Noriyuki Minezawa

List of Publications by Year
in descending order

17	712	687363 13	888059 17
papers	citations	h-index	g-index

18	18	18	951
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum mechanical/molecular mechanical trajectory surface hopping molecular dynamics simulation by spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2020, 152, 024119.	3.0	8
2	Trajectory surface hopping molecular dynamics simulation by spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2019, 150, 204120.	3.0	13
3	Vertical excitation energies of linear cyanine dyes by spin-flip time-dependent density functional theory. Chemical Physics Letters, 2015, 622, 115-119.	2.6	13
4	Optimizing minimum free-energy crossing points in solution: Linear-response free energy/spin-flip density functional theory approach. Journal of Chemical Physics, 2014, 141, 164118.	3.0	12
5	State-specific solvation effect on the intramolecular charge transfer reaction in solution: A linear-response free energy TDDFT method. Chemical Physics Letters, 2014, 608, 140-144.	2.6	16
6	Excited-State Hydrogen Atom Transfer Reaction in Solvated 7-Hydroxy-4-methylcoumarin. Journal of Physical Chemistry B, 2013, 117, 15386-15394.	2.6	18
7	Excited-state free energy surfaces in solution: Time-dependent density functional theory/reference interaction site model self-consistent field method. Journal of Chemical Physics, 2013, 138, 244101.	3.0	10
8	Automated Search for Minimum Energy Conical Intersection Geometries between the Lowest Two Singlet States S₀/S₁-MECIs by the Spin-Flip TDDFT Method. Journal of Chemical Theory and Computation, 2013, 9, 4116-4123.	5.3	56
9	Optimizing conical intersections of solvated molecules: The combined spin-flip density functional theory/effective fragment potential method. Journal of Chemical Physics, 2012, 137, 034116.	3.0	30
10	Fragment Molecular Orbital Molecular Dynamics with the Fully Analytic Energy Gradient. Journal of Chemical Theory and Computation, 2012, 8, 5008-5012.	5.3	47
11	Photoisomerization of Stilbene: A Spin-Flip Density Functional Theory Approach. Journal of Physical Chemistry A, 2011, 115, 7901-7911.	2.5	129
12	Modeling Solvent Effects on Electronic Excited States. Journal of Physical Chemistry Letters, 2011, 2, 2184-2192.	4.6	107
13	Implementation of the analytic energy gradient for the combined time-dependent density functional theory/effective fragment potential method: Application to excited-state molecular dynamics simulations. Journal of Chemical Physics, 2011, 134, 054111.	3.0	36
14	Electronic spectra of coumarin-151 in polar solvents: Linear response free energy approach. Chemical Physics Letters, 2010, 492, 193-197.	2.6	10
15	Optimizing Conical Intersections by Spinâ^'Flip Density Functional Theory: Application to Ethylene. Journal of Physical Chemistry A, 2009, 113, 12749-12753.	2.5	155
16	Efficient implementation of three-dimensional reference interaction site model self-consistent-field method: Application to solvatochromic shift calculations. Journal of Chemical Physics, 2007, 126, 054511.	3.0	27
17	Intramolecular Charge-Transfer State Formation of 4-(N,N-Dimethylamino)benzonitrile in Acetonitrile Solution:Â RISM-SCF Study. Journal of Physical Chemistry A, 2005, 109, 5445-5453.	2.5	25