Gregory S Tschumper

List of Publications by Year
in descending order

115 papers	4,417 citations	117453 34 h-index	110170 64 g-index
121 all docs	121 docs citations	121 times ranked	4081 citing authors

#	Article	IF	Citations
1	Atomic and Molecular Electron Affinities:â€‰ Photoelectron Experiments and Theoretical Computations. Chemical Reviews, 2002, 102, 231-282.	23.0	1,152
2	Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses. Journal of Chemical Physics, 2002, 116, 690-701.	1.2	262
3	CCSD(T) Complete Basis Set Limit Relative Energies for Low-Lying Water Hexamer Structures. Journal of Physical Chemistry A, 2009, 113, 3555-3559.	1.1	188
4	Predicting electron affinities with density functional theory: Some positive results for negative ions. Journal of Chemical Physics, 1997, 107, 2529-2541.	1.2	114
5	Epigenetic Modification, Dehydration, and Molecular Crowding Effects on the Thermodynamics of i-Motif Structure Formation from C-Rich DNA. Biochemistry, 2014, 53, 1586-1594.	1.2	109
6	Hydrogen Bonding in Alcohol Clusters:â€‰ A Comparative Study by Infrared Cavity Ringdown Laser Absorption Spectroscopy. Journal of Physical Chemistry A, 2000, 104, 1423-1429.	1.1	105
7	Ab Initio Studies of Ï€Â·Â·Â·Ï€ Interactions:Â The Effects of Quadruple Excitationsâ€. Journal of Physical Chemistry A, 2004, 108, 2941-2948.	1.1	84
8	Interstaple Dithiol Cross-Linking in Au₂₅(SR)₁₈ Nanomolecules: A Combined Mass Spectrometric and Computational Study. Journal of the American Chemical Society, 2011, 133, 20258-20266.	6.6	79
9	Structures, thermochemistry, and electron affinities of the PFn and PFâ¯n series, n=1â€“6. Journal of Chemical Physics, 1996, 104, 3676-3683.	1.2	76
10	Indolizineâ€Based Donors as Organic Sensitizer Components for Dyeâ€Sensitized Solar Cells. Advanced Energy Materials, 2015, 5, 1401629.	10.2	71
11	Anchoring the potential energy surface of the cyclic water trimer. Journal of Chemical Physics, 2004, 121, 11023.	1.2	68
12	Real versus artifactual symmetry-breaking effects in Hartreeâ€“Fock, density-functional, and coupled-cluster methods. Journal of Chemical Physics, 2004, 120, 7298-7306.	1.2	68
13	Development of a 3-body:many-body integrated fragmentation method for weakly bound clusters and application to water clusters (H2O)n= 3 â¯ 10, 16, 17. Journal of Chemical Physics, 2011, 135, 044123.	1.2	68
14	Multicentered integrated QM:QM methods for weakly bound clusters: An efficient and accurate 2-body:many-body treatment of hydrogen bonding and van der Waals interactions. Chemical Physics Letters, 2006, 427, 185-191.	1.2	64
15	Getting down to the Fundamentals of Hydrogen Bonding: Anharmonic Vibrational Frequencies of (HF)₂ and (H₂O)₂ from Ab Initio Electronic Structure Computations. Journal of Chemical Theory and Computation, 2014, 10, 5426-5435.	2.3	63
16	Benchmark Structures and Harmonic Vibrational Frequencies Near the CCSD(T) Complete Basis Set Limit for Small Water Clusters: (H₂O)_{nÂ=Â2, 3, 4, 5, 6}. Journal of Chemical Theory and Computation, 2015, 11, 2126-2136.	2.3	63
17	A multicentered approach to integrated QM/QM calculations. Applications to multiply hydrogen bonded systems. Journal of Computational Chemistry, 2003, 24, 1563-1568.	1.5	61
