Pilarisetty Tarakeshwar

List of Publications by Year
in descending order

104 papers	6,729 citations	71061 41 h-index	60583 81 g-index
107 all docs	107 docs citations	107 times ranked	6159 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.	23.0	984
2	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
3	Structures, energies, vibrational spectra, and electronic properties of water monomer to decamer. Journal of Chemical Physics, 2000, 112, 9759-9772.	1.2	291
4	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
5	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
6	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
7	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
8	Substituent Effects on the Edge-to-Face Aromatic Interactions. Journal of the American Chemical Society, 2005, 127, 4530-4537.	6.6	190
9	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
10	A Nickel Phosphine Complex as a Fast and Efficient Hydrogen Production Catalyst. Journal of the American Chemical Society, 2015, 137, 1109-1115.	6.6	137
11	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
12	Characterization of Weak NHâ^'Ï€ Intermolecular Interactions of Ammonia with Various Substituted Ï€-Systems. Journal of the American Chemical Society, 2006, 128, 5416-5426.	6.6	107
13	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
14	Simple and accurate correlation of experimental redox potentials and DFT-calculated HOMO/LUMO energies of polycyclic aromatic hydrocarbons. Journal of Molecular Modeling, 2013, 19, 2845-2848.	0.8	104
15	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
16	Electrochemical Capture and Release of Carbon Dioxide. ACS Energy Letters, 2017, 2, 454-461.	8.8	100
17	Role of Lewis Acid(AlCl3)â^'Aromatic Ring Interactions in Friedelâ^'Craft's Reaction:Â An ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 2253-2255.	1.1	96
18	Origin of the magic numbers of water clusters with an excess electron. Journal of Chemical Physics, 2005, 122, 044309.	1.2	94

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19	Fluorobenzeneâ‹¯water and difluorobenzeneâ‹¯water systems: An ab initio investigation. Journal of Chemical Physics, 1999, 110, 8501-8512.	1.2	91
20	Surface-Enhanced Raman Scattering on Semiconducting Oxide Nanoparticles: Oxide Nature, Size, Solvent, and pH Effects. Journal of Physical Chemistry C, 2011, 115, 8994-9004.	1.5	79
21	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
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	Structures, energetics, and spectra of hydrated hydroxide anion clusters. Journal of Chemical Physics, 2004, 121, 4657-4664.	1.2	70
24	Electrochemical Capture and Release of Carbon Dioxide Using a Disulfideâ€“Thiocarbonate Redox Cycle. Journal of the American Chemical Society, 2017, 139, 1033-1036.	6.6	67
25	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
26	Ab Initio Study of Benzeneâ‹¯BX3(X = H, F, Cl) Interactions. Journal of Physical Chemistry B, 1999, 103, 184-191.	1.2	58
27	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
28	Structures, energies, and spectra of aqua-silver (I) complexes. Journal of Chemical Physics, 2003, 119, 7725-7736.	1.2	57
29	Hydration profiles of aromatic amino acids: conformations and vibrations ofl-phenylalanineâ€“(H2O)nclusters. Physical Chemistry Chemical Physics, 2006, 8, 4783-4791.	1.3	57
30	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
31	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
32	Role of molecular orbitals of the benzene in electronic nanodevices. Journal of Chemical Physics, 2005, 122, 094706.	1.2	54
33	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
34	Catalytic Mechanism of Enzymes:Â Preorganization, Short Strong Hydrogen Bond, and Charge Bufferingâ€. Biochemistry, 2002, 41, 5300-5306.	1.2	52
35	Chemically Induced Magnetism in Atomically Precise Gold Clusters. Small, 2014, 10, 907-911.	5.2	52
36	Ground state vibrations of citric acid and the citrate trianionâ€”an ab initio study. Spectrochimica Acta Part A: Molecular Spectroscopy, 1994, 50, 2327-2343.	0.1	51

