Seung Kyu Min

List of Publications by Year
in descending order

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		186265	175258
50	3,781	28	52
papers	citations	h-index	g-index

54	54	54	4187
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Coupled- and Independent-Trajectory Approaches Based on the Exact Factorization Using the PyUNIxMD Package. Topics in Current Chemistry, 2022, 380, 8.	5.8	4
2	Proton affinity and gas phase basicity of diamandoid molecules: diamantane to C₁₃₁H₁₁₆. Physical Chemistry Chemical Physics, 2022, 24, 3470-3477.	2.8	2
3	Spatial distribution modulation of mixed building blocks in metal-organic frameworks. Nature Communications, 2022, 13, 1027.	12.8	13
4	Singlet Oxygen Generation from Polyaminoglycerol by Spin-Flip-Based Electron Transfer. Jacs Au, 2022, 2, 933-942.	7.9	8
5	Electrochemical Formation of a Covalentâ€“Ionic Stage-1 Graphite Intercalation Compound with Trifluoroacetic Acid. Chemistry of Materials, 2022, 34, 217-231.	6.7	6
6	Independent trajectory mixed quantum-classical approaches based on the exact factorization. Journal of Chemical Physics, 2022, 156, 174109.	3.0	11
7	Generalized Formulation of the Density Functional Tight Binding-Based Restricted Ensemble Kohnâ€“Sham Method with Onsite Correction to Long-Range Correction. Journal of Chemical Theory and Computation, 2022, 18, 3391-3409.	5.3	2
8	Coupled- and Independent-Trajectory Approaches Based on the Exact Factorization Using the PyUNIxMD Package. Topics in Current Chemistry Collections, 2022, , 153-179.	0.5	1
9	pH-Responsive Amphiphilic Polyether Micelles with Superior Stability for Smart Drug Delivery. Biomacromolecules, 2021, 22, 2043-2056.	5.4	34
10	Study of the Decoherence Correction Derived from the Exact Factorization Approach for Nonadiabatic Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 3852-3862.	5.3	27
11	<scp>PyUNIxMD</scp>: A <scp>Pythonâ€based</scp> excited state molecular dynamics package. Journal of Computational Chemistry, 2021, 42, 1755-1766.	3.3	24
12	Machine Learning-Assisted Excited State Molecular Dynamics with the State-Interaction State-Averaged Spin-Restricted Ensemble-Referenced Kohnâ€“Sham Approach. Journal of Chemical Theory and Computation, 2021, 17, 694-702.	5.3	12
13	Selfâ€Assembly of Mitochondriaâ€Targeted Photosensitizer to Increase Photostability and Photodynamic Therapeutic Efficacy in Hypoxia. Chemistry - A European Journal, 2020, 26, 10695-10701.	3.3	15
14	Effect of Pt Crystal Surface on Hydrogenation of Monolayer h-BN and Its Conversion to Graphene. Chemistry of Materials, 2020, 32, 4584-4590.	6.7	9
15	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
16	Tailorable Degradation of pH-Responsive All-Polyether Micelles: Unveiling the Role of Monomer Structure and Hydrophilicâ€“Hydrophobic Balance. Macromolecules, 2019, 52, 5884-5893.	4.8	19
17	Theoretical modelling of the dynamics of primary photoprocess of cyclopropanone. Physical Chemistry Chemical Physics, 2019, 21, 2489-2498.	2.8	23
18	Metal-organic framework based on hinged cube tessellation as transformable mechanical metamaterial. Science Advances, 2019, 5, eaav4119.	10.3	28

