

K P Katin

List of Publications by Year in descending order

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84
papers

1,273
citations

361413

20
h-index

477307

29
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84
all docs

84
docs citations

84
times ranked

574
citing authors

#	ARTICLE	IF	CITATIONS
1	Probing of Neural Networks as a Bridge from Ab Initio Relevant Characteristics to Differential Scanning Calorimetry Measurements of High-Energy Compounds. <i>Physica Status Solidi - Rapid Research Letters</i> , 2022, 16, 2100191.	2.4	11
2	Raman and IR spectra of a 2D Thiophene-Tetrathia-Annulene monolayer calculated via density-functional theory. <i>Materials Chemistry and Physics</i> , 2022, 275, 125181.	4.0	1
3	Novel cucurbit[6]uril-based [3]rotaxane supramolecular ionic liquid as a green and excellent corrosion inhibitor for the chemical industry. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 633, 127837.	4.7	36
4	Headspace μ -solid phase extraction of 1,4-dioxane and 2-methyl-1,3-dioxolane from shampoo samples in a home-mode device and large volume injection of deep eutectic solvent: Theoretical and experimental studies. <i>Microchemical Journal</i> , 2022, 173, 107040.	4.5	5
5	Novel gossypol-indole modification as a green corrosion inhibitor for low-carbon steel in aggressive alkaline-saline solution. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 637, 128207.	4.7	70
6	Ab Initio Insight into the Interaction of Metal-Decorated Fluorinated Carbon Fullerenes with Anti-COVID Drugs. <i>International Journal of Molecular Sciences</i> , 2022, 23, 2345.	4.1	6
7	Phenylamine/Amide Grafted in Silica as Sensing Nanocomposites for the Removal of Carbamazepine: A DFT Approach. <i>Chemosensors</i> , 2022, 10, 76.	3.6	3
8	Fluorinated carbon and boron nitride fullerenes for drug Delivery: Computational study of structure and adsorption. <i>Journal of Molecular Liquids</i> , 2022, 353, 118773.	4.9	9
9	Synthesis and characterization of chitosan-vermiculite-lignin ternary composite as an adsorbent for effective removal of uranyl ions from aqueous solution: Experimental and theoretical analyses. <i>International Journal of Biological Macromolecules</i> , 2022, 209, 1234-1247.	7.5	22
10	New mixed-ligand iron(III) complexes containing thiocarbohydrazones: Preparation, characterization, and chemical reactivity analysis through theoretical calculations. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	3.5	3
11	Graphene nanoflakes and fullerenes doped with aluminum: features of Al-C interaction and adsorption characteristics of carbon shell. <i>Letters on Materials</i> , 2022, 12, 148-152.	0.7	7
12	Covalent and van der Waals interactions in a vertical heterostructure composed of boron and carbon. <i>Physical Review B</i> , 2022, 105, .	3.2	14
13	Moiré diamanes based on the hydrogenated or fluorinated twisted bigraphene: The features of atomic and electronic structures, Raman and infrared spectra. <i>Applied Surface Science</i> , 2021, 537, 148011.	6.1	21
14	Interlayer Heat Conductivity and Thermal Stability of Distorted Bilayer Graphene. <i>JETP Letters</i> , 2021, 113, 169-175.	1.4	7
15	Development of sensitive and accurate solid-phase microextraction procedure for preconcentration of As(III) ions in real samples. <i>Scientific Reports</i> , 2021, 11, 5481.	3.3	9
16	Ab initio Study of Hydrogen Adsorption on Metal-Decorated Borophene-Graphene Bilayer. <i>Energies</i> , 2021, 14, 2473.	3.1	8
17	Improved lithium-ion batteries and their communication with hydrogen power. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 17019-17036.	7.1	14
18	Optimization of vortex-assisted ionic liquid dispersive liquid-liquid microextraction by experimental design prior to hydride generation atomic absorption spectrometry for determination of selenium species in food, beverage and water samples. <i>Journal of Food Composition and Analysis</i> , 2021, 99, 103871.	3.9	19

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19	Experimental and theoretical investigation for the spectrophotometric determination of thiabendazole in fruit samples. <i>Microchemical Journal</i> , 2021, 168, 106488.	4.5	33
20	Enhanced properties of covalently coupled borophene-graphene layers through fluorination and hydrogenation. <i>Applied Surface Science</i> , 2021, 562, 150150.	6.1	17
21	Stone-Ångström Wales Bilayer Graphene: Structure, Stability, and Interlayer Heat Transfer. <i>JETP