18	Intrinsic Conformational Preferences of Substituted Cyclohexanes and Tetrahydropyrans Evaluated at the CCSD(T) Complete Basis Set Limit:Â Implications for the Anomeric Effect. Journal of Physical Chemistry A, 2005, 109, 11073-11079.	1.1	58

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19	Efficient and Accurate Methods for the Geometry Optimization of Water Clusters: Application of Analytic Gradients for the Two-Body:Many-Body QM:QM Fragmentation Method to (H₂O)_n = 3â€“10. Journal of Chemical Theory and Computation, 2011, 7, 2753-2760.	2.3	53
20	Gauging the applicability of ONIOM (MO/MO) methods to weak chemical interactions in large systems: hydrogen bonding in alcohol dimers. Computational and Theoretical Chemistry, 2002, 592, 137-147.	1.5	52
21	Effects of Hydrogen Bonding on Vibrational Normal Modes of Pyrimidine. Journal of Physical Chemistry A, 2010, 114, 6803-6810.	1.1	49
22	Assessing the accuracy of some popular DFT methods for computing harmonic vibrational frequencies of water clusters. Journal of Chemical Physics, 2015, 143, 214103.	1.2	49
23	Characterizing the Potential Energy Surface of the Water Dimer with DFT:Â Failures of Some Popular Functionals for Hydrogen Bonding. Journal of Physical Chemistry A, 2006, 110, 7268-7271.	1.1	48
24	Hydrocarbon/Water Interactions: Encouraging Energetics and Structures from DFT but Disconcerting Discrepancies for Hessian Indices. Journal of Chemical Theory and Computation, 2012, 8, 1646-1656.	2.3	47
25	Probing Phenylalanine/Adenine Ï€-Stacking Interactions in Protein Complexes with Explicitly Correlated and CCSD(T) Computations. Journal of Physical Chemistry B, 2008, 112, 14291-14295.	1.2	46
26	Accurate Interaction Energies for Problematic Dispersion-Bound Complexes: Homogeneous Dimers of NCCN, P2, and PCCP. Journal of Chemical Theory and Computation, 2011, 7, 2842-2851.	2.3	46
27	Charge Transfer and Blue Shifting of Vibrational Frequencies in a Hydrogen Bond Acceptor. Journal of Physical Chemistry A, 2013, 117, 5435-5446.	1.1	46
28	Electron affinities of the oxides of aluminum, silicon, phosphorus, sulfur, and chlorine. Journal of Chemical Physics, 1999, 110, 6240-6245.	1.2	44
29	Wavefunction methods for the accurate characterization of water clusters. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 199-224.	6.2	43
30	N-body:Many-body QM:QM vibrational frequencies: Application to small hydrogen-bonded clusters. Journal of Chemical Physics, 2013, 139, 184113.	1.2	42
31	Multicentred QM/QM methods for overlapping model systems. Molecular Physics, 2005, 103, 309-315.	0.8	41
32	Integrated quantum mechanical approaches for extended Ï€ systems: Multicentered QM/QM studies of the cyanogen and diacetylene trimers. Chemical Physics Letters, 2005, 407, 362-367.	1.2	39
33	Assignment of the infrared spectra of the methanol trimer. Journal of Chemical Physics, 1999, 111, 3027-3034.	1.2	37
34	Intrinsic conformational preferences of and an anomeric-like effect in 1-substituted silacyclohexanes. International Journal of Quantum Chemistry, 2007, 107, 2261-2265.	1.0	37
35	A high level theoretical investigation of the cyclic hydrogen fluoride trimer. Journal of Chemical Physics, 1997, 106, 9627-9633.	1.2	34
36	A Computational and Experimental Study of Thieno[3,4â€b]thiophene as a Proaromatic Ï€â€Bridge in Dyeâ€Sensitized Solar Cells. Chemistry - A European Journal, 2016, 22, 694-703.	1.7	34

