Seung Kyu Min

List of Publications by Year
in descending order

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Version: 2024-02-01

		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	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
2	Fast DNA sequencing with a graphene-based nanochannel device. Nature Nanotechnology, 2011, 6, 162-165.	31.5	517
3	Near-field focusing and magnification through self-assembled nanoscale spherical lenses. Nature, 2009, 460, 498-501.	27.8	338
4	Comprehensive Energy Analysis for Various Types of Ï€-Interaction. Journal of Chemical Theory and Computation, 2009, 5, 515-529.	5.3	253
5	Chromium Porphyrin Arrays As Spintronic Devices. Journal of the American Chemical Society, 2011, 133, 9364-9369.	13.7	167
6	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
7	Coupled-Trajectory Quantum-Classical Approach to Electronic Decoherence in Nonadiabatic Processes. Physical Review Letters, 2015, 115, 073001.	7.8	126
8	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
9	Application of quantum chemistry to nanotechnology: electron and spin transport in molecular devices. Chemical Society Reviews, 2009, 38, 2319.	38.1	119
10	Quantum-Classical Nonadiabatic Dynamics: Coupled- vs Independent-Trajectory Methods. Journal of Chemical Theory and Computation, 2016, 12, 2127-2143.	5.3	117
11	Magic and Antimagic Protonated Water Clusters: Exotic Structures with Unusual Dynamic Effects. Angewandte Chemie - International Edition, 2006, 45, 3795-3800.	13.8	108
12	Is the Molecular Berry Phase an Artifact of the Born-Oppenheimer Approximation?. Physical Review Letters, 2014, 113, 263004.	7.8	93
13	The exact forces on classical nuclei in non-adiabatic charge transfer. Journal of Chemical Physics, 2015, 142, 084303.	3.0	83
14	Surface Hopping Dynamics beyond Nonadiabatic Couplings for Quantum Coherence. Journal of Physical Chemistry Letters, 2018, 9, 1097-1104.	4.6	80
15	Noncovalent Interactions of DNA Bases with Naphthalene and Graphene. Journal of Chemical Theory and Computation, 2013, 9, 2090-2096.	5.3	73
16	Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting, DNA Sequencing, and Cancerous DNA Recognition. ACS Nano, 2014, 8, 1827-1833.	14.6	65
17	Structure and spectral features of H+(H2O)7: Eigen versus Zundel forms. Journal of Chemical Physics, 2006, 125, 234305.	3.0	52
18	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

#	Article	IF	Citations
19	Magic Structures and Quantum Conductance of[110]Silver Nanowires. Physical Review Letters, 2006, 96, 096104.	7.8	47
20	CO₂ Capturing Mechanism in Aqueous Ammonia: NH₃-Driven Decompositionâ^'Recombination Pathway. Journal of Physical Chemistry Letters, 2011, 2, 689-694.	4.6	47
21	The origin of dips for the graphene-based DNA sequencing device. Physical Chemistry Chemical Physics, 2011, 13, 14293.	2.8	44
22	Hydrated copper and gold monovalent cations:Ab initiostudy. Journal of Chemical Physics, 2005, 122, 064314.	3.0	41
23	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
24	pH-Responsive Amphiphilic Polyether Micelles with Superior Stability for Smart Drug Delivery. Biomacromolecules, 2021, 22, 2043-2056.	5.4	34
25	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
26	Semiclassical analysis of the electronâ€"nuclear coupling in electronic nonâ€"adiabatic processes. Annalen Der Physik, 2015, 527, 546-555.	2.4	32
27	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
28	Dissolution Nature of Cesium Fluoride by Water Moleculesâ€. Journal of Physical Chemistry B, 2006, 110, 3808-3815.	2.6	28
29	Comparison of cationic, anionic and neutral hydrogen bonded dimers. Physical Chemistry Chemical Physics, 2010, 12, 6278.	2.8	28
30	Metal-organic framework based on hinged cube tessellation as transformable mechanical metamaterial. Science Advances, 2019, 5, eaav4119.	10.3	28
31	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
32	<scp>PyUNIxMD</scp>: A <scp>Pythonâ€based</scp> excited state molecular dynamics package. Journal of Computational Chemistry, 2021, 42, 1755-1766.	3.3	24
33	Theoretical modelling of the dynamics of primary photoprocess of cyclopropanone. Physical Chemistry Chemical Physics, 2019, 21, 2489-2498.	2.8	23
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	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
36	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

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37	Spatial distribution modulation of mixed building blocks in metal-organic frameworks. Nature Communications, 2022, 13, 1027.	12.8	13
38	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
39	Adsorption of Carbon Tetrahalides on Coronene and Graphene. Journal of Physical Chemistry C, 2017, 121, 14968-14974.	3.1	11
40	Independent trajectory mixed quantum-classical approaches based on the exact factorization. Journal of Chemical Physics, 2022, 156, 174109.	3.0	11
41	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
42	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
43	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
44	Singlet Oxygen Generation from Polyaminoglycerol by Spin-Flip-Based Electron Transfer. Jacs Au, 2022, 2, 933-942.	7.9	8
45	Electrochemical Formation of a Covalentâ€“Ionic Stage-1 Graphite Intercalation Compound with Trifluoroacetic Acid. Chemistry of Materials, 2022, 34, 217-231.	6.7	6
46	Coupled- and Independent-Trajectory Approaches Based on the Exact Factorization Using the PyUNIxMD Package. Topics in Current Chemistry, 2022, 380, 8.	5.8	4
47	Proton affinity and gas phase basicity of diamandoid molecules: diamantane to C₁₃₁H₁₁₆. Physical Chemistry Chemical Physics, 2022, 24, 3470-3477.	2.8	2
48	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
49	Chiral Transformation in Protonated and Deprotonated Adipic Acids through Multistep Internal Proton Transfer. Chemistry - A European Journal, 2010, 16, 10373-10379.	3.3	1
50	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