Thomas Sommerfeld

List of Publications by Year
in descending order

42 papers	1,036 citations	394421 19 h-index	434195 31 g-index
42 all docs	42 docs citations	42 times ranked	743 citing authors

#	Article	IF	Citations
1	Lifetimes of Be₃^{2â€“} and Mg₃^{2â€“} Cluster Dianions. Journal of Physical Chemistry A, 2021, 125, 3579-3588.	2.5	4
2	CAP/EA-ADC method for metastable anions: Computational aspects and application to Ï€* resonances of norbornadiene and 1,4-cyclohexadiene. Journal of Chemical Physics, 2021, 155, 054103.	3.0	13
3	Autodetachment over Broad Photon Energy Ranges in the Anion Photoelectron Spectra of [O₂â€“M]^{â¯} (M = Glyoxal, Methylglyoxal, or) Tj ETQq1 1 0.784314 rgBT /Over	2.5	7
4	Computing resonance energies directly: method comparison for a model potential. European Physical Journal D, 2021, 75, 1.	1.3	9
5	Resonant states in cyanogen NCCN. Physical Chemistry Chemical Physics, 2020, 22, 23141-23147.	2.8	9
6	Temporary anion states of fluorine substituted benzenes probed by charge transfer in O2â¯Â·C6H6â¯xFx (x = 0â€“5) ionâ€“molecule complexes. Journal of Chemical Physics, 2020, 152, 204309.	3.0	7
7	Combination of a Voronoi-Type Complex Absorbing Potential with the XMS-CASPT2 Method and Pilot Applications. Journal of Chemical Theory and Computation, 2020, 16, 2606-2616.	5.3	14
8	Excluded-volume descriptors for dipole-bound anions: Amine N-oxides as a test case. Journal of Chemical Physics, 2020, 152, 054102.	3.0	6
9	Emerging Nonvalence Anion States of [Isoprene-HÂ·]Â·H₂O Accessed via Detachment of OH^{â€“}Â·Isoprene. Journal of Physical Chemistry A, 2020, 124, 2279-2287.	2.5	7
10	Temporary Anion States of Ethene Interacting with Single Molecules of Methane, Ethane, and Water. Journal of Physical Chemistry A, 2018, 122, 2580-2586.	2.5	5
11	Ring-opening attachment as an explanation for the long lifetime of the octafluorooxolane anion. Journal of Chemical Physics, 2018, 149, 084305.	3.0	10
12	Resonance Energies and Lifetimes from the Analytic Continuation of the Coupling Constant Method: Robust Algorithms and a Critical Analysis. Journal of Chemical Theory and Computation, 2017, 13, 2550-2560.	5.3	7
13	Theoretical approaches for treating non-valence correlation-bound anions. Journal of Chemical Physics, 2017, 147, 214114.	3.0	34
14	Low-lying Ï€âˆ— resonances associated with cyano groups: A CAP/SAC-CI study. Chemical Physics, 2017, 482, 169-177.	1.9	15
15	Projected <scp>CAP</scp>/<scp>SAC</scp>â€<scp>CI</scp> method with smooth <scp>V</scp>oronoi potential for calculating resonance states. Journal of Computational Chemistry, 2016, 37, 242-249.	3.3	19
16	Low-Lying Ï€* Resonances of Standard and Rare DNA and RNA Bases Studied by the Projected CAP/SACâ€“CI Method. Journal of Physical Chemistry A, 2016, 120, 1545-1553.	2.5	36
17	Short-range stabilizing potential for computing energies and lifetimes of temporary anions with extrapolation methods. Journal of Chemical Physics, 2015, 142, 034105.	3.0	28
18	Complex Absorbing Potentials with Voronoi Isosurfaces Wrapping Perfectly around Molecules. Journal of Chemical Theory and Computation, 2015, 11, 4627-4633.	5.3	43

