

Puspitapallab Chaudhuri

List of Publications by Year in descending order

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50
papers

699
citations

623734

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580821

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50
all docs

50
docs citations

50
times ranked

629
citing authors

#	ARTICLE	IF	CITATIONS
1	Encapsulation of atomic hydrogen and gaseous molecules in single-walled boron-nitrogen nanotubes: A computational study. Applied Surface Science, 2022, 579, 152098.	6.1	0
2	Density functional study of glycine adsorption on single-walled BN nanotubes. Applied Surface Science, 2021, 536, 147686.	6.1	12
3	Mechanical alloying synthesis of Sm ₃ NbO ₇ defect fluorite and structural characterization by X-ray diffraction, Raman spectroscopy and DFT calculation. Ceramics International, 2021, 47, 8936-8943.	4.8	4
4	Density functional study of adsorption of atoms and molecules on single-walled BN nanotubes. Applied Surface Science Advances, 2021, 4, 100084.	6.8	2
5	Experimental and theoretical characterization of SmAlO ₃ perovskite synthesized by mechanical alloying. Journal of Solid State Chemistry, 2021, 298, 122097.	2.9	2
6	Vibrational Spectra of Atmospherically Relevant Hydrogen-Bonded MSA-(H ₂ SO ₄) _n (n = 1-3) Clusters. Journal of Physical Chemistry A, 2021, 125, 8791-8802.	2.5	0
7	Atmospherically Relevant Hydrogen-Bonded Interactions between Methanesulfonic Acid and H ₂ SO ₄ Clusters: A Computational Study. Journal of Physical Chemistry A, 2020, 124, 11072-11085.	2.5	8
8	Paper: In-situ high-pressure Raman scattering and ab-initio studies in Cu ₂ Sb up to 45 GPa. Journal of Alloys and Compounds, 2020, 827, 154372.	5.5	2
9	Structural and optical properties of a mechanically alloyed thermoelectric lamellar SnSe solid solution. Journal of Applied Physics, 2019, 126, .	2.5	6
10	First-principles study of nanotubes of carbon, boron and nitrogen. Applied Surface Science, 2019, 490, 242-250.	6.1	14
11	Spin-spin coupling constants in linear substituted HCN clusters. Molecular Physics, 2019, 117, 693-704.	1.7	3
12	NMR spin-spin coupling constants in hydrogen-bonded glycine clusters. International Journal of Quantum Chemistry, 2018, 118, e25608.	2.0	4
13	Effect of hydrogen-bonded interactions on the energetics and spectral properties of the astromolecule aminoacetonitrile. International Journal of Quantum Chemistry, 2018, 118, e25459.	2.0	1
14	Conductance through glycine in a graphene nanogap. Journal of Nanoparticle Research, 2018, 20, 1.	1.9	2
15	Electronic structure and quantum transport properties of boron and nitrogen substituted graphene monolayers. Current Applied Physics, 2017, 17, 957-961.	2.4	7
16	Electrical properties of SnSe under high-pressure. Computational Condensed Matter, 2016, 9, 77-81.	2.1	23
17	NMR properties of hydrogen-bonded glycine cluster in gas phase. Journal of Molecular Structure, 2016, 1123, 55-65.	3.6	6
18	Pressure-induced polymorphism in nanostructured SnSe. Journal of Applied Crystallography, 2016, 49, 213-221.	4.5	20

