List of Publications by Year in descending order

45 papers	4,854 citations	136885 32 h-index	254106 43 g-index
45 all docs	45 docs citations	45 times ranked	3903 citing authors

#	Article	IF	Citations
1	Hydrogen multicenter bonds and reversible hydrogen storage. Journal of Chemical Physics, 2009, 130, 114301.	1.2	23
2	Structures, energetics, and spectra of aqua-cesium (I) complexes: An ab initio and experimental study. Journal of Chemical Physics, 2007, 126, 074302.	1.2	55
3	Cationâ^Ï€â^'Anion Interaction:â€‰ A Theoretical Investigation of the Role of Induction Energies. Journal of Physical Chemistry A, 2007, 111, 7980-7986.	1.1	101
4	Understanding of Assembly Phenomena by Aromaticâ^'Aromatic Interactions:Â Benzene Dimer and the Substituted Systems. Journal of Physical Chemistry A, 2007, 111, 3446-3457.	1.1	617
5	Hydration and Dissociation of Hydrogen Fluoric Acid (HF). Journal of Physical Chemistry A, 2006, 110, 7918-7924.	1.1	38
6	Study of interactions of various ionic species with solvents toward the design of receptors. Theoretical Chemistry Accounts, 2006, 115, 127-135.	0.5	49
7	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.	1.2	20
8	Modulation of the Electronic Structure of Semiconducting Nanotubes Resulting from Different Metal Contacts. Journal of Physical Chemistry B, 2005, 109, 7601-7604.	1.2	20
9	Substituent Effects on the Edge-to-Face Aromatic Interactions. Journal of the American Chemical Society, 2005, 127, 4530-4537.	6.6	190
10	Clusters to functional molecules, nanomaterials, and molecular devices. , 2005, , 963-993.		3
11	p-benzoquinone-benzene clusters as potential nanomechanical devices: A theoretical study. Journal of Chemical Physics, 2004, 121, 841-846.	1.2	26
12	Theoretical Approaches to the Design of Functional Nanomaterials. Theoretical and Computational Chemistry, 2004, 15, 119-170.	0.2	5
13	Theoretical Investigations of Anionâ^'Ï€ Interactions:â€‰ The Role of Anions and the Nature of Ï€ Systems. Journal of Physical Chemistry A, 2004, 108, 1250-1258.	1.1	260
14	Insights into the Structures, Energetics, and Vibrations of Monovalent Cationâ^'(Water)1-6Clustersâ€. Journal of Physical Chemistry A, 2004, 108, 2949-2958.	1.1	158
15	Ab initiostudies of neutral and anionic p-benzoquinoneâ€“water clusters. Journal of Chemical Physics, 2003, 118, 8681-8686.	1.2	29
16	Cationâ^'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.	1.1	226
17	Highly Stereospecific Epimerization of Î±-Amino Acids:Â Conducted Tour Mechanism. Journal of Organic Chemistry, 2003, 68, 6571-6575.	1.7	7
18	Geometrical and Electronic Structures of Gold, Silver, and Goldâ^'Silver Binary Clusters:Â Origins of Ductility of Gold and Goldâ^'Silver Alloy Formation. Journal of Physical Chemistry B, 2003, 107, 9994-10005.	1.2	283

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19	Structures, energies, and spectra of aqua-silver (I) complexes. Journal of Chemical Physics, 2003, 119, 7725-7736.	1.2	57
20	Electronic structure of silver subnanowires in self-assembled organic nanotubes: Density functional calculations. Physical Review B, 2003, 67, .	1.1	29
21	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.	1.2	43
22	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.	1.2	70
23	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.	1.1	18
24	Catalytic Mechanism of Enzymes:Â Preorganization, Short Strong Hydrogen Bond, and Charge Bufferingâ€. Biochemistry, 2002, 41, 5300-5306.	1.2	52
25	Assembling Phenomena of Calix[4]hydroquinone Nanotube Bundles by One-Dimensional Short Hydrogen Bonding and Displaced Ï€â‹¯Ï€ Stacking. Journal of the American Chemical Society, 2002, 124, 14268-14279.	6.6	106
26	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.	1.7	24
27	An Electrochemically Controllable Nanomechanical Molecular System Utilizing Edge-to-Face and Face-to-Face Aromatic Interactions. Organic Letters, 2002, 4, 3971-3974.	2.4	56
28	Comparison of the nature of Ï€ and conventional H-bonds: a theoretical investigation. Journal of Molecular Structure, 2002, 615, 227-238.	1.8	31
29	Olefinic vs Aromatic Ï€â‹¯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.	6.6	193
30	Ïƒ to Ï€ conformational transition: Interactions of the water trimer with Ï€ systems. Journal of Chemical Physics, 2001, 114, 1295-1305.	1.2	36
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.	1.2	34
32	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.	1.2	52
33	Fluorobenzene and p-difluorobenzene microsolvated by methanol: An infrared spectroscopic and ab initio theoretical investigation. Journal of Chemical Physics, 2000, 112, 1844-1858.	1.2	59
34	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.	1.2	58
35	van der Waals isomers and ionic reactivity of the cluster system para-chlorofluorobenzene/methanol. Journal of Chemical Physics, 2000, 112, 1170-1177.	1.2	34
36	Structures, vibrational frequencies, and infrared spectra of the hexa-hydrated benzene clusters. Journal of Chemical Physics, 2000, 113, 6160-6168.	1.2	33

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37	Structures, energies, vibrational spectra, and electronic properties of water monomer to decamer. Journal of Chemical Physics, 2000, 112, 9759-9772.	1.2	291
38	Molecular Clusters of Ï€-Systems:â€‰ Theoretical Studies of Structures, Spectra, and Origin of Interaction Energies. Chemical Reviews, 2000, 100, 4145-4186.	23.0	984
39	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.	1.2	125
40	Fluorobenzeneâ‹¯water and difluorobenzeneâ‹¯water systems: An ab initio investigation. Journal of Chemical Physics, 1999, 110, 8501-8512.	1.2	91
41	Ab Initio Study of Benzeneâˆ’BX3(X = H, F, Cl) Interactions. Journal of Physical Chemistry B, 1999, 103, 184-191.	1.2	58
42	A Theoretical Investigation of Benzeneâˆ’AlX3and Etheneâˆ’AlX3(X = H, F, Cl) Interactions. Journal of Physical Chemistry A, 1999, 103, 9116-9124.	1.1	41
43	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.	1.1	96
44	Benzene-hydrogen halide interactions: Theoretical studies of binding energies, vibrational frequencies, and equilibrium structures. Journal of Chemical Physics, 1998, 108, 7217-7223.	1.2	73
45	De Novo Design Theory: Nanomaterials and Molecular Devices. , 0, , 1111-1120.		0