Tamar Stein

List of Publications by Year
in descending order

24 papers	5,639 citations	471509 17 h-index	642732 23 g-index
25 all docs	25 docs citations	25 times ranked	5887 citing authors

#	Article	IF	Citations
1	Isomerization of hydrogen cyanide and hydrogen isocyanide in a cluster environment: quantum chemical study. Journal of Chemical Physics, 2022, 156, 054307.	3.0	3
2	Stereoselective Dielsâ€“Alder Reactions of gem-Diborylalkenes: Toward the Synthesis of gem-Diboron-Based Polymers. Journal of the American Chemical Society, 2021, 143, 6211-6220.	13.7	19
3	Molecular dynamics reveals formation path of benzonitrile and other molecules in conditions relevant to the interstellar medium. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	6
4	The Effect of Cluster Size on the Intra-Cluster Ionic Polymerization Process. Molecules, 2021, 26, 4782.	3.8	2
5	Electrochemical deposition of N-heterocyclic carbene monolayers on metal surfaces. Nature Communications, 2020, 11, 5714.	12.8	32
6	Molecular growth upon ionization of van der Waals clusters containing HCCH and HCN is a pathway to prebiotic molecules. Physical Chemistry Chemical Physics, 2020, 22, 20337-20348.	2.8	8
7	Photoredoxâ€Mediated Reaction of gemâ€Diborylalkenes: Reactivity Toward Diverse 1,1â€Bisborylalkanes. Chemistry - A European Journal, 2020, 26, 5360-5364.	3.3	24
8	Molecular Formation upon Ionization of van der Waals Clusters and Implication to Astrochemistry. Israel Journal of Chemistry, 2020, 60, 842-849.	2.3	10
9	Probing solvation and reactivity in ionized polycyclic aromatic hydrocarbonâ€“water clusters with photoionization mass spectrometry and electronic structure calculations. Faraday Discussions, 2019, 217, 414-433.	3.2	18
10	Ab initio dynamics and photoionization mass spectrometry reveal ionâ€“molecule pathways from ionized acetylene clusters to benzene cation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E4125-E4133.	7.1	24
11	Mechanisms of the Formation of Adenine, Guanine, and Their Analogues in UV-Irradiated Mixed NH₃:H₂O Molecular Ices Containing Purine. Astrobiology, 2017, 17, 771-785.	3.0	25
12	Probing Ionic Complexes of Ethylene and Acetylene with Vacuum-Ultraviolet Radiation. Journal of Physical Chemistry A, 2016, 120, 5053-5064.	2.5	11
13	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
14	Seniority-based coupled cluster theory. Journal of Chemical Physics, 2014, 141, 244104.	3.0	110
15	Seniority zero pair coupled cluster doubles theory. Journal of Chemical Physics, 2014, 140, 214113.	3.0	147
16	Stability of Hemi-Bonded vs Proton-Transferred Structures of (H₂O)₂⁺, (H₂S)₂⁺, and (H₂Se)₂⁺ Studied with Projected Hartreeâ€“Fock Methods. Journal of Physical Chemistry A, 2014, 118, 7261-7266.	2.5	26
17	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	4.6	145
18	Calculation of transition dipole moment in fluorescent proteinsâ€”towards efficient energy transfer. Physical Chemistry Chemical Physics, 2012, 14, 4109.	2.8	60

#	Article	IF	Citations
19	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2012, 8, 1515-1531.	5.3	765
20	Charge-Transfer-Like Ï€â†'Ï€* Excitations in Time-Dependent Density Functional Theory: A Conundrum and Its Solution. Journal of Chemical Theory and Computation, 2011, 7, 2408-2415.	5.3	221
21	Fundamental Gaps in Finite Systems from Eigenvalues of a Generalized Kohn-Sham Method. Physical Review Letters, 2010, 105, 266802.	7.8	377
22	Prediction of charge-transfer excitations in coumarin-based dyes using a range-separated functional tuned from first principles. Journal of Chemical Physics, 2009, 131, 244119.	3.0	313
23	Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory. Journal of the American Chemical Society, 2009, 131, 2818-2820.	13.7	729
24	Accelerated Multiphosphorylated Peptide Synthesis. Organic Process Research and Development, 0, , .	2.7	3