List of Publications by Year in descending order

45 papers	4,854 citations	136950 32 h-index	254184 43 g-index
45 all docs	45 docs citations	45 times ranked	3903 citing authors

#	Article	IF	Citations
1	Molecular Clusters of Ï€-Systems:â€‰ Theoretical Studies of Structures, Spectra, and Origin of Interaction Energies. Chemical Reviews, 2000, 100, 4145-4186.	47.7	984
2	Understanding of Assembly Phenomena by Aromaticâˆ’Aromatic Interactions:Â Benzene Dimer and the Substituted Systems. Journal of Physical Chemistry A, 2007, 111, 3446-3457.	2.5	617
3	Structures, energies, vibrational spectra, and electronic properties of water monomer to decamer. Journal of Chemical Physics, 2000, 112, 9759-9772.	3.0	291
4	Geometrical and Electronic Structures of Gold, Silver, and Goldâˆ’Silver Binary Clusters:Â Origins of Ductility of Gold and Goldâˆ’Silver Alloy Formation. Journal of Physical Chemistry B, 2003, 107, 9994-10005.	2.6	283
5	Theoretical Investigations of Anionâˆ’Ï€ Interactions:â€‰ The Role of Anions and the Nature of Ï€ Systems. Journal of Physical Chemistry A, 2004, 108, 1250-1258.	2.5	260
6	Cationâˆ’Ï€ Interactions:â€‰ A Theoretical Investigation of the Interaction of Metallic and Organic Cations with Alkenes, Arenes, and Heteroarenes. Journal of Physical Chemistry A, 2003, 107, 1228-1238.	2.5	226
7	Olefinic vs Aromatic Ï€âˆ’H Interaction:Â A Theoretical Investigation of the Nature of Interaction of First-row Hydrides with Ethene and Benzene. Journal of the American Chemical Society, 2001, 123, 3323-3331.	13.7	193
8	Substituent Effects on the Edge-to-Face Aromatic Interactions. Journal of the American Chemical Society, 2005, 127, 4530-4537.	13.7	190
9	Insights into the Structures, Energetics, and Vibrations of Monovalent Cationâˆ’(Water)1-6Clustersâ€. Journal of Physical Chemistry A, 2004, 108, 2949-2958.	2.5	158
10	A theoretical investigation of the nature of the Ï€-H interaction in etheneâ€“H2O, benzeneâ€“H2O, and benzeneâ€“(H2O)2. Journal of Chemical Physics, 1999, 111, 5838-5850.	3.0	125
11	Assembling Phenomena of Calix[4]hydroquinone Nanotube Bundles by One-Dimensional Short Hydrogen Bonding and Displaced Ï€âˆ’Ï€ Stacking. Journal of the American Chemical Society, 2002, 124, 14268-14279.	13.7	106
12	Cationâˆ’Ï€âˆ’Anion Interaction:â€‰ A Theoretical Investigation of the Role of Induction Energies. Journal of Physical Chemistry A, 2007, 111, 7980-7986.	2.5	101
13	Role of Lewis Acid(AlCl3)âˆ’Aromatic Ring Interactions in Friedelâˆ’Craft's Reaction:Â An ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 2253-2255.	2.5	96
14	Fluorobenzeneâ‹¯water and difluorobenzeneâ‹¯water systems: An ab initio investigation. Journal of Chemical Physics, 1999, 110, 8501-8512.	3.0	91
15	Benzene-hydrogen halide interactions: Theoretical studies of binding energies, vibrational frequencies, and equilibrium structures. Journal of Chemical Physics, 1998, 108, 7217-7223.	3.0	73
16	Anisole-(H2O)n (n=1â€“3) complexes: An experimental and theoretical investigation of the modulation of optimal structures, binding energies, and vibrational spectra in both the ground and first excited states. Journal of Chemical Physics, 2002, 117, 8805-8822.	3.0	70
17	Fluorobenzene and p-difluorobenzene microsolvated by methanol: An infrared spectroscopic and ab initio theoretical investigation. Journal of Chemical Physics, 2000, 112, 1844-1858.	3.0	59
18	Ab Initio Study of Benzeneâˆ’BX3(X = H, F, Cl) Interactions. Journal of Physical Chemistry B, 1999, 103, 184-191.	2.6	58