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19	Excess Electrons Bound to Molecular Systems with a Vanishing Dipole but Large Molecular Quadrupole. Journal of Physical Chemistry A, 2014, 118, 7320-7329.	2.5	31
20	Method for Visualizing and Quantifying the Nonvalence Character of Excess Electrons. Journal of Chemical Theory and Computation, 2013, 9, 4866-4873.	5.3	13
21	Combined photoelectron, collision-induced dissociation, and computational studies of parent and fragment anions of N-paranitrophenylsulfonylalanine and N-paranitrophenylalanine. Journal of Chemical Physics, 2013, 139, 224308.	3.0	0
22	Characterizing the excess electron of Li(NH3)4. Journal of Chemical Physics, 2012, 137, 244302.	3.0	18
23	Benchmark Calculations of the Energies for Binding Excess Electrons to Water Clusters. Journal of Chemical Theory and Computation, 2012, 8, 893-900.	5.3	39
24	CAP/SAC-CI method for calculating resonance states of metastable anions. Chemical Physics Letters, 2012, 537, 107-112.	2.6	59
25	Al(CN)3â^'6 and Al(NC)3â^'6 trianions. Physical Chemistry Chemical Physics, 2011, 13, 18393.	2.8	3
26	Empirical Correlation Methods for Temporary Anions. Journal of Physical Chemistry A, 2011, 115, 6675-6682.	2.5	28
27	Synthesis of Nâ€alkoxybenzimidoyl azides and their reactions in electrophilic media. Journal of Physical Organic Chemistry, 2010, 23, 227-237.	1.9	6
28	Al 4 â^' cluster anion: Electronic structure, excited states, and electron detachment. Journal of Chemical Physics, 2010, 132, 124305.	3.0	5
29	Correlation-bound anions of NaCl clusters. Journal of Chemical Physics, 2010, 133, 114301.	3.0	33
30	Discrete Variable Representation Implementation of the One-Electron Polarization Model. Journal of Chemical Theory and Computation, 2010, 6, 2388-2394.	5.3	5
31	Excess Electrons Bound to Small Ammonia Clusters. Journal of Physical Chemistry A, 2008, 112, 11817-11823.	2.5	21
32	Reply to â€œComment on â€˜Instability of the Al42â^' â€˜All-Metal Aromaticâ€™ Ion and Its Implicationsâ€™â€• Journal of Physical Chemistry A, 2008, 112, 7986-7986.	2.5	17
33	Model Potential Approaches for Describing the Interaction of Excess Electrons with Water Clusters: Incorporation of Long-Range Correlation Effects. Journal of Physical Chemistry A, 2008, 112, 11021-11035.	2.5	68
34	Doorway mechanism for dissociative electron attachment to fructose. Journal of Chemical Physics, 2007, 126, 124301.	3.0	38
35	Comment on â€œAb initio studies of (H2O)14â^' clusters: Existence of surface and interior-bound extra electronsâ€•[J. Chem. Phys. 125, 024307 (2006)]. Journal of Chemical Physics, 2007, 126, 027101.	3.0	7
36	Intersections of potential energy surfaces of short-lived states: The complex analogue of conical intersections. Journal of Chemical Physics, 2004, 120, 3201-3214.	3.0	50

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37	Complex absorbing potentials in the framework of electron propagator theory. II. Application to temporary anions. Journal of Chemical Physics, 2003, 118, 6188-6199.	3.0	92
38	A Fresh Look at Aromatic Dianions. Journal of the American Chemical Society, 2002, 124, 1119-1124.	13.7	65
39	Efficient method to perform CAP/CI calculations for temporary anions. International Journal of Quantum Chemistry, 2001, 82, 218-226.	2.0	66
40	Electron-induced Chemistry of 5-Chlorouracil. ChemPhysChem, 2001, 2, 677-679.	2.1	24
41	Resonance States of Atomic Di-anions. Physical Review Letters, 2000, 85, 956-959.	7.8	27
42	Lifetimes of Metastable Dianions:Â CN22-, C42-, and CO32-. Journal of Physical Chemistry A, 2000, 104, 8806-8813.	2.5	48