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37	Synthesis of the ABC Ring System of Azaspiracid. 2. A Systematic Study into the Effect of C16 and C17 Substitution on Bis-spirocyclization. Organic Letters, 2002, 4, 2181-2184.	2.4	33
38	Analytic gradients for the multicentred integrated QM:QM method for weakly bound clusters: efficient and accurate 2-body:many-body geometry optimizations. Molecular Physics, 2007, 105, 2777-2782.	0.8	32
39	An Alternative Mechanism for the Dimerization of Formic Acid. Journal of Physical Chemistry A, 2003, 107, 10208-10216.	1.1	30
40	Basis set dependence of higher-order correlation effects in Ï€-type interactions. Journal of Chemical Physics, 2012, 136, 014103.	1.2	27
41	Subtle basis set effects on hydrogen bonded systems. Molecular Physics, 1999, 96, 493-504.	0.8	26
42	Probing the effects of heterogeneity on delocalized Ï€â‹¯Ï€ interaction energies. Physical Chemistry Chemical Physics, 2008, 10, 2775.	1.3	25
43	Examination of Tyrosine/Adenine Stacking Interactions in Protein Complexes. Journal of Physical Chemistry B, 2013, 117, 14001-14008.	1.2	25
44	Elucidating the Effects of Fluoro and Nitro Substituents on Halogen Bond Driven Assemblies of Pyridyl-Capped Ï€-Conjugated Molecules. Crystal Growth and Design, 2016, 16, 6648-6653.	1.4	25
45	The hydroperoxyl radical dimer: Triplet ring or singlet string?. Journal of Chemical Physics, 1997, 106, 5102-5108.	1.2	24
46	Homogeneous and Heterogeneous Noncovalent Dimers of Formaldehyde and Thioformaldehyde: Structures, Energetics, and Vibrational Frequencies. Journal of Physical Chemistry A, 2014, 118, 3376-3385.	1.1	24
47	Spectroscopic and computational insight into weak noncovalent interactions in crystalline pyrimidine. Chemical Physics Letters, 2011, 501, 319-323.	1.2	22
48	Probing Dative and Dihydrogen Bonding in Ammonia Borane with Electronic Structure Computations and Raman under Nitrogen Spectroscopy. Journal of Physical Chemistry A, 2017, 121, 5884-5893.	1.1	22
49	Systematic Experimental and Computational Studies of Substitution and Hybridization Effects in Solid-State Halogen Bonded Assemblies. Crystal Growth and Design, 2018, 18, 3244-3254.	1.4	20
50	Computational and ESR Studies of Electron Attachment to Decafluorocyclopentane, Octafluorocyclobutane, and Hexafluorocyclopropane:Â Electron Affinities of the Molecules and the Structures of Their Stable Negative Ions as Determined from13C and19F Hyperfine Coupling Constants. Journal of the American Chemical Society, 2005, 127, 10573-10583.	6.6	18
51	A Robust Pyridyl-NHC-Ligated Rhenium Photocatalyst for CO2 Reduction in the Presence of Water and Oxygen. Inorganics, 2018, 6, 22.	1.2	18
52	Comparison of polarization consistent and correlation consistent basis sets for noncovalent interactions. International Journal of Quantum Chemistry, 2009, 109, 91-96.	1.0	17
53	Peptide Bond Formation via Glycine Condensation in the Gas Phase. Journal of Physical Chemistry B, 2014, 118, 8583-8590.	1.2	17
54	Vibrational Spectroscopy of N-Methyliminodiacetic Acid (MIDA)-Protected Boronate Ester: Examination of the Bâ€“N Dative Bond. Journal of Physical Chemistry A, 2011, 115, 6426-6431.	1.1	16

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55	Quantifying the Effects of Halogen Bonding by Haloaromatic Donors on the Acceptor Pyrimidine. ChemPhysChem, 2017, 18, 1267-1273.	1.0	16
