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	Ab Initio Molecular Dynamics Simulations of Solvated Electrons in Ammonia Clusters. Journal of Physical Chemistry B, 2020, 124, 7205-7216.	2.6	7
2	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
3	Tribute to Peter J. Rossky. Journal of Physical Chemistry B, 2020, 124, 10591-10593.	2.6	0
4	Excess electron solvation in ammonia clusters. Journal of Chemical Physics, 2019, 151, 204304.	3.0	13
5	Ab initio molecular dynamics study of solvated electrons in methanol clusters. Physical Chemistry Chemical Physics, 2018, 20, 28741-28750.	2.8	8
6	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
7	Excess electrons in methanol clusters: Beyond the one-electron picture. Journal of Chemical Physics, 2016, 145, 164313.	3.0	5
8	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
9	Hydrated Electrons in Water Clusters: Inside or Outside, Cavity or Noncavity?. Journal of Chemical Theory and Computation, 2015, 11, 1745-1755.	5.3	27
10	Hydration dynamics in water clusters via quantum molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 204317.	3.0	4
11	Theoretical Studies of Spectroscopy and Dynamics of Hydrated Electrons. Chemical Reviews, 2012, 112, 5641-5674.	47.7	169
12	Comment on â€œDoes the Hydrated Electron Occupy a Cavity?â€• Science, 2011, 331, 1387-1387.	12.6	77
13	Quantum-classical simulation of electron localization in negatively charged methanol clusters. Journal of Chemical Physics, 2011, 135, 084501.	3.0	8
14	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
15	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
16	Response of Observables for Cold Anionic Water Clusters to Cluster Thermal History. Journal of Physical Chemistry A, 2010, 114, 2331-2337.	2.5	33
17	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
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	Excess electron relaxation dynamics at water/air interfaces. Journal of Chemical Physics, 2007, 126, 234707.	3.0	56
20	Nuclear quantum effects on the nonadiabatic decay mechanism of an excited hydrated electron. Journal of Chemical Physics, 2007, 127, 174508.	3.0	29
21	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
22	Excess electron localization sites in neutral water clusters. Journal of Chemical Physics, 2006, 125, 014308.	3.0	47
23	Characterization of Excess Electrons in Water-Cluster Anions by Quantum Simulations. Science, 2005, 309, 914-917.	12.6	220
24	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
25	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
26	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
27	Non-linear response and hydrogen bond dynamics for electron solvation in methanol. Chemical Physics Letters, 2000, 316, 465-470.	2.6	36
28	A Comprehensive Liquid Simulation Study of Neat Formic Acid. Journal of Physical Chemistry B, 2000, 104, 8287-8294.	2.6	30
29	A quantum chemical study of negatively charged methanol clusters. Journal of Chemical Physics, 1999, 110, 10364-10369.	3.0	37
30	Nonadiabatic molecular dynamics simulation of photoexcitation experiments for the solvated electron in methanol. Journal of Chemical Physics, 1999, 110, 10953-10962.	3.0	35
31	A dynamical analysis of energy level fluctuations for an excess electron in methanol. Chemical Physics Letters, 1998, 282, 239-244.	2.6	18
32	Equilibrium structure, fluctuations, and spectroscopy of a solvated electron in methanol. Journal of Chemical Physics, 1997, 107, 1970-1980.	3.0	55
33	Alternative Mechanisms for Solvation Dynamics of Laser-Induced Electrons in Methanol. Journal of Physical Chemistry A, 1997, 101, 5469-5476.	2.5	17
34	A New Five-Site Pair Potential for Formic Acid in Liquid Simulations. Journal of Physical Chemistry A, 1997, 101, 2662-2665.	2.5	46
35	Role of the Câ‹¯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
36	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

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37	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
38	Molecular Orbital Studies of Crystalline Nitroanilines. The Journal of Physical Chemistry, 1996, 100, 9638-9648.	2.9	35
39	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
40	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
41	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
42	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
43	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
44	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
45	Molecular orbital study of acetic acid aggregation. 1. Monomers and dimers. The Journal of Physical Chemistry, 1993, 97, 12197-12204.	2.9	143
46	Acidity of hydroxamic acids: an ab initio and semiempirical study. Journal of the American Chemical Society, 1993, 115, 5754-5761.	13.7	82
47	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
48	Molecular orbital studies of C-H...O hydrogen-bonded complexes. The Journal of Physical Chemistry, 1993, 97, 7899-7909.	2.9	130
49	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
50	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
51	Molecular orbital study of the structures of hydroxamic acids. The Journal of Physical Chemistry, 1992, 96, 3709-3712.	2.9	32
52	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