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37	Vibrational frequencies of cysteine and serine zwitterionsâ€"an ab initio assignment. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1995, 51, 925-928.	2.0	51
38	Study of interactions of various ionic species with solvents toward the design of receptors. Theoretical Chemistry Accounts, 2006, 115, 127-135.	0.5	49
39	Dopamine Adsorption on TiO₂ Anatase Surfaces. Journal of Physical Chemistry C, 2014, 118, 20688-20693.	1.5	47
40	Pseudocarbynes: Charge-Stabilized Carbon Chains. Journal of Physical Chemistry Letters, 2016, 7, 1675-1681.	2.1	46
41	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
42	Conformational effects on vibrational frequencies of cysteine and serine: an ab initio study. Computational and Theoretical Chemistry, 1994, 305, 205-224.	1.5	41
43	A Theoretical Investigation of Benzeneâ^'AlX3and Etheneâ^'AlX3(X = H, F, Cl) Interactions. Journal of Physical Chemistry A, 1999, 103, 9116-9124.	1.1	41
44	Catalytic Hydrogen Evolution by Fe(II) Carbonyls Featuring a Dithiolate and a Chelating Phosphine. Inorganic Chemistry, 2014, 53, 8919-8929.	1.9	39
45	Hydration and Dissociation of Hydrogen Fluoric Acid (HF). Journal of Physical Chemistry A, 2006, 110, 7918-7924.	1.1	38
46	Role of Catalytic Residues in Enzymatic Mechanisms of Homologous Ketosteroid Isomerasesâ€,â€¡. Biochemistry, 2000, 39, 13891-13896.	1.2	37
47	Exploring Gas-Phase Ionâ^'Ionophore Interactions: Infrared Spectroscopy of Argon-Tagged Alkali Ion-Crown Ether Complexes. Journal of Physical Chemistry A, 2010, 114, 1514-1520.	1.1	37
48	Ïƒ to Ï€ conformational transition: Interactions of the water trimer with Ï€ systems. Journal of Chemical Physics, 2001, 114, 1295-1305.	1.2	36
49	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
50	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
51	Structures, vibrational frequencies, and infrared spectra of the hexa-hydrated benzene clusters. Journal of Chemical Physics, 2000, 113, 6160-6168.	1.2	33
52	Photoinduced Kinetics of SERS in Bioinorganic Hybrid Systems. A Case Study: Dopamineâ^'TiO₂. Journal of Physical Chemistry B, 2010, 114, 14642-14645.	1.2	33
53	Metal contacts in carbon nanotube field-effect transistors: Beyond the Schottky barrier paradigm. Physical Review B, 2008, 77, .	1.1	32
54	Comparison of the nature of Ï€ and conventional H-bonds: a theoretical investigation. Journal of Molecular Structure, 2002, 615, 227-238.	1.8	31

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55	CO₂ Preactivation in Photoinduced Reduction via Surface Functionalization of TiO₂ Nanoparticles. Journal of Physical Chemistry Letters, 2013, 4, 475-479.	2.1	30
56	Conformations and vibrations of dicarboxylic acids. An ab initio study. Computational and Theoretical Chemistry, 1996, 362, 77-99.	1.5	29
57	Ab initiostudies of neutral and anionic p-benzoquinoneâ€“water clusters. Journal of Chemical Physics, 2003, 118, 8681-8686.	1.2	29
58	Electronic structure of silver subnanowires in self-assembled organic nanotubes: Density functional calculations. Physical Review B, 2003, 67, .	1.1	29
59	Quantum confinement effects on the surface enhanced Raman spectra of hybrid systems moleculeâ€¬TiO₂ nanoparticles. International Journal of Quantum Chemistry, 2011, 111, 1659-1670.	1.0	29
60	Nature of Hydrogen Interaction and Saturation on Small Titanium Clusters. Journal of Physical Chemistry A, 2008, 112, 2846-2854.	1.1	28
61	p-benzoquinone-benzene clusters as potential nanomechanical devices: A theoretical study. Journal of Chemical Physics, 2004, 121, 841-846.	1.2	26
62	SERS as a Probe of Charge-Transfer Pathways in Hybrid Dye/Moleculeâ€“Metal Oxide Complexes. Journal of Physical Chemistry C, 2014, 118, 3774-3782.	1.5	25
63	Dimer to Monomer Phase Transition in Alkali-Metal Fullerides: Magnetic Susceptibility Changes. Physical Review Letters, 2000, 84, 2425-2428.	2.9	24
64	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
65	Insights into the Structure of Cyclohexane from Femtosecond Degenerate Four-Wave Mixing Spectroscopy and Ab Initio Calculations. Journal of the American Chemical Society, 2003, 125, 16455-16462.	6.6	24
66	Geometric and electronic structures of hydrogenated transition metal (Sc, Ti, Zr) clusters. Physical Review B, 2009, 79, .	1.1	24
67	An ab initio study of pyruvic acid. Computational and Theoretical Chemistry, 1998, 430, 51-56.	1.5	23
68	Hydrogen multicenter bonds and reversible hydrogen storage. Journal of Chemical Physics, 2009, 130, 114301.	1.2	23
69	Pseudorotation in pyrrolidine: rotational coherence spectroscopy and ab initio calculations of a large amplitude intramolecular motion. Physical Chemistry Chemical Physics, 2010, 12, 72-81.	1.3	23
70	Structural, energetic, and electronic properties of hydrogenated titanium clusters. Journal of Chemical Physics, 2008, 128, 194714.	1.2	22
71	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
72	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

