C N Ramachandran

List of Publications by Year
in descending order

50 papers	802 citations	516710 16 h-index	526287 27 g-index
50 all docs	50 docs citations	50 times ranked	863 citing authors

#	Article	IF	Citations
1	Blue Shift in Xâ^'H Stretching Frequency of Molecules Due to Confinement. Journal of Physical Chemistry A, 2006, 110, 2-4.	2.5	96
2	Water clusters in a confined nonpolar environment. Chemical Physics Letters, 2005, 410, 348-351.	2.6	94
3	Hostâ€“guest interaction in endohedral fullerenes. Chemical Physics Letters, 2008, 461, 87-92.	2.6	54
4	Revisiting the potential energy surface for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:mtext>He</mml:mtext><mml:mo>+</mml:mo><mml:msubsup><mml:mrow><mml:mtext>H</mr Chemical Physics Letters, 2009, 469, 26-30.	2.6	46
5	A highly sensitive pyridine-dicarbohydrazide based chemosensor for colorimetric recognition of Cu²⁺, AMP^{2â^'}, F^{â^'}and AcO^{â^'}ions. New Journal of Chemistry, 2018, 42, 8567-8576.	2.8	35
6	Hydrogen Peroxide Clusters:Â The Role of Open Book Motif in Cage and Helical Structures. Journal of Physical Chemistry A, 2006, 110, 6294-6300.	2.5	33
7	Guest species trapped inside carbon nanotubes. Chemical Physics Letters, 2009, 473, 146-150.	2.6	33
8	Natural Gas Evolution in a Gas Hydrate Melt: Effect of Thermodynamic Hydrate Inhibitors. Journal of Physical Chemistry B, 2017, 121, 153-163.	2.6	26
9	A multifunctional triazine-based nanoporous polymer as a versatile organocatalyst for CO₂utilization and Câ€“C bond formation. Chemical Communications, 2019, 55, 11607-11610.	4.1	24
10	Triazole-appended pyrano[2,3-c]pyrazolone based colorimetric chemosensors for recognition of Fe³⁺ ions and their molecular logic gate behavior. Analytical Methods, 2019, 11, 3230-3243.	2.7	22
11	Time-Dependent Density Functional Theoretical Study of the Absorption Properties of BN-Substituted C60Fullerenes. Journal of Physical Chemistry A, 2007, 111, 6901-6903.	2.5	21
12	Nitrogen Amelioration-Driven Carbon Dioxide Capture by Nanoporous Polytriazine. Langmuir, 2019, 35, 4893-4901.	3.5	21
13	Density functional theoretical studies of the isomers of croconic acid and their dimers. Computational and Theoretical Chemistry, 2011, 973, 28-32.	2.5	20
14	Interaction of rare gas dimers in the confines of a carbon nanotube. Chemical Physics Letters, 2015, 618, 42-45.	2.6	19
15	Carbon dioxide induced bubble formation in a CH₄â€“CO₂â€“H₂O ternary system: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2016, 18, 3746-3754.	2.8	19
16	Encapsulation of paramagnetic diatomic molecules B 2 , O 2 and Ge 2 inside C 60. Chemical Physics Letters, 2014, 610-611, 251-255.	2.6	17
17	Water clustering in the presence of a CO2 molecule. Computational and Theoretical Chemistry, 2011, 966, 84-90.	2.5	16
18	Hydrogen-tetrahydrofuran mixed hydrates: AÂcomputational study. International Journal of Hydrogen Energy, 2018, 43, 19559-19566.	7.1	14