56	Examination of the structures, energetics, and vibrational frequencies of small sulfurâ€containing prototypical dimers, (H 2 S) 2 and H 2 O/H 2 S. Journal of Computational Chemistry, 2019, 40, 229-236.	1.5	16
57	Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie - International Edition, 2020, 59, 11399-11407.	7.2	16
58	Anharmonic vibrational frequencies of ammonia borane (BH3NH3). Journal of Chemical Physics, 2021, 154, 041104.	1.2	15
59	Structures, Energetics and Vibrational Frequency Shifts of Hydrated Pyrimidine. ChemPhysChem, 2011, 12, 3262-3273.	1.0	14
60	Competition between Hydrophilic and Argyrophilic Interactions in Surface Enhanced Raman Spectroscopy. ChemPhysChem, 2016, 17, 2782-2786.	1.0	14
61	The onset of electron-induced proton-transfer in hydrated azabenzene cluster anions. Physical Chemistry Chemical Physics, 2016, 18, 704-712.	1.3	14
62	A comparison between the CISD[TQ] wave function and other highly correlated methods: Molecular geometry and harmonic vibrational frequencies of MgH2. Journal of Chemical Physics, 1998, 108, 7511-7515.	1.2	13
63	Synergistic effects of halogen bond and Ï€â€“Ï€ interactions in thiophene-based building blocks. RSC Advances, 2015, 5, 82544-82548.	1.7	13
64	Effect of â€œXâ€•Ligands on the Photocatalytic Reduction of CO₂ to CO with Re(pyridylNHCâ€CF₃)(CO)₃X Complexes. European Journal of Inorganic Chemistry, 2020, 2020, 1844-1851.	1.0	13
65	Photoelectron Spectroscopic and Computational Study of Hydrated Pyrimidine Anions. Journal of Physical Chemistry A, 2014, 118, 11901-11907.	1.1	12
66	Dissociation Energy of the H₂OÂ·Â·Â·HF Dimer. Journal of Physical Chemistry A, 2018, 122, 4902-4908.	1.1	12
67	Binding of the atomic cations hydrogen through argon to water and hydrogen sulfide. Physical Chemistry Chemical Physics, 2018, 20, 25967-25973.	1.3	12
68	Intermolecular Interactions and Vibrational Perturbations within Mixtures of 1-Ethyl-3-methylimidazolium Thiocyanate and Water. Journal of Physical Chemistry C, 2018, 122, 27673-27680.	1.5	12
69	Reliable structures and energetics for two new delocalized Ï€â‹¯Ï€ prototypes: cyanogen dimer and diacetylene dimer. Physical Chemistry Chemical Physics, 2007, 9, 1550-1558.	1.3	11
70	Anchoring the potential energy surface of the nitrogen/water dimer, N2â‹¯H2O, with explicitly correlated coupled-cluster computations. Computational and Theoretical Chemistry, 2013, 1021, 109-113.	1.1	11
71	Characterization of Furan- and Thiophene-Containing Bispyridyl Oligomers via Spectroscopic, Electrochemical, and TD-DFT Methods. Journal of Physical Chemistry C, 2019, 123, 15176-15185.	1.5	11
72	Probing non-covalent interactions driving molecular assembly in organo-electronic building blocks. CrystEngComm, 2019, 21, 3151-3157.	1.3	11

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73	Hydrogen bonding in the mixed HF/HCl dimer: Is it better to give or receive?. Journal of Computational Chemistry, 2018, 39, 839-843.	1.5	10
74	Torsional Profiles of Thiophene and Furan Oligomers: Probing the Effects of Heterogeneity and Chain Length. Journal of Physical Chemistry A, 2021, 125, 6228-6237.	1.1	10
75	Ab initio theoretical studies of potential energy surfaces in the photodissociation of the vinyl radical. I. Ãƒ state dissociation. Journal of Chemical Physics, 2003, 119, 6524-6538.	1.2	9