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19	Design and photoisomerization dynamics of a new family of synthetic 2-stroke light driven molecular rotary motors. Chemical Communications, 2019, 55, 5247-5250.	4.1	34
20	Formulation and Implementation of the Spin-Restricted Ensemble-Referenced Kohnâ€“Sham Method in the Context of the Density Functional Tight Binding Approach. Journal of Chemical Theory and Computation, 2019, 15, 3021-3032.	5.3	10
21	Non-adiabatic dynamics of ring opening in cyclohexa-1,3-diene described by an ensemble density-functional theory method. Molecular Physics, 2019, 117, 1128-1141.	1.7	33
22	Surface Hopping Dynamics beyond Nonadiabatic Couplings for Quantum Coherence. Journal of Physical Chemistry Letters, 2018, 9, 1097-1104.	4.6	80
23	Direct Nonadiabatic Dynamics by Mixed Quantum-Classical Formalism Connected with Ensemble Density Functional Theory Method: Application to trans-Penta-2,4-dieniminium Cation. Journal of Chemical Theory and Computation, 2018, 14, 4499-4512.	5.3	30
24	Fulgides as Light-Driven Molecular Rotary Motors: Computational Design of a Prototype Compound. Journal of Physical Chemistry Letters, 2018, 9, 4995-5001.	4.6	48
25	Ab Initio Nonadiabatic Dynamics with Coupled Trajectories: A Rigorous Approach to Quantum (De)Coherence. Journal of Physical Chemistry Letters, 2017, 8, 3048-3055.	4.6	123
26	Adsorption of Carbon Tetrahalides on Coronene and Graphene. Journal of Physical Chemistry C, 2017, 121, 14968-14974.	3.1	11
27	Quantum-Classical Nonadiabatic Dynamics: Coupled- vs Independent-Trajectory Methods. Journal of Chemical Theory and Computation, 2016, 12, 2127-2143.	5.3	117
28	Coupled-Trajectory Quantum-Classical Approach to Electronic Decoherence in Nonadiabatic Processes. Physical Review Letters, 2015, 115, 073001.	7.8	126
29	Semiclassical analysis of the electronâ€nuclear coupling in electronic nonâ€adiabatic processes. Annalen Der Physik, 2015, 527, 546-555.	2.4	32
30	The exact forces on classical nuclei in non-adiabatic charge transfer. Journal of Chemical Physics, 2015, 142, 084303.	3.0	83
31	Is the Molecular Berry Phase an Artifact of the Born-Oppenheimer Approximation?. Physical Review Letters, 2014, 113, 263004.	7.8	93
32	Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting, DNA Sequencing, and Cancerous DNA Recognition. ACS Nano, 2014, 8, 1827-1833.	14.6	65
33	Noncovalent Interactions of DNA Bases with Naphthalene and Graphene. Journal of Chemical Theory and Computation, 2013, 9, 2090-2096.	5.3	73
34	Theoretical Design of Nanomaterials and Nanodevices: Nanolensing, Supermagnetoresistance, and Ultrafast DNA Sequencing. Journal of Physical Chemistry C, 2011, 115, 16247-16257.	3.1	20
35	Chromium Porphyrin Arrays As Spintronic Devices. Journal of the American Chemical Society, 2011, 133, 9364-9369.	13.7	167
36	The origin of dips for the graphene-based DNA sequencing device. Physical Chemistry Chemical Physics, 2011, 13, 14293.	2.8	44

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37	CO₂ Capturing Mechanism in Aqueous Ammonia: NH₃-Driven Decompositionâ^'Recombination Pathway. Journal of Physical Chemistry Letters, 2011, 2, 689-694.	4.6	47
38	Fast DNA sequencing with a graphene-based nanochannel device. Nature Nanotechnology, 2011, 6, 162-165.	31.5	517
39	Efficient electron dynamics with the planewave-based real-time time-dependent density functional theory: Absorption spectra, vibronic electronic spectra, and coupled electron-nucleus dynamics. Journal of Chemical Physics, 2011, 135, 244112.	3.0	8
40	Chiral Transformation in Protonated and Deprotonated Adipic Acids through Multistep Internal Proton Transfer. Chemistry - A European Journal, 2010, 16, 10373-10379.	3.3	1
41	Comparison of cationic, anionic and neutral hydrogen bonded dimers. Physical Chemistry Chemical Physics, 2010, 12, 6278.	2.8	28
42	Near-field focusing and magnification through self-assembled nanoscale spherical lenses. Nature, 2009, 460, 498-501.	27.8	338
43	Application of quantum chemistry to nanotechnology: electron and spin transport in molecular devices. Chemical Society Reviews, 2009, 38, 2319.	38.1	119
44	Comprehensive Energy Analysis for Various Types of Ï€-Interaction. Journal of Chemical Theory and Computation, 2009, 5, 515-529.	5.3	253
45	Complete basis set limit of Ab initio binding energies and geometrical parameters for various typical types of complexes. Journal of Computational Chemistry, 2008, 29, 1208-1221.	3.3	144
46	Dissolution Nature of Cesium Fluoride by Water Moleculesâ€. Journal of Physical Chemistry B, 2006, 110, 3808-3815.	2.6	28
47	Structure and spectral features of H+(H2O)7: Eigen versus Zundel forms. Journal of Chemical Physics, 2006, 125, 234305.	3.0	52
48	Magic and Antimagic Protonated Water Clusters: Exotic Structures with Unusual Dynamic Effects. Angewandte Chemie - International Edition, 2006, 45, 3795-3800.	13.8	108
49	Magic Structures and Quantum Conductance of[110]Silver Nanowires. Physical Review Letters, 2006, 96, 096104.	7.8	47
50	Hydrated copper and gold monovalent cations:Ab initiostudy. Journal of Chemical Physics, 2005, 122, 064314.	3.0	41