#	ARTICLE	IF	CITATIONS
19	Hydrogen-bonded glycine-HCN complexes in gas phase: structure, energetics, electric properties and cooperativity. <i>Molecular Physics</i> , 2015, 113, 447-462.	1.7	7
20	NMR spin-spin coupling constants in microhydrated ortho-aminobenzoic acid. <i>Molecular Physics</i> , 2015, 113, 497-507.	1.7	2
21	Effect of Hydrogen Bond Formation on the NMR Properties of Glycine-HCN Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10274-10285.	2.5	20
22	Effects of Microhydration on the Electronic Properties of <i>ortho</i> -Aminobenzoic Acid. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5675-5684.	2.5	6
23	Effect of hydrogen bond formation on the NMR properties of microhydrated ortho-aminobenzoic acid. <i>Molecular Physics</i> , 2013, 111, 403-412.	1.7	13
24	Effect of hydrogen bond formation on the elastic molecular scattering: a case study with methanol. <i>Molecular Physics</i> , 2012, 110, 297-306.	1.7	11
25	Rayleigh light scattering from hydrogen-bonded dimers of small astrophysical molecules. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2822-2827.	2.0	11
26	An ab initio quantum chemical characterization of structure and vibrational spectra of anthranilic acid. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1709-1718.	2.0	8
27	Many-body energy decomposition of hydrogen-bonded glycine clusters in gas-phase. <i>Chemical Physics Letters</i> , 2010, 491, 86-90.	2.6	9
28	EFFECT OF APERIODICITY ON THE CHARGE TRANSFER THROUGH DNA MOLECULES. <i>International Journal of Modern Physics B</i> , 2010, 24, 5683-5694.	2.0	1
29	Conformational behavior of different possible ways of oligoglycine formation in a solvent-free environment. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 25-32.	1.5	4
30	Rayleigh scattering properties of small polyglycine molecules. <i>Computational and Theoretical Chemistry</i> , 2006, 760, 15-20.	1.5	31
31	Total elastic cross section for H^+ scattering at thermal energies. <i>Physical Review A</i> , 2004, 69, .	2.5	11
32	Electronic excitation of N_2 by positron impact. <i>Physical Review A</i> , 2004, 69, .	2.5	28
33	Antiatom-atom scattering with the close-coupling model. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2004, 221, 12-20.	1.4	1
34	Positron impact electronic excitation of N_2 . <i>Nuclear Instruments & Methods in Physics Research B</i> , 2004, 221, 69-75.	1.4	21
35	Relative strength of hydrogen bond interaction in alcohol-water complexes. <i>Chemical Physics Letters</i> , 2004, 400, 494-499.	2.6	135
36	Quantifying multiple-body interaction terms in H-bonded HCN chains with many-body perturbation/coupled-cluster theories. <i>Journal of Chemical Physics</i> , 2003, 118, 10593-10601.	3.0	67

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37	Antihydrogen-hydrogen elastic scattering at thermal energies using an atomic-orbital technique. Physical Review A, 2003, 67, .	2.5	17
38	Orthopositronium-sodium scattering using the close-coupling approximation in the integral representation. Physical Review A, 2002, 65, .	2.5	7
39	An ab initio study of the peptide bond formation between alanine and glycine: electron correlation effects on the structure and binding energy. Computational and Theoretical Chemistry, 2002, 577, 267-279.	1.5	27
40	Positronium formation from hydrogen negative ion, H ⁻ . Brazilian Journal of Physics, 2001, 31, 1-7.	1.4	3
41	Generalized Position and Momentum Tsallis Entropies. International Journal of Theoretical Physics, 2000, 39, 2423-2438.	1.2	18
42	Momentum-space non-hydrogenic wavefunction of quantum defect theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 95-99.	1.5	4
43	Close-coupling calculations of elastic and inelastic positron-helium scattering. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 129-136.	1.5	3
44	Ps-He scattering using the three-state positronium close-coupling approximation. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 1657-1667.	1.5	35
45	Positron-helium scattering: Resonance and differential cross sections. Nuclear Physics A, 1998, 631, 715-719.	1.5	3
46	The effect of core electrons in Na scattering. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 1631-1636.	1.5	5
47	Close-coupling calculations of positronium formation in positron-helium scattering. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 3057-3063.	1.5	15
48	Differential cross sections for target excitation and positronium formation in positron-helium scattering. Physical Review A, 1998, 57, 984-989.	2.5	9
49	Resonance in positron - helium scattering at medium energy. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, L81-L85.	1.5	14
50	Ps - H scattering using the three-state positronium close-coupling approximation. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 4643-4652.	1.5	37