76	A systematic assessment of density functionals and ONIOM schemes for the study of hydrogen bonding between water and the side chains of serine, threonine, asparagine, and glutamine. Computational and Theoretical Chemistry, 2006, 771, 65-71.	1.5	9
77	Anchoring the hydrogen sulfide dimer potential energy surface to juxtapose (H2S)2 with (H2O)2. Journal of Chemical Physics, 2020, 152, 214306.	1.2	9
78	Extending the ONIOM integrated MO/MO approach to hydrogen bonding in biologic systems: Serine-water and threonine-water dimers. International Journal of Quantum Chemistry, 2004, 96, 294-302.	1.0	8
79	Water network-mediated, electron-induced proton transfer in [C5H5N â‹… (H2O)n]â^' clusters. Journal of Chemical Physics, 2015, 143, 144305.	1.2	8
80	Superconvergent Perturbation Theory for an Anharmonic Oscillator. Journal of Mathematical Chemistry, 2002, 31, 105-120.	0.7	7
81	Reliable Electron Affinities of Perfluorocyclopropane and Perfluorocyclobutane from Convergent ab Initio Computations. Journal of Physical Chemistry A, 2006, 110, 1975-1977.	1.1	7
82	Energetics of Oxaspirocycle Prototypes:â€‰ 1,7-Dioxaspiro[5.5]undecane and 1,7,9-Trioxadispiro[5.1.5.3]hexadecane. Journal of Organic Chemistry, 2006, 71, 9212-9216.	1.7	7
83	Anchoring the potential energy surface of the diacetylene dimer. Molecular Physics, 2009, 107, 923-928.	0.8	7
84	2-body:Many-body QM:QM study of structures, energetics, and vibrational frequencies for microhydrated halide ions. Molecular Physics, 2019, 117, 1413-1420.	0.8	7
85	Characterization of Competing Halogen- and Hydrogen-Bonding Motifs in Simple Mixed Dimers of HCN and HX (X = F, Cl, Br, and I). Journal of Physical Chemistry A, 2022, 126, 3688-3695.	1.1	7
86	Chemically accurate conformational energies for aziridine-2-carbonitrile. Journal of Chemical Physics, 2001, 114, 225.	1.2	6
87	Anchoring the potential energy surface of an important atmospheric van der Waals dimer, the H2Oâ‹¯O2 complex. Computational and Theoretical Chemistry, 2015, 1072, 21-27.	1.1	6
88	A Raman Spectroscopic and Computational Study of New Aromatic Pyrimidine-Based Halogen Bond Acceptors. Inorganics, 2019, 7, 119.	1.2	6
89	Dissociation energy of the HCNâ‹¯HF dimer. Chemical Physics Letters, 2020, 748, 137382.	1.2	6
90	Effects of Heterogeneity in Small Ï€-Type Dimers: Homogeneous and Mixed Dimers of Diacetylene and Cyanogen. Journal of Chemical Theory and Computation, 2012, 8, 4279-4284.	2.3	5

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91	Characterizing the Bï£¿P Stretching Vibration in Phosphorusâ€Substituted Phosphine Boranes. ChemPhysChem, 2014, 15, 1867-1871.	1.0	5
92	Communication: Gas phase vibrational spectroscopy of the azide-water complex. Journal of Chemical Physics, 2018, 149, 191101.	1.2	5
93	An ab Initio Excursion on the Lowest 18 Electronic Surfaces of the NCl + NCl System:â€‰ Some Insight into the Long-Range Self-Quenching Pathways of the First Excited State of NCl. Journal of Physical Chemistry A, 2002, 106, 8453-8460.	1.1	4
94	Intramolecular Hydrogen Bonding in Î±-Epoxy Alcohols: A Conformational Analysis of 1,2-Dialkyl-2,3-epoxycyclopentanol Diastereomers. Chemistry Letters, 2018, 47, 156-159.	0.7	4
95	Energetics and Vibrational Signatures of Nucleobase Argyrophilic Interactions. ACS Omega, 2018, 3, 12936-12943.	1.6	4
