LÃ¡szlÃ³ Turi

List of Publications by Year
in descending order

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52	2,579	159585	182427
papers	citations	30 h-index	51 g-index

54	54	54	1547
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Correcting for basis set superposition error in aggregates containing more than two molecules: ambiguities in the calculation of the counterpoise correction. The Journal of Physical Chemistry, 1993, 97, 2488-2490.	2.9	262
2	Characterization of Excess Electrons in Water-Cluster Anions by Quantum Simulations. Science, 2005, 309, 914-917.	12.6	220
3	Theoretical Studies of Spectroscopy and Dynamics of Hydrated Electrons. Chemical Reviews, 2012, 112, 5641-5674.	47.7	169
4	Analytical investigations of an electronâ€“water molecule pseudopotential. II. Development of a new pair potential and molecular dynamics simulations. Journal of Chemical Physics, 2002, 117, 6186-6195.	3.0	147
5	Molecular orbital study of acetic acid aggregation. 1. Monomers and dimers. The Journal of Physical Chemistry, 1993, 97, 12197-12204.	2.9	143
6	Molecular orbital studies of C-H...O hydrogen-bonded complexes. The Journal of Physical Chemistry, 1993, 97, 7899-7909.	2.9	130
7	Acidity of hydroxamic acids: an ab initio and semiempirical study. Journal of the American Chemical Society, 1993, 115, 5754-5761.	13.7	82
8	Ab Initio Molecular Orbital Analysis of Dimers ofcis-Formic Acid. Implications for Condensed Phases. The Journal of Physical Chemistry, 1996, 100, 11285-11291.	2.9	79
9	Proximity Effects on Nuclear Spin-Spin Coupling Constants. 1. J(CH) Couplings in the Vicinity of an Atom Bearing Lone Pairs. The Journal of Physical Chemistry, 1994, 98, 8858-8861.	2.9	78
10	Comment on â€œDoes the Hydrated Electron Occupy a Cavity?â€• Science, 2011, 331, 1387-1387.	12.6	77
11	Molecular Orbital Study of Crystalline Acetic Acid. 2. Aggregates in One, Two, and Three Dimensions. Journal of the American Chemical Society, 1994, 116, 8714-8721.	13.7	71
12	Role of the Câˆ’HÂ·Â·Â·O Hydrogen Bonds in Liquids:Â A Monte Carlo Simulation Study of Liquid Formic Acid Using a Newly Developed Pair-Potential. Journal of Physical Chemistry B, 1997, 101, 5429-5436.	2.6	69
13	Excess electron relaxation dynamics at water/air interfaces. Journal of Chemical Physics, 2007, 126, 234707.	3.0	56
14	Equilibrium structure, fluctuations, and spectroscopy of a solvated electron in methanol. Journal of Chemical Physics, 1997, 107, 1970-1980.	3.0	55
15	Analytical investigations of an electronâ€“water molecule pseudopotential. I. Exact calculations on a model system. Journal of Chemical Physics, 2001, 114, 7805-7815.	3.0	54
16	Gas-Phase Structure and Acidity of Formohydroxamic Acid and Formamide: A Comparative ab Initio Study. The Journal of Physical Chemistry, 1995, 99, 131-136.	2.9	49
17	Excess electron localization sites in neutral water clusters. Journal of Chemical Physics, 2006, 125, 014308.	3.0	47
18	Interior- and surface-bound excess electron states in large water cluster anions. Journal of Chemical Physics, 2009, 130, 124319.	3.0	47

