Tapas Kar

List of Publications by Year in descending order

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94 papers	4,720 citations	147566 31 h-index	98622 67 g-index
96 all docs	96 docs citations	96 times ranked	4460 citing authors

#	Article	IF	Citations
1	Fundamental Properties of the CHÂ·Â·Â·O Interaction:Â Is It a True Hydrogen Bond?. Journal of the American Chemical Society, 1999, 121, 9411-9422.	6.6	940
2	Red- versus Blue-Shifting Hydrogen Bonds:Â Are There Fundamental Distinctions?. Journal of Physical Chemistry A, 2002, 106, 1784-1789.	1.1	331
3	Comparison of Various Types of Hydrogen Bonds Involving Aromatic Amino Acids. Journal of the American Chemical Society, 2002, 124, 13257-13264.	6.6	328
4	Strength of the CÎ±HÂ·Â·O Hydrogen Bond of Amino Acid Residues. Journal of Biological Chemistry, 2001, 276, 9832-9837.	1.6	267
5	Influence of Hybridization and Substitution on the Properties of the CHÂ·Â·Â·O Hydrogen Bond. Journal of Physical Chemistry A, 2001, 105, 10607-10612.	1.1	224
6	Comparison of Cooperativity in CHÂ·Â·Â·O and OHÂ·Â·Â·O Hydrogen Bonds. Journal of Physical Chemistry A, 2004, 108, 9161-9168.	1.1	183
7	The Nonexistence of Specially Stabilized Hydrogen Bonds in Enzymes. Journal of the American Chemical Society, 1995, 117, 6970-6975.	6.6	142
8	Insertion of Lithium Ions into Carbon Nanotubes:Â An ab Initio Study. Journal of Physical Chemistry A, 2001, 105, 10397-10403.	1.1	98
9	Comparison between hydrogen and dihydrogen bonds among H3BNH3, H2BNH2, and NH3. Journal of Chemical Physics, 2003, 119, 1473-1482.	1.2	95
10	Comparison of ab Initio Hartreeâ^'Fock and Kohnâ^'Sham Orbitals in the Calculation of Atomic Charge, Bond Index, and Valence. Journal of Physical Chemistry A, 2000, 104, 9953-9963.	1.1	93
11	Effect of Solvent upon CHÂ·Â·Â·O Hydrogen Bonds with Implications for Protein Folding. Journal of Physical Chemistry B, 2005, 109, 3681-3689.	1.2	92
12	Noncovalent Ï€â^'Ï€ Stacking and CH---Ï€ Interactions of Aromatics on the Surface of Single-Wall Carbon Nanotubes: An MP2 Study. Journal of Physical Chemistry C, 2008, 112, 20070-20075.	1.5	87
13	Boronâ^'Nitrogen (BN) Substitution of Fullerenes:Â C60to C12B24N24CBN Ball. Journal of Physical Chemistry A, 2002, 106, 2970-2978.	1.1	86
14	Three-center four-electron bonds and their indices. Chemical Physics Letters, 1992, 192, 14-20.	1.2	79
15	Effect of adjoining aromatic ring upon excited state proton transfer, o-hydroxybenzaldehyde. Computational and Theoretical Chemistry, 1999, 467, 37-49.	1.5	76
16	Effects of Peripheral Substituents and Axial Ligands on the Electronic Structure and Properties of Iron Phthalocyanine. Inorganic Chemistry, 2004, 43, 7151-7161.	1.9	68
17	Spectroscopic and Structural Signature of the CHâ^'O Hydrogen Bond. Journal of Physical Chemistry A, 2008, 112, 11854-11860.	1.1	59
18	Activation and Cleavage of Hâ^'R Bonds through Intermolecular H...H Bonding upon Reaction of Proton Donors HR with 18-Electron Transition Metal Hydrides. Journal of Physical Chemistry A, 1999, 103, 514-520.	1.1	52