96	Computational Investigation on Electronic Structures and Properties of 4,6-Bis(nitroimino)-1,3,5-triazinan-2-one: An Insensitive Munition Compound. Journal of Physical Chemistry A, 2019, 123, 3504-3509.	1.1	4
97	Probing the Effects of Electron Deficient Aryl Substituents and a Ï€â€System Extended NHC Ring on the Photocatalytic CO₂ Reduction Reaction with Reâ€pyNHCâ€Aryl Complexes**. ChemPhotoChem, 2021, 5, 353-361.	1.5	4
98	Concerning the stability of dichlorodiazene. Chemical Physics Letters, 2003, 370, 418-424.	1.2	3
99	Big Changes for Small Noncovalent Dimers: Revisiting the Potential Energy Surfaces of (P₂)₂ and (PCCP)₂ with CCSD(T) Optimizations and Vibrational Frequencies. Journal of Chemical Theory and Computation, 2016, 12, 1534-1541.	2.3	3
100	Dissociation in Binary Acid/Base Clusters: An Examination of Inconsistencies Introduced Into the Many-Body Expansion by NaÃ¯ve Fragmentation Schemes. Annual Reports in Computational Chemistry, 2017, , 93-115.	0.9	3
101	Co-Localization of DNA i-Motif-Forming Sequences and 5-Hydroxymethyl-cytosines in Human Embryonic Stem Cells. Molecules, 2019, 24, 3619.	1.7	3
102	Characterization of the potential energy surfaces of two small but challenging noncovalent dimers: (P₂)₂ and (PCCP)₂. Journal of Computational Chemistry, 2014, 35, 479-487.	1.5	2
103	Cis/Trans Energetics in Epoxide, Thiirane, Aziridine and Phosphirane Containing Cyclopentanols: Effects of Intramolecular OHâ‹¯O, S, N and P Contacts. Molecules, 2019, 24, 2523.	1.7	2
104	Competition between Solventâ€“Solvent and Solventâ€“Solute Interactions in the Microhydration of the Hexafluorophosphate Anion, PF6â€“(H2O)n=1,2. Journal of Physical Chemistry A, 2020, 124, 8744-8752.	1.1	2
105	Solvation of Isoelectronic Halide and Alkali Metal Ions by Argon Atoms. Journal of Physical Chemistry A, 2021, 125, 10524-10531.	1.1	2
106	Correlation of Solid-State Order to Optoelectronic Behavior in Heterocyclic Oligomers. CrystEngComm, 0, , .	1.3	2
107	Raman and SERS Spectroscopy of N-Methyliminodiacetic Acid (MIDA)-Protected Boronate Esters. , 2010, , .		1
108	Fundamental vibrational frequencies of isolated 2-phosphaethynolate and 2-phosphaethynthiolate anions: OCPâ€“Âand SCPâ€“. Molecular Physics, 0, , e1967495.	0.8	1

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109	Relative energetics of CH3CH2O, CH3CHOH, and CH2CH2OH radical products from ethanol dehydrogenation. Journal of Chemical Physics, 2021, 155, 114306.	1.2	1
110	Subtle basis set effects on hydrogen bonded systems. , 0, .		1
111	Raman Spectroscopic Investigations of Noncovalent Interactions between Pyrimidine and Hydrogen Bonded Networks. , 2010, , .		0
112	Boyd Group Electronegativity Influence on the Parr Global Electrophilicity of Vilsmeier Reagentâ€Derived Imidates: New Insights toward Improving Mitsunobu Chemistry. Helvetica Chimica Acta, 2015, 98, 582-588.	1.0	0
113	Frontispiz: Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie, 2020, 132, .	1.6	0
114	Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie, 2020, 132, 11496-11504.	1.6	0
115	Frontispiece: Observation of the Lowâ€Frequency Spectrum of the Water Trimer as a Sensitive Test of the Waterâ€Trimer Potential and the Dipoleâ€Moment Surface. Angewandte Chemie - International Edition, 2020, 59, .	7.2	0