Science, 2016, 2, 316-324.	11.3	176
14	Direct simulation of electron transfer in the cobalt hexammine(<scp>ii</scp>/<scp>iii</scp>) self-exchange reaction. Physical Chemistry Chemical Physics, 2016, 18, 26117-26124.	2.8	13
15	Deriving the exact nonadiabatic quantum propagator in the mapping variable representation. Faraday Discussions, 2016, 195, 269-289.	3.2	32
16	Mean field ring polymer molecular dynamics for electronically nonadiabatic reaction rates. Faraday Discussions, 2016, 195, 253-268.	3.2	36
17	Anomalous orbital admixture in ammine complexes. Journal of Organometallic Chemistry, 2015, 792, 6-12.	1.8	5
18	Simulating Excited State Dynamics in Systems with Multiple Avoided Crossings Using Mapping Variable Ring Polymer Molecular Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 4219-4223.	4.6	37

#	Article	IF	Citations
19	Dynamically consistent method for mixed quantum-classical simulations: A semiclassical approach. Journal of Chemical Physics, 2015, 142, 184102.	3.0	33
20	Tuning the Ground State Symmetry of Acetylenyl Radicals. ACS Central Science, 2015, 1, 270-278.	11.3	5
21	Tuning Spin-States of Carbynes and Silylynes: A Long Jump with One Leg. Journal of the American Chemical Society, 2014, 136, 13388-13398.	13.7	11
22	Seeking Small Molecules for Singlet Fission: A Heteroatom Substitution Strategy. Journal of the American Chemical Society, 2014, 136, 12638-12647.	13.7	121
23	The Low-Lying Electronic States of Pentacene and Their Roles in Singlet Fission. Journal of the American Chemical Society, 2014, 136, 5755-5764.	13.7	197
24	Mapping variable ring polymer molecular dynamics: A path-integral based method for nonadiabatic processes. Journal of Chemical Physics, 2013, 139, 124102.	3.0	119
25	Flux-correlation approach to characterizing reaction pathways in quantum systems: a study of condensed-phase proton-coupled electron transfer. Molecular Physics, 2012, 110, 1009-1015.	1.7	17
26	Direct simulation of electron transfer using ring polymer molecular dynamics: Comparison with semiclassical instanton theory and exact quantum methods. Journal of Chemical Physics, 2011, 135, 074106.	3.0	105
27	Exact quantum statistics for electronically nonadiabatic systems using continuous path variables. Journal of Chemical Physics, 2010, 133, 234103.	3.0	71
28	Semiclassical description of electronically nonadiabatic dynamics via the initial value representation. Journal of Chemical Physics, 2007, 127, 084114.	3.0	97