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19	Boronâ^'Nitrogen (BN) Substitution Patterns in C/BN Hybrid Fullerenes:â€‰ C60-2x(BN)x (x = 1â^'7). Journal of Physical Chemistry A, 2001, 105, 8376-8384.	1.1	49
20	Competition between Rotamerization and Proton Transfer ino-Hydroxybenzaldehyde. Journal of the American Chemical Society, 1998, 120, 10497-10503.	6.6	48
21	B₃N₃ Borazine Substitution in Hexaâ€periâ€Hexabenzocoronene: Computational Analysis and Scholl Reaction of Hexaphenylborazine. ChemPhysChem, 2012, 13, 1173-1181.	1.0	47
22	Effects of Peripheral Substituents on the Electronic Structure and Properties of Unligated and Ligated Metal Phthalocyanines, Metal = Fe, Co, Zn. Journal of Chemical Theory and Computation, 2005, 1, 1201-1210.	2.3	46
23	Borazine and Benzene Homo- and Heterodimers. Journal of Physical Chemistry A, 2009, 113, 3353-3359.	1.1	46
24	Density functional theory calculations of ozone adsorption on sidewall single-wall carbon nanotubes with Stone-Wales defects. Chemical Physics Letters, 2007, 445, 281-287.	1.2	45
25	Cooperativity of conventional and unconventional hydrogen bonds involving imidazole. International Journal of Quantum Chemistry, 2006, 106, 843-851.	1.0	39
26	A theoretical study of functionalized single-wall carbon nanotubes: ONIOM calculations. Chemical Physics Letters, 2004, 392, 176-180.	1.2	38
27	Tunable optical properties of icosahedral, dodecahedral, and tetrahedral clusters. Physical Review B, 2005, 71, .	1.1	38
28	Analysis of the Reactivities of Protein Câ^'H Bonds to H Atom Abstraction by OH Radical. Journal of the American Chemical Society, 2010, 132, 16450-16459.	6.6	38
29	Tuning spectral properties of fullerenes by substitutional doping. Physical Review B, 2004, 69, .	1.1	37
30	Rules for BN-Substitution in BCNâ^'Fullerenes. Separation of BN and C Domains. Journal of Physical Chemistry A, 2003, 107, 8630-8637.	1.1	35
31	Excited State Intramolecular Proton Transfer in Anionic Analogues of Malonaldehyde. Journal of Physical Chemistry A, 1997, 101, 5901-5909.	1.1	34
32	How the electron-deficient cavity of heterocalixarenes recognizes anions: insights from computation. Physical Chemistry Chemical Physics, 2017, 19, 24696-24705.	1.3	29
33	Molecular orbital theory of bond order and valency. Journal of Chemical Education, 1988, 65, 674.	1.1	28
34	Hardness and Chemical Potential Profiles for Some Open-Shell HAB â†' HBA Type Reactions. Ab Initio and Density Functional Study. Journal of Physical Chemistry A, 1998, 102, 5967-5973.	1.1	28
35	Structure, Stability, and Bonding of BC2N:Â An ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 10134-10141.	1.1	27
36	Substitution Patterns in Mono-BN-Fullerenes:Â Cn(n= 20, 24, 28, 32, 36, and 40). Journal of Physical Chemistry A, 2004, 108, 7681-7685.	1.1	27

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37	Comparison of atomic charges, valencies and bond orders in some hydrogen-bonded complexes calculated from Mulliken and LÃ¶wdin SCF density matrices. Computational and Theoretical Chemistry, 1987, 153, 93-101.	1.5	26
38	Some remarks on multi-center bond index. Chemical Physics Letters, 1999, 299, 518-526.	1.2	26
39	Effect of basis set on Mulliken and LÃ¶wdin atomic charges, bond orders and valencies of some polar molecules. Computational and Theoretical Chemistry, 1988, 165, 47-54.	1.5	25
40	An attempt towards coordination supramolecularity from Mn(II), Ni(II) and Cd(II) with a new hexadentate [N4O2] symmetrical Schiff base ligand: Syntheses, crystal structures, electrical conductivity and optical properties. Polyhedron, 2008, 27, 3359-3370.	1.0	25
41	Competition between carboxylic and phenolic groups for the preferred sites at the periphery of graphene â€“ A DFT study. Carbon, 2014, 80, 405-418.	5.4	24
42	Comparison of methods for calculating the properties of intramolecular hydrogen bonds. Excited state proton transfer. Journal of Chemical Physics, 1999, 111, 849-858.	1.2	23
43	Actinyls in Expanded Porphyrin:Â A Relativistic Density-Functional Studyâ€. Journal of Physical Chemistry A, 2004, 108, 3056-3063.	1.1	23
44	Open-ended modified single-wall carbon nanotubes: A theoretical study of the effects of purification. Chemical Physics Letters, 2006, 423, 126-130.	1.2	23
45	Origin of the bridge bond in [1,1,1]propellane. Chemical Physics Letters, 1996, 256, 201-206.	1.2	21
46	The Polar Mechanism for the Nitration of Benzene with Nitronium Ion: Ab Initio Structures of Intermediates and Transition States. Journal of Organic Chemistry, 2013, 78, 9522-9525.	1.7	20
47	Site and chirality selective chemical modifications of boron nitride nanotubes (BNNTs) via Lewis acidâ€“base interactions. Physical Chemistry Chemical Physics, 2015, 17, 3850-3866.	1.3	20
48	Comparison of BN and AlN Substitution on the Structure and Electronic and Chemical Properties of C60 Fullerene. Journal of Physical Chemistry A, 2003, 107, 4056-4065.	1.1	19
49	Theoretical Study of the Effect of Structural Modifications on the Hyperpolarizabilities of Indigo Derivatives. Journal of Physical Chemistry A, 2009, 113, 2623-2631.	1.1	19
50	IR Characterization of Tip-Functionalized Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 20955-20961.	1.5	19
51	Proton and Lithium Ion Transfer between Two Water Molecules with an External Restraining Force. Journal of the American Chemical Society, 1995, 117, 1344-1351.	6.6	18
52	A Study of the Mechanism of the Reaction between Ozone and the Chlorine Atom Using Density Functional Theory. Journal of Physical Chemistry A, 2001, 105, 4065-4070.	1.1	18
53	AlN, GaN, Al Ga1â^'N nanotubes and GaN/Al Ga1â^'N nanotube heterojunctions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 877-881.	0.9	18
54	Aluminum doping makes boron nitride nanotubes (BNNTs) an attractive adsorbent of hydrazine (N2H4). Structural Chemistry, 2018, 29, 375-382.	1.0	18

