Tamar Stein

List of Publications by Year
in descending order

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24 papers	5,639 citations	471061 17 h-index	642321 23 g-index
25 all docs	25 docs citations	25 times ranked	5887 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2012, 8, 1515-1531.	2.3	765
3	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.	6.6	729
4	Fundamental Gaps in Finite Systems from Eigenvalues of a Generalized Kohn-Sham Method. Physical Review Letters, 2010, 105, 266802.	2.9	377
5	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.	1.2	313
6	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.	2.3	221
7	Seniority zero pair coupled cluster doubles theory. Journal of Chemical Physics, 2014, 140, 214113.	1.2	147
8	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	2.1	145
9	Seniority-based coupled cluster theory. Journal of Chemical Physics, 2014, 141, 244104.	1.2	110
10	Calculation of transition dipole moment in fluorescent proteinsâ€"towards efficient energy transfer. Physical Chemistry Chemical Physics, 2012, 14, 4109.	1.3	60
11	Electrochemical deposition of N-heterocyclic carbene monolayers on metal surfaces. Nature Communications, 2020, 11, 5714.	5.8	32
12	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.	1.1	26
13	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.	1.5	25
14	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.	3.3	24
15	Photoredoxâ€Mediated Reaction of gemâ€Diborylalkenes: Reactivity Toward Diverse 1,1â€Bisborylalkanes. Chemistry - A European Journal, 2020, 26, 5360-5364.	1.7	24
16	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.	6.6	19
17	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.	1.6	18
18	Probing Ionic Complexes of Ethylene and Acetylene with Vacuum-Ultraviolet Radiation. Journal of Physical Chemistry A, 2016, 120, 5053-5064.	1.1	11

#	Article	IF	Citations
19	Molecular Formation upon Ionization of van der Waals Clusters and Implication to Astrochemistry. Israel Journal of Chemistry, 2020, 60, 842-849.	1.0	10
20	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.	1.3	8
21	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, .	3.3	6
22	Isomerization of hydrogen cyanide and hydrogen isocyanide in a cluster environment: quantum chemical study. Journal of Chemical Physics, 2022, 156, 054307.	1.2	3
23	Accelerated Multiphosphorylated Peptide Synthesis. Organic Process Research and Development, 0, , .	1.3	3
24	The Effect of Cluster Size on the Intra-Cluster Ionic Polymerization Process. Molecules, 2021, 26, 4782.	1.7	2