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19	A New Five-Site Pair Potential for Formic Acid in Liquid Simulations. Journal of Physical Chemistry A, 1997, 101, 2662-2665.	2.5	46
20	Molecular Orbital Studies of the Nitromethane-Ammonia Complex. An Unusually Strong C-H.cntdot..cntdot..cntdot.N Hydrogen Bond. The Journal of Physical Chemistry, 1995, 99, 639-641.	2.9	43
21	A quantum chemical study of negatively charged methanol clusters. Journal of Chemical Physics, 1999, 110, 10364-10369.	3.0	37
22	Non-linear response and hydrogen bond dynamics for electron solvation in methanol. Chemical Physics Letters, 2000, 316, 465-470.	2.6	36
23	Quantized time correlation function approach to nonadiabatic decay rates in condensed phase: Application to solvated electrons in water and methanol. Journal of Chemical Physics, 2006, 125, 064501.	3.0	36
24	Molecular orbital studies of crystal formation: the aggregation and nucleation of 1,3-diones. The Journal of Physical Chemistry, 1992, 96, 5819-5824.	2.9	35
25	Molecular Orbital Studies of Crystalline Nitroanilines. The Journal of Physical Chemistry, 1996, 100, 9638-9648.	2.9	35
26	Nonadiabatic molecular dynamics simulation of photoexcitation experiments for the solvated electron in methanol. Journal of Chemical Physics, 1999, 110, 10953-10962.	3.0	35
27	Response of Observables for Cold Anionic Water Clusters to Cluster Thermal History. Journal of Physical Chemistry A, 2010, 114, 2331-2337.	2.5	33
28	Molecular orbital study of the structures of hydroxamic acids. The Journal of Physical Chemistry, 1992, 96, 3709-3712.	2.9	32
29	Critical evaluation of approximate quantum decoherence rates for an electronic transition in methanol solution. Journal of Chemical Physics, 2004, 120, 3688-3698.	3.0	31
30	A Comprehensive Liquid Simulation Study of Neat Formic Acid. Journal of Physical Chemistry B, 2000, 104, 8287-8294.	2.6	30
31	Nuclear quantum effects on the nonadiabatic decay mechanism of an excited hydrated electron. Journal of Chemical Physics, 2007, 127, 174508.	3.0	29
32	Hydrated Electrons in Water Clusters: Inside or Outside, Cavity or Noncavity?. Journal of Chemical Theory and Computation, 2015, 11, 1745-1755.	5.3	27
33	Nuclear quantum effects in electronically adiabatic quantum time correlation functions: Application to the absorption spectrum of a hydrated electron. Journal of Chemical Physics, 2009, 131, 024119.	3.0	25
34	Molecular Orbital Study of Crystalline 1,3-Cyclohexanedione. 2. Aggregates in Two and Three Dimensions. Chemistry of Materials, 1994, 6, 1313-1316.	6.7	19
35	A quantum chemical analysis of the intermolecular interactions between the molecules of the typically aprotic, dipolar acetone. Chemical Physics Letters, 1997, 275, 35-39.	2.6	19
36	A dynamical analysis of energy level fluctuations for an excess electron in methanol. Chemical Physics Letters, 1998, 282, 239-244.	2.6	18

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37	Alternative Mechanisms for Solvation Dynamics of Laser-Induced Electrons in Methanol. Journal of Physical Chemistry A, 1997, 101, 5469-5476.	2.5	17
38	On the applicability of one- and many-electron quantum chemistry models for hydrated electron clusters. Journal of Chemical Physics, 2016, 144, 154311.	3.0	17
39	A new electron-methanol molecule pseudopotential and its application for the solvated electron in methanol. Journal of Chemical Physics, 2010, 132, 154507.	3.0	15
40	Electronic Excited State Lifetimes of Anionic Water Clusters: Dependence on Charge Solvation Motif. Journal of Physical Chemistry Letters, 2017, 8, 2304-2309.	4.6	15
41	Excess electron solvation in ammonia clusters. Journal of Chemical Physics, 2019, 151, 204304.	3.0	13
42	Computational studies on aspartic proteases. I. Active-site protonation and hydration in the substrate-free crystalline state. International Journal of Quantum Chemistry, 1992, 42, 1537-1551.	2.0	12
43	Analysis of localization sites for an excess electron in neutral methanol clusters using approximate pseudopotential quantum-mechanical calculations. Journal of Chemical Physics, 2010, 133, 144510.	3.0	8
44	Quantum-classical simulation of electron localization in negatively charged methanol clusters. Journal of Chemical Physics, 2011, 135, 084501.	3.0	8
45	Ab initio molecular dynamics study of solvated electrons in methanol clusters. Physical Chemistry Chemical Physics, 2018, 20, 28741-28750.	2.8	8
46	Ab Initio Molecular Dynamics Simulations of Solvated Electrons in Ammonia Clusters. Journal of Physical Chemistry B, 2020, 124, 7205-7216.	2.6	7
47	Excess electrons in methanol clusters: Beyond the one-electron picture. Journal of Chemical Physics, 2016, 145, 164313.	3.0	5
48	Combined Effects from Solvation and Nuclear Quantum Fluctuations on Autoionization Mechanisms in Aqueous Clusters. Journal of Physical Chemistry B, 2020, 124, 2198-2208.	2.6	5
49	Hydration dynamics in water clusters via quantum molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 204317.	3.0	4
50	Transferability of the -COOH...?OOC- dyad Geometry from the gas phase to crystals and proteins. Theoretica Chimica Acta, 1995, 90, 41-50.	0.8	1
51	A Molecular Orbital Study of 6:l 1,3-Dione Complexes with Fluorinated Benzenes. Molecular Crystals and Liquid Crystals, 1992, 219, 63-69.	0.3	0
52	Tribute to Peter J. Rossky. Journal of Physical Chemistry B, 2020, 124, 10591-10593.	2.6	0