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55	The effect on acidity of size and shape of carboxylated single-wall carbon nanotubes. A DFT-SLDB study. Chemical Physics Letters, 2008, 460, 225-229.	1.2	17
56	Is there any three-center CBC bond in 1, 5-C2B3H5 and 1,5-C2B3H3?. International Journal of Quantum Chemistry, 1995, 53, 407-412.	1.0	16
57	Theoretical investigation on the mechanism of LiH+NH3â†'LiNH2+H2 reaction. Computational and Theoretical Chemistry, 2008, 857, 111-114.	1.5	15
58	A novel approach for the design of a highly selective sulfate-ion-selective electrode. Chemical Communications, 2009, , 325-327.	2.2	15
59	An accurate pair potential function for diatomic systems. Chemical Physics Letters, 2014, 591, 69-77.	1.2	15
60	Bâ•N Bond Cleavage and BN Ring Expansion at the Surface of Boron Nitride Nanotubes by Iminoborane. Journal of Physical Chemistry C, 2015, 119, 3253-3259.	1.5	15
61	Theoretical insight into a feasible strategy of capturing, storing and releasing toxic HCN at the surface of doped BN-sheets by charge modulation. Applied Surface Science, 2019, 496, 143714.	3.1	15
62	Electronic Structure, Stability, and Nature of Bonding of the Complexes of C2H2 and C2H4 with H+, Li+, and Na+ Ions. Extensive ab Initio and Density Functional Study. Journal of Physical Chemistry A, 2001, 105, 7737-7744.	1.1	14
63	Underlying source of the relation between polypeptide conformation and strength of NHÂ·Â·Â·O hydrogen bonds. Journal of Molecular Structure, 2007, 844-845, 166-172.	1.8	14
64	Nanoscale stabilization of zintl compounds: 1D ionic Liâ€"P double helix confined inside a carbon nanotube. Nanoscale, 2016, 8, 3454-3460.	2.8	14
65	Ab initio investigation of the nature of bonding in LiX dimers with first row substituents. Computational and Theoretical Chemistry, 1988, 180, 149-160.	1.5	13
66	Spectroscopy, crystal structure, valance molecular orbital energy level diagram and DFT study of cis-[Cr(2,2â€²-bipy)2Cl2](Cl)0.38(PF6)0.62. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 882-886.	2.0	13
67	Unusual Low-Vibrational Câ•O Mode of COOH Can Distinguish between Carboxylated Zigzag and Armchair Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 26072-26083.	1.5	13
68	Substituent Effects upon Protonation-Induced Red Shift of Phenylâ^'Pyridine Copolymers. Journal of Physical Chemistry B, 2002, 106, 534-539.	1.2	12
69	Reliability of Approximate Methods to Study Tip-Functionalized Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 25401-25406.	1.5	12
70	Site Preferences of Carboyxl Groups on the Periphery of Graphene and Their Characteristic IR Spectra. Journal of Physical Chemistry C, 2013, 117, 18206-18215.	1.5	12
71	Role of the central atom in three-centre bonding. Computational and Theoretical Chemistry, 1993, 283, 313-315.	1.5	11
72	Three-center bond index profiles. Computational and Theoretical Chemistry, 1996, 370, 45-49.	1.5	11