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19	Formation of a nanobubble and its effect on the structural ordering of water in a CH₄â€“N₂â€“CO₂â€“H₂O mixture. Physical Chemistry Chemical Physics, 2018, 20, 9157-9166.	2.8	13
20	Structure, Stability, and Properties of Boron Encapsulated Complexes of C₆₀, C₅₉B, and C₅₉N. Journal of Physical Chemistry A, 2017, 121, 1708-1714.	2.5	12
21	Self-Assembling and Luminescent Properties of Chiral Bisoxadiazole Derivatives in Solution and Liquid-Crystalline Phases. Journal of Physical Chemistry B, 2017, 121, 1922-1929.	2.6	12
22	Optoelectronic Properties of Cycloparaphenyleneâ€“Carbon Nanotube Based Molecular Architectures. Journal of Physical Chemistry C, 2018, 122, 19904-19912.	3.1	12
23	Charge transport and optical properties of the complexes of indigo wrapped over carbon nanotubes. Physical Chemistry Chemical Physics, 2016, 18, 14040-14045.	2.8	11
24	Hostâ€“guest and guestâ€“guest interactions in noble gas hydrates. Molecular Physics, 2018, 116, 54-63.	1.7	11
25	Isatinâ€Triazoleâ€Functionalized Rhodamine: A Dual Sensor for Cu2+and Fe3+Ions and Its Application to Cell Imaging. ChemistrySelect, 2019, 4, 7532-7540.	1.5	11
26	Structure and Properties of Small Aurocarbons: A Selective Study. Journal of Physical Chemistry A, 2013, 117, 6803-6808.	2.5	9
27	Effect of surface roughness on adsorption and distribution of methane at the water-methane interface. Journal of Molecular Liquids, 2018, 266, 856-863.	4.9	9
28	Catalytic reduction of SO2 by CO using carbon intercalated gold clusters. Chemical Physics Letters, 2019, 726, 111-116.	2.6	9
29	Atoms and molecules in a confined environment. European Physical Journal D, 2021, 75, 1.	1.3	9
30	Effect of multiple and adjacent cage occupancies on host-guest interaction and NMR chemical shifts in gas hydrates. Computational and Theoretical Chemistry, 2016, 1092, 57-67.	2.5	8
31	Spinâ€“Spin Coupling in Nitrogen Atom Encapsulated C_{60,} C₅₉N, and Their Respective Dimers. Journal of Physical Chemistry A, 2016, 120, 6990-6997.	2.5	7
32	Effect of confinement on structure, energy and vibrational spectra of (HF) , nâ€¯=â€¯1â€“4. Chemical Physics Letters, 2019, 733, 136670.	2.6	7
33	Synthesis of a Highly Efficient Multifunctional Copper (II)â€Pyridyl Complex for Adsorption and Photocatalytic Degradation of Organic Dyes. ChemistrySelect, 2019, 4, 4952-4961.	1.5	7
34	Structural, optoelectronic and charge transport properties of the complexes of indigo encapsulated in carbon nanotubes. Physical Chemistry Chemical Physics, 2018, 20, 15158-15167.	2.8	6
35	A comprehensive study of the optoelectronic properties of donor-acceptor based derivatives of 1,3,4-oxadiazole. Chemical Physics Letters, 2017, 679, 102-111.	2.6	5
36	Hydracyanation of acetylene on carbon intercalated gold clusters: Co-operativity and site specificity. Chemical Physics Letters, 2020, 761, 138059.	2.6	5

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37	Revisiting the structural pattern and the stability of (H2O)20 clusters using the dispersion corrected density functional method. Chemical Physics Letters, 2015, 626, 39-42.	2.6	4
38	Density functional studies of fused dodecahedral and irregular-dodecahedral water cages. RSC Advances, 2015, 5, 74270-74273.	3.6	4
39	Electronic and optical absorption properties of the derivatives of 1,3,4-Oxadiazole. Chemical Data Collections, 2016, 5-6, 88-95.	2.3	4
40	Density functional studies of the catalytic oxidation of CO using small aurocarbons. Chemical Physics Impact, 2021, 2, 100023.	3.5	4
41	Encapsulation of the interstellar abundant H₃⁺ in a C₆₀ fullerene. International Journal of Quantum Chemistry, 2011, 111, 3695-3700.	2.0	3
42	Adsorption and dissolution of methane at the surface of the methanol-water mixture. Fluid Phase Equilibria, 2018, 473, 310-317.	2.5	3
43	Optoelectronic and charge transport properties of the complex of carbon nanotube with perylene bisimide. International Journal of Quantum Chemistry, 2019, 119, e26026.	2.0	2
44	Density functional studies on the conversion of hydrogen cyanide to vinyl isocyanide using carbon-supported platinum catalysts. Computational and Theoretical Chemistry, 2021, 1205, 113442.	2.5	2
45	Density functional studies of endosulphan and its interaction with glycine and GABA#. Journal of Chemical Sciences, 2012, 124, 203-207.	1.5	1
46	Spin density transfer from guest to host in endohedral heterofullerene dimers. Physical Chemistry Chemical Physics, 2019, 21, 7605-7612.	2.8	1
47	Clustering of Auro-acetylenes via C-Auâ€¦ Ïâ€ Interactions: Gold-Hydrogen Analogy. Chemical Physics Letters, 2022, , 139387.	2.6	1
48	Switching the charge transfer characteristics of quaterthiophene from p-type to n-type via interactions with carbon nanotubes. Physical Chemistry Chemical Physics, 2019, 21, 24820-24827.	2.8	0
49	Cisâ€“trans isomerisation and absorption properties of the ring-extended azobenzene. Molecular Physics, 0, , Â.	1.7	0
50	Stacked dimers of Fe-porphyrin with hydrazine and pyrazine as linkers. Chemical Physics Letters, 2021, 779, 138826.	2.6	0