# Shih-I Lu

List of Publications by Year
in descending order



| 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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | A diffusion quantum Monte Carlo study of geometries and harmonic frequencies of molecules. Journal of Chemical Physics, 2004, 120, 14-17. | 1.2 | 11 |
| 6 | 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 |
| 7 | 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 |
| 8 | Electron affinities with diffusion quantum Monte Carlo for C2 and BO molecules. Journal of Chemical Physics, 2004, 121, 10495-10497. | 1.2 | 10 |
| 9 | 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 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | Computational investigation of first hyperpolarizability in substituted hydrazones. Chemical Physics Letters, 2013, 581, 42-46. | 1.2 | 3 |
| 21 | 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 |
| 22 | 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 |
| 23 | 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 |
| 24 | Application of discrete solvent reaction field to second-order susceptibility of organic molecular crystal. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 2 |
| 25 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | 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 |
| 30 | Geometry of (E)-benzaldehyde phenylhydrazone in ethanol. Computational and Theoretical Chemistry, 2011, 976, 197-200. | 1.1 | 0 |
| 31 | 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 |