Deping Hu

List of Publications by Year in descending order

26 papers	939 citations	623734 14 h-index	552781 26 g-index
31 all docs	31 docs citations	31 times ranked	977 citing authors

#	Article	IF	Citations
1	Heavyâ€Atomâ€Free Roomâ€Temperature Phosphorescent Rylene Imide for Highâ€Performing Organic Photovoltaics. Advanced Science, 2022, 9, e2103975.	11.2	12
2	Ultrafast Internal Conversion Dynamics through the on-the-Fly Simulation of Transient Absorption Pumpâ€“Probe Spectra with Different Electronic Structure Methods. Journal of Physical Chemistry Letters, 2022, 13, 661-668.	4.6	13
3	Investigation of nonadiabatic dynamics in the photolysis of methyl nitrate (CH₃ONO₂) by on-the-fly surface hopping simulation. Physical Chemistry Chemical Physics, 2021, 23, 25597-25611.	2.8	8
4	Analysis of bath motion in MM-SQC dynamics via dimensionality reduction approach: Principal component analysis. Journal of Chemical Physics, 2021, 154, 094122.	3.0	12
5	On-the-Fly Symmetrical Quasi-Classical Dynamics with Meyerâ€“Miller Mapping Hamiltonian for the Treatment of Nonadiabatic Dynamics at Conical Intersections. Journal of Chemical Theory and Computation, 2021, 17, 3267-3279.	5.3	16
6	Brightening up Circularly Polarized Luminescence of Monosubstituted Polyacetylene by Conformation Control: Mechanism, Switching, and Sensing. Angewandte Chemie, 2021, 133, 22089-22097.	2.0	20
7	Brightening up Circularly Polarized Luminescence of Monosubstituted Polyacetylene by Conformation Control: Mechanism, Switching, and Sensing. Angewandte Chemie - International Edition, 2021, 60, 21918-21926.	13.8	82
8	Spectral Fingerprint of Excited-State Energy Transfer in Dendrimers through Polarization-Sensitive Transient-Absorption Pumpâ€“Probe Signals: On-the-Fly Nonadiabatic Dynamics Simulations. Journal of Physical Chemistry Letters, 2021, 12, 9710-9719.	4.6	12
9	Prediction of the excited-state reaction channels in photo-induced processes of nitrofurantoin using first-principle calculations and dynamics simulations. Chemosphere, 2021, 281, 130831.	8.2	2
10	Achieving Pure Green Electroluminescence with CIEy of 0.69 and EQE of 28.2% from an Azaâ€Fused Multiâ€Resonance Emitter. Angewandte Chemie, 2020, 132, 17652-17656.	2.0	72
11	Achieving Pure Green Electroluminescence with CIEy of 0.69 and EQE of 28.2% from an Azaâ€Fused Multiâ€Resonance Emitter. Angewandte Chemie - International Edition, 2020, 59, 17499-17503.	13.8	211
12	Online highâ€pH reversedâ€phase liquid chromatography Ã— lowâ€pH reversedâ€phase liquid chromatography tandem electrospray ionization mass spectrometry combined with pulse elution gradient in the first dimension for the analysis of alkaloids in Macleaya cordata (willd.) R. Br. Journal of Separation Science, 2020, 43, 1423-1430.	2.5	5
13	Performance of trajectory surface hopping method in the treatment of ultrafast intersystem crossing dynamics. Journal of Chemical Physics, 2019, 150, 164126.	3.0	8
14	Pulsed elution modulation for on-line comprehensive two-dimensional liquid chromatography coupling reversed phase liquid chromatography and hydrophilic interaction chromatography. Journal of Chromatography A, 2019, 1583, 98-107.	3.7	21
15	Analysis of trajectory similarity and configuration similarity in on-the-fly surface-hopping simulation on multi-channel nonadiabatic photoisomerization dynamics. Journal of Chemical Physics, 2018, 149, 244104.	3.0	18
16	Ultrafast unidirectional chiral rotation in the Zâ€“E photoisomerization of two azoheteroarene photoswitches. Physical Chemistry Chemical Physics, 2018, 20, 25910-25917.	2.8	9
17	Inclusion of Machine Learning Kernel Ridge Regression Potential Energy Surfaces in On-the-Fly Nonadiabatic Molecular Dynamics Simulation. Journal of Physical Chemistry Letters, 2018, 9, 2725-2732.	4.6	113
18	â€œWatchingâ€•the Dark State in Ultrafast Nonadiabatic Photoisomerization Process of a Light-Driven Molecular Rotary Motor. Journal of Physical Chemistry A, 2017, 121, 1240-1249.	2.5	38

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19	The behavior of hydroxide and hydronium ions at the hexadecaneâ€“water interface studied with second harmonic generation and zeta potential measurements. Soft Matter, 2017, 13, 7962-7968.	2.7	27
20	Analysis of the Geometrical Evolution in On-the-Fly Surface-Hopping Nonadiabatic Dynamics with Machine Learning Dimensionality Reduction Approaches: Classical Multidimensional Scaling and Isometric Feature Mapping. Journal of Chemical Theory and Computation, 2017, 13, 4611-4623.	5.3	41
21	Nonadiabatic dynamics simulation of keto isocytosine: a comparison of dynamical performance of different electronic-structure methods. Physical Chemistry Chemical Physics, 2017, 19, 19168-19177.	2.8	28
22	Study of Adsorption Behavior and Inhibition Mechanism of Mild Steel in Hydrochloric Acid by a Novel Thiadiazole Derivative. Electrochemistry, 2015, 83, 262-267.	1.4	6
23	Rigidâ€“Flexible Coupling High Ionic Conductivity Polymer Electrolyte for an Enhanced Performance of LiMn₂O₄/Graphite Battery at Elevated Temperature. ACS Applied Materials & Interfaces, 2015, 7, 4720-4727.	8.0	108
24	Computational Investigation of Acene-Modified Zinc-Porphyrin Based Sensitizers for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2015, 119, 8417-8430.	3.1	22
25	Nonadiabatic dynamics and photoisomerization of biomimetic photoswitches. Chemical Physics, 2015, 463, 95-105.	1.9	9
26	Theoretical analysis of excited states and energy transfer mechanism in conjugated dendrimers. Journal of Computational Chemistry, 2015, 36, 151-163.	3.3	26