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73	Vibrational frequencies of proline and hydroxyproline An ab initio study. Computational and Theoretical Chemistry, 1996, 365, 167-181.	1.5	19
74	Stereoselective synthesis of substituted tetrahydrofurans - identification and analysis by proton NMR and MNDO, MM2 calculations. Tetrahedron, 1991, 47, 297-304.	1.0	18
75	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
76	Single-Molecule Conductance through Hydrogen Bonds: The Role of Resonances. Journal of Physical Chemistry Letters, 2016, 7, 2977-2980.	2.1	16
77	Polarizability as a Molecular Descriptor for Conductance in Organic Molecular Circuits. Journal of Physical Chemistry C, 2016, 120, 26054-26060.	1.5	16
78	Proline and hydroxyproline zwitterionsâ€"an ab initio study. Computational and Theoretical Chemistry, 1997, 417, 255-263.	1.5	14
79	On the microscopic interaction of para-chlorofluorobenzene with water. Journal of Chemical Physics, 2001, 115, 10045-10047.	1.2	14
80	Pseudocarbynes: Linear Carbon Chains Stabilized by Metal Clusters. Journal of Physical Chemistry C, 2020, 124, 19355-19361.	1.5	14
81	Modulation of Molecular Conductance Induced by Electrode Atomic Species and Interface Geometry. Journal of Physical Chemistry B, 2006, 110, 7456-7462.	1.2	13
82	Electrodeâ€"Molecule Interface Effects on Molecular Conductance. IEEE Nanotechnology Magazine, 2009, 8, 16-21.	1.1	12
83	Probing the Nature of Charge Transfer at Nanoâ€"Bio Interfaces: Peptides on Metal Oxide Nanoparticles. Journal of Physical Chemistry Letters, 2014, 5, 3555-3559.	2.1	11
84	On the Structure, Magnetic Properties, and Infrared Spectra of Iron Pseudocarbynes in the Interstellar Medium. Astrophysical Journal, 2019, 879, 2.	1.6	11
85	Vibrational signatures of Watsonâ€"Crick base pairing in adenineâ€"thymine mimics. Physical Chemistry Chemical Physics, 2013, 15, 11520.	1.3	9
86	Molecular Structure of p-Cyclohexylaniline. Comparison of Results Obtained by X-ray Diffraction with Gas Phase Laser Experiments and ab Initio Calculations. Journal of Physical Chemistry A, 2000, 104, 11593-11600.	1.1	8
87	4-Aminobenzimidazoleâ€"1-Methylthymine: A Model for Investigating Hoogsteen Base-Pairing between Adenine and Thymine. Journal of Physical Chemistry A, 2011, 115, 11403-11411.	1.1	8
88	Probing Raman Enhancement in a Dopamineâ€"Ti₂O₄ Hybrid Using Stretched Molecular Geometries. Journal of Physical Chemistry A, 2014, 118, 1196-1202.	1.1	8
89	INSIGHTS FROM THEORETICAL INVESTIGATIONS OF AQUEOUS CLUSTERS. , 2002, , 1642-1683.		7
90	Highly Stereospecific Epimerization of Î±-Amino Acids:Â Conducted Tour Mechanism. Journal of Organic Chemistry, 2003, 68, 6571-6575.	1.7	7

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91	Electronic transport across hydrogen bonds in organic electronics. International Journal of Nanotechnology, 2015, 12, 297.	0.1	7
92	Improving Seebeck coefficient of thermoelectrochemical cells by controlling ligand complexation at metal redox centers. Applied Physics Letters, 2021, 118, .	1.5	7
93	Interface Study of Metal Electrode and Semiconducting Carbon Nanotubes: Effects of Electrode Atomic Species. IEEE Nanotechnology Magazine, 2008, 7, 124-127.	1.1	6
94	Experimental, Simulation, and Computational Study of the Interaction of Reduced Forms of N â€Methylâ€4,4â€™â€Bipyridinium with CO 2. ChemElectroChem, 2020, 7, 469-475.	1.7	6
95	Theoretical Approaches to the Design of Functional Nanomaterials. Theoretical and Computational Chemistry, 2004, 15, 119-170.	0.2	5
96	Stability and Quenching of Plasmon Resonance Absorption in Magnetic Gold Nanoparticles. Journal of Physical Chemistry Letters, 2011, 2, 2996-3001.	2.1	5
97	Solvent Effects on the Dynamic Polarizability and Raman Response of Moleculeâ€“Metal Oxide Hybrid Clusters. ChemPhysChem, 2016, 17, 2590-2595.	1.0	4
98	Clusters to functional molecules, nanomaterials, and molecular devices. , 2005, , 963-993.		3
99	Supersonic jet studies of solvation effects on the spectroscopy and photophysics of 4-diethylaminopyridine. Physical Chemistry Chemical Physics, 2007, 9, 4981.	1.3	3
100	An Electrochemically Controllable Nanomechanical Molecular System Utilizing Edge-to-Face and Face-to-Face Aromatic Interactions. Organic Letters, 2003, 5, 961-961.	2.4	0
101	Interface study of metal electrode and semiconducting carbon nanotubes: effects of electrode atomic species. , 2006, , .		0
102	Electronic and vibrational properties of magnetic core-shell nanoparticles. , 2012, , .		0
103	De Novo Design Theory: Nanomaterials and Molecular Devices. , 0, , 1111-1120.		0
104	Nanosensors for Biomedical Applications: A Tutorial. Nanostructure Science and Technology, 2018, , 145-167.	0.1	0