Shih-I Lu

List of Publications by Year
in descending order

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31	206	1162367 8	1058022 14
papers	citations	h-index	g-index

31	31	31	224
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The role of distributed atomic point charges and polarizabilities of solvent molecules on oneâ€•and twoâ€•photon absorption spectra of aqueous p â€•nitroaniline. Journal of the Chinese Chemical Society, 2021, 68, 429-433.	0.8	0
2	Discrete Solvent Reaction Field Calculations for One- and Two-Photon Absorptions of Solution-Phase Dimethylaminonitrostilbene Molecule. Journal of Physical Chemistry A, 2019, 123, 5334-5340.	1.1	3
3	Application of discrete solvent reaction field model with self-consistent atomic charges and atomic polarizabilities to calculate the Ï‡(1) and Ï‡(2) of organic molecular crystals. Chemical Physics Letters, 2018, 691, 8-13.	1.2	4
4	Calculations of Electronic Excitation Energies and Excess Electric Dipole Moments of Solvated p-Nitroaniline with the EOM-CCSD-PCM Method. Journal of Physical Chemistry A, 2018, 122, 6062-6070.	1.1	7
5	Application of discrete solvent reaction field to second-order susceptibility of organic molecular crystal. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	2
6	On the performance of range-separated hybrid in computations of dynamic quadratic polarizability of solution-phase organic molecules: a comparison to MP2(Full) calculation. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	3
7	Assessment of the global and range-separated hybrids for computing the dynamic second-order hyperpolarizability of solution-phase organic molecules. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	5
8	Computational investigation of first hyperpolarizability in substituted hydrazones. Chemical Physics Letters, 2013, 581, 42-46.	1.2	3
9	Density functional theory calculations of dynamic first hyperpolarizabilities for organic molecules in organic solvent: Comparison to experiment. Journal of Chemical Physics, 2011, 135, 134104.	1.2	37
10	Geometry of (E)-benzaldehyde phenylhydrazone in ethanol. Computational and Theoretical Chemistry, 2011, 976, 197-200.	1.1	0
11	Computational study of static first hyperpolarizability of donorâ€“acceptor substituted (E)â€benzaldehyde phenylhydrazone. Journal of Computational Chemistry, 2011, 32, 730-736.	1.5	28
12	The K-band Î»max values of the ultravioletâ€“visible spectra of some hydrazones in ethanol by a TD-DFT/PCM approach. Chemical Physics Letters, 2010, 494, 198-201.	1.2	4
13	Gibbs energy of activation for thermal isomerization of (1Z)â€acetaldehyde hydrazone and (1Z)â€acetaldehyde N,Nâ€dimethylhydrazone by Gaussianâ€4 theory and CCSD(T)/CBS computations. Journal of Computational Chemistry, 2009, 30, 2176-2180.	1.5	3
14	Study on the Z/E thermal isomerization of acetaldehyde N,N-dimethylhydrazone in cyclohexane by density functional theory computations. Computational and Theoretical Chemistry, 2009, 893, 84-87.	1.5	1
15	Adding an explicit solvent molecule to polarized continuum model for computational study on the conformational population of a highly fluorinated hydrazone. Computational and Theoretical Chemistry, 2009, 901, 31-33.	1.5	2
16	Computational note on thermal isomerization of trimethylacetaldehyde N,N-dimethylhydrazone in vacuum and cyclohexane. Computational and Theoretical Chemistry, 2007, 822, 151-152.	1.5	0
17	Accuracy of a Random Walk-Based Approach in the Determination of Equilibrium Bond Lengths and Harmonic Frequencies for Some Doublet First-Row Diatomic Radicals. ACS Symposium Series, 2006, , 29-41.	0.5	0
18	Theoretical study of transition state structure and reaction enthalpy of the F+H2â†'HF+H reaction by a diffusion quantum Monte Carlo approach. Journal of Chemical Physics, 2005, 122, 194323.	1.2	5

#	Article	IF	Citations
19	A diffusion quantum Monte Carlo study on the lowest singlet and triplet electronic states of BN molecule. Journal of Chemical Physics, 2005, 123, 174313.	1.2	6
20	Accuracy of a random-walk-based approach in the determination of equilibrium bond lengths and harmonic frequencies for some doublet first-row diatomic radicals. Journal of Chemical Physics, 2005, 123, 074104.	1.2	0
21	A diffusion quantum Monte Carlo study of geometries and harmonic frequencies of molecules. Journal of Chemical Physics, 2004, 120, 14-17.	1.2	11
22	Diffusion quantum Monte Carlo for equilibrium structures and harmonic frequencies of ethane and ozone molecules. Journal of Chemical Physics, 2004, 120, 10423-10425.	1.2	5
23	The accuracy of diffusion quantum Monte Carlo simulations in the determination of molecular equilibrium structures. Journal of Chemical Physics, 2004, 121, 10365-10369.	1.2	1
24	Ornsteinâ€“Uhlenbeck diffusion quantum Monte Carlo study on the bond lengths and harmonic frequencies of some first-row diatomic molecules. Journal of Chemical Physics, 2004, 120, 3185-3188.	1.2	10
25	Random walks based approach to study on molecular structures and torsional barrier heights of hydrogen peroxide. Chemical Physics Letters, 2004, 394, 271-274.	1.2	7
26	Electron affinities with diffusion quantum Monte Carlo for C2 and BO molecules. Journal of Chemical Physics, 2004, 121, 10495-10497.	1.2	10
27	Computing potential energy curve for hydrogen fluoride in Ornstein-Uhlenbeck diffusion quantum Monte Carlo method. Chemical Physics Letters, 2003, 381, 672-676.	1.2	4
28	Ornsteinâ€“Uhlenbeck diffusion quantum Monte Carlo calculations on BH and HF with the floating spherical Gaussian orbitals and spherical Gaussian geminals. Chemical Physics, 2003, 287, 297-302.	0.9	7
29	Performance of Ornsteinâ€“Uhlenbeck diffusion quantum Monte Carlo for first-row diatomic dissociation energies and dipole moments. Journal of Chemical Physics, 2003, 118, 6152-6156.	1.2	10
30	Accurate atomization energies and dipole moments from Ornsteinâ€“Uhlenbeck diffusion quantum Monte Carlo calculations for small first-row polyatomic molecules. Journal of Chemical Physics, 2003, 118, 9528-9532.	1.2	13
31	A diffusion quantum Monte Carlo method based on floating spherical Gaussian orbitals and Gaussian geminals: Dipole moment of lithium hydride molecule. Journal of Chemical Physics, 2001, 114, 3898-3904.	1.2	15