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73	Structure and Properties of [8]BN-Circulenes: Inorganic Analogues of [8]Circulenes. Journal of Physical Chemistry C, 2015, 119, 15541-15546.	1.5	11
74	Evaluation of Lignans from Piper cubeba against Schistosoma mansoni Adult Worms: A Combined Experimental and Theoretical Study. Chemistry and Biodiversity, 2019, 16, e1800305.	1.0	11
75	Three-center bonding in LiXHn, HBeXHn, and H2BXHn, dimers with first-row substituents: a comparative study. Computational and Theoretical Chemistry, 1993, 283, 177-183.	1.5	10
76	Do phenolic and carboxylic groups coexist at the tips of oxidized single-wall carbon nanotubes (o-SWNTs)?. Carbon, 2014, 73, 194-205.	5.4	10
77	Electronic properties and metal-ligand bonding situation in Eu(III) complexes containing tris(pyrazolyl)borate and phenantroline ligands. Journal of Luminescence, 2017, 182, 137-145.	1.5	9
78	Ultraviolet Optical Absorption Spectra of Water Clusters: From Molecular Dimer to Nanoscaled Cage-Like Hexakaidecahedron. Journal of Computational and Theoretical Nanoscience, 2007, 4, 453-466.	0.4	9
79	The remarkable stability of the LiBH2 and HBeBH2 dimers. Bî—»B double bond or multi-center bonds?. Chemical Physics Letters, 1993, 214, 615-620.	1.2	8
80	Synthesis, characterization, and density functional study of some manganese(III) Schiff-base complexes. Journal of Coordination Chemistry, 2012, 65, 980-993.	0.8	8
81	Computational Study of the Thermodynamics of New Particle Formation Initiated by Complexes of H₂SO₄â€“H₂Oâ€“NH_x, CH₃SO₃Hâ€“H₂Oâ€“NH_x, and HO₂â€“H₂Oâ€“NH_x. ACS Earth and Space Chemistry, 2019, 3, 1415-1425.	1.2	6
82	Proton transfer in H5O2+ and H3O2? with an external restraining force. International Journal of Quantum Chemistry, 1995, 56, 567-575.	1.0	5
83	Periodicity in proton conduction along a Hâ€bonded chain. Application to biomolecules. International Journal of Quantum Chemistry, 2008, 108, 607-616.	1.0	5
84	Electronic Structure and Spectroscopic Properties of the Two Structural Isomers of Donorâ^'Acceptor Substituted Sesquifulvalene in the Gas and Solution PhasesA Case Study of Sudden Polarization. Journal of Physical Chemistry A, 2006, 110, 12684-12692.	1.1	3
85	Performance of polarization-consistent vs. correlation-consistent basis sets for CCSD(T) prediction of water dimer interaction energy. Journal of Molecular Modeling, 2019, 25, 313.	0.8	3
86	N/Oâ†'B dative bonds supplemented by Nâ€“HN/HC hydrogen bonds make BN-cages an attractive candidate for DNA-nucleobase adsorption â€“ an MP2 prediction. Physical Chemistry Chemical Physics, 2022, 24, 16862-16875.	1.3	3
87	Improved pair-potential function for diatomic systems. Chemical Physics Letters, 2014, 593, 77-82.	1.2	2
88	Solvation Enhances the Distinction between Carboxylated Armchair and Zigzag Single-Wall Carbon Nanotubes (SWNT-COOH). Journal of Physical Chemistry C, 2017, 121, 9516-9527.	1.5	2
89	Local aromaticity in polyacenes manifested by individual proton and carbon shieldings: DFT mapping of aromaticity. Magnetic Resonance in Chemistry, 2020, 58, 145-153.	1.1	2
90	Hydrogen Bonding in Polyfluoride Ions. Bulletin of the Chemical Society of Japan, 1986, 59, 1283-1284.	2.0	1

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91	Pauliâ€“Rydbergâ€“London Potential: An Accurate Pair Potential Function for Diatomic Systems. Journal of Nanoscience and Nanotechnology, 2014, 14, 3993-4001.	0.9	1
92	Pilot program to integrate nanotechnology at Utah's high schools. , 2006, , .		0
93	Segmentation and additive approach: A reliable technique to study noncovalent interactions of large molecules at the surface of singleâ€wall carbon nanotubes. Journal of Computational Chemistry, 2016, 37, 1953-1961.	1.5	0
94	Can HCCH/HBNH Break Bâ•N/Câ•C Bonds of Single-Wall BN/Carbon Nanotubes at Their Surface?. Journal of Physical Chemistry C, 2017, 121, 26044-26053.	1.5	0