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19	Interaction of the water dimer with Ï€-systems: A theoretical investigation of structures, energies, and vibrational frequencies. Journal of Chemical Physics, 2000, 112, 1769-1781.	3.0	58
20	Structures, energies, and spectra of aqua-silver (I) complexes. Journal of Chemical Physics, 2003, 119, 7725-7736.	3.0	57
21	An Electrochemically Controllable Nanomechanical Molecular System Utilizing Edge-to-Face and Face-to-Face Aromatic Interactions. Organic Letters, 2002, 4, 3971-3974.	4.6	56
22	Structures, energetics, and spectra of aqua-cesium (I) complexes: An ab initio and experimental study. Journal of Chemical Physics, 2007, 126, 074302.	3.0	55
23	Structure and stability of fluorine-substituted benzene-argon complexes: The decisive role of exchange-repulsion and dispersion interactions. Journal of Chemical Physics, 2001, 115, 6018-6029.	3.0	52
24	Catalytic Mechanism of Enzymes:Â Preorganization, Short Strong Hydrogen Bond, and Charge Bufferingâ€. Biochemistry, 2002, 41, 5300-5306.	2.5	52
25	Study of interactions of various ionic species with solvents toward the design of receptors. Theoretical Chemistry Accounts, 2006, 115, 127-135.	1.4	49
26	Nature of the interaction of paramagnetic atoms (A=4N,4P,3O,3S) with Ï€ systems and C60: A theoretical investigation of Aâ‹…â‹…â‹…C6H6 and endohedral fullerenes A@C60. Journal of Chemical Physics, 2002, 116, 10684-10691.	3.0	43
27	A Theoretical Investigation of Benzeneâˆ’AlX3and Etheneâˆ’AlX3(X = H, F, Cl) Interactions. Journal of Physical Chemistry A, 1999, 103, 9116-9124.	2.5	41
28	Hydration and Dissociation of Hydrogen Fluoric Acid (HF). Journal of Physical Chemistry A, 2006, 110, 7918-7924.	2.5	38
29	Ïƒ to Ï€ conformational transition: Interactions of the water trimer with Ï€ systems. Journal of Chemical Physics, 2001, 114, 1295-1305.	3.0	36
30	van der Waals isomers and ionic reactivity of the cluster system para-chlorofluorobenzene/methanol. Journal of Chemical Physics, 2000, 112, 1170-1177.	3.0	34
31	Ab initio studies of Ï€-water tetramer complexes: Evolution of optimal structures, binding energies, and vibrational spectra of Ï€-(H2O)n (n=1â€“4) complexes. Journal of Chemical Physics, 2001, 114, 4016-4024.	3.0	34
32	Structures, vibrational frequencies, and infrared spectra of the hexa-hydrated benzene clusters. Journal of Chemical Physics, 2000, 113, 6160-6168.	3.0	33
33	Comparison of the nature of Ï€ and conventional H-bonds: a theoretical investigation. Journal of Molecular Structure, 2002, 615, 227-238.	3.6	31
34	Ab initiostudies of neutral and anionic p-benzoquinoneâ€“water clusters. Journal of Chemical Physics, 2003, 118, 8681-8686.	3.0	29
35	Electronic structure of silver subnanowires in self-assembled organic nanotubes: Density functional calculations. Physical Review B, 2003, 67, .	3.2	29
36	p-benzoquinone-benzene clusters as potential nanomechanical devices: A theoretical study. Journal of Chemical Physics, 2004, 121, 841-846.	3.0	26

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37	A New Type of Ionophore Family Utilizing the Cation-Olefinic Ï€ Interaction:Â Theoretical Study of [n]Beltenes. Journal of Organic Chemistry, 2002, 67, 1848-1851.	3.2	24
38	Hydrogen multicenter bonds and reversible hydrogen storage. Journal of Chemical Physics, 2009, 130, 114301.	3.0	23
39	Why the hydration energy of Au+ is larger for the second water molecule than the first one: Skewed orbitals overlap. Journal of Chemical Physics, 2005, 123, 074328.	3.0	20
40	Modulation of the Electronic Structure of Semiconducting Nanotubes Resulting from Different Metal Contacts. Journal of Physical Chemistry B, 2005, 109, 7601-7604.	2.6	20
41	Insights into the Nature of SiH4â^'BH3Complex:Â Theoretical Investigation of New Mechanistic Pathways Involving SiH3â€¢and BH4â€¢Radicals. Journal of Physical Chemistry A, 2002, 106, 6817-6822.	2.5	18
42	Highly Stereospecific Epimerization of Î±-Amino Acids:Â Conducted Tour Mechanism. Journal of Organic Chemistry, 2003, 68, 6571-6575.	3.2	7
43	Theoretical Approaches to the Design of Functional Nanomaterials. Theoretical and Computational Chemistry, 2004, 15, 119-170.	0.4	5
44	Clusters to functional molecules, nanomaterials, and molecular devices. , 2005, , 963-993.		3
45	De Novo Design Theory: Nanomaterials and Molecular Devices. , 0, , 1111-1120.		0