Istvan Szabo

List of Publications by Year in descending order

32 papers	1,251 citations	304701 22 h-index	454934 30 g-index
32 all docs	32 docs citations	32 times ranked	1299 citing authors

#	Article	IF	Citations
1	Revealing a double-inversion mechanism for the Fâ¯+CH3Cl SN2 reaction. Nature Communications, 2015, 6, 5972.	12.8	134
2	Influence of the leaving group on the dynamics of a gas-phase SN2 reaction. Nature Chemistry, 2016, 8, 151-156.	13.6	116
3	Room-Temperature Optical Picocavities below 1 nm³ Accessing Single-Atom Geometries. Journal of Physical Chemistry Letters, 2018, 9, 7146-7151.	4.6	88
4	Dynamics of the Fâ¯ + CH3Cl â† Clâ¯ + CH3F SN2 reaction on a chemically accurate potential energy surface. Chemical Science, 2013, 4, 4362.	7.4	70
5	Mode-Specific S_N2 Reaction Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 3322-3327.	4.6	63
6	Dynamics and Novel Mechanisms of S_N2 Reactions on ab Initio Analytical Potential Energy Surfaces. Journal of Physical Chemistry A, 2017, 121, 9005-9019.	2.5	55
7	High-level ab initio potential energy surface and dynamics of the F^{â¯}+ CH₃I S_N2 and proton-transfer reactions. Chemical Science, 2017, 8, 3164-3170.	7.4	53
8	Molecular simulations unravel the molecular principles that mediate selective permeability of carboxysome shell protein. Scientific Reports, 2020, 10, 17501.	3.3	52
9	Double-Inversion Mechanisms of the X^{â€“} + CH₃Y [X,Y = F, Cl, Br, I] S_N2 Reactions. Journal of Physical Chemistry A, 2015, 119, 3134-3140.	2.5	49
10	Deciphering Front-Side Complex Formation in S_N2 Reactions via Dynamics Mapping. Journal of Physical Chemistry Letters, 2017, 8, 2917-2923.	4.6	49
11	Controlling the structure and photophysics of fluorophore dimers using multiple cucurbit[8]uril clampings. Chemical Science, 2020, 11, 812-825.	7.4	48
12	EXPERIMENTAL ENERGY LEVELS AND PARTITION FUNCTION OF THE ¹²C₂ MOLECULE. Astrophysical Journal, Supplement Series, 2016, 224, 44.	7.7	45
13	Modular supramolecular dimerization of optically tunable extended aryl viologens. Chemical Science, 2019, 10, 8806-8811.	7.4	43
14	Hostâ€“Guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as a Hybrid System in CO₂ Reduction. ACS Catalysis, 2020, 10, 751-761.	11.2	43
15	Tracking Nanoelectrochemistry Using Individual Plasmonic Nanocavities. Nano Letters, 2017, 17, 4840-4845.	9.1	42
16	ExoMol line lists XXXI: spectroscopy of lowest eights electronic states of C2. Monthly Notices of the Royal Astronomical Society, 2018, 480, 3397-3411.	4.4	37
17	On the Choice of the Ab Initio Level of Theory for Potential Energy Surface Developments. Journal of Physical Chemistry A, 2014, 118, 646-654.	2.5	36
18	Anomalously Large Spectral Shifts near the Quantum Tunnelling Limit in Plasmonic Rulers with Subatomic Resolution. Nano Letters, 2019, 19, 2051-2058.	9.1	35

#	Article	IF	Citations
19	Accurate ab initio potential energy surface, thermochemistry, and dynamics of the Fâ˙ + CH3F SN2 and proton-abstraction reactions. Journal of Chemical Physics, 2015, 142, 244301.	3.0	33
20	Cucurbit[8]uril-mediated pseudo[2,3]rotaxanes. Chemical Communications, 2019, 55, 13227-13230.	4.1	29
21	Inhibiting Analyte Theft in Surface-Enhanced Raman Spectroscopy Substrates: Subnanomolar Quantitative Drug Detection. ACS Sensors, 2019, 4, 2988-2996.	7.8	27
22	Benchmark ab Initio Characterization of the Complex Potential Energy Surface of the Cl^{â€“} + CH₃I Reaction. Journal of Physical Chemistry A, 2017, 121, 5748-5757.	2.5	23
23	Smart supramolecular sensing with cucurbit[n]urils: probing hydrogen bonding with SERS. Faraday Discussions, 2017, 205, 505-515.	3.2	20
24	Benchmark ab initio and dynamical characterization of the stationary points of reactive atom + alkane and S_N2 potential energy surfaces. Physical Chemistry Chemical Physics, 2020, 22, 4298-4312.	2.8	17
25	Mode-specific multi-channel dynamics of the Fâ˙ + CHD2Cl reaction on a global ab initio potential energy surface. Journal of Chemical Physics, 2016, 145, 134303.	3.0	15
26	Rotational Mode Specificity in the F^{â€“} + CH₃Y [Y = F and Cl] S_N2 Reactions. Journal of Physical Chemistry A, 2015, 119, 12231-12237.	2.5	9
27	Temperature-Dependent, Effective Structures of the ¹⁴NH₃ and ¹⁴ND₃ Molecules. Journal of Physical Chemistry A, 2012, 116, 4356-4362.	2.5	8
28	Toward Understanding CB[7]-Based Supramolecular Diels-Alder Catalysis. Frontiers in Chemistry, 2020, 8, 587084.	3.6	6
29	Gas-phase structures reflect the pain-relief potency of enkephalin peptides. Physical Chemistry Chemical Physics, 2019, 21, 22700-22703.	2.8	3
30	Combining data integration and molecular dynamics for target identification in Î±-Synuclein-aggregating neurodegenerative diseases: Structural insights on Synaptojanin-1 (Synj1). Computational and Structural Biotechnology Journal, 2020, 18, 1032-1042.	4.1	3
31	1 Host-guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as Hybrid System in CO2 Reduction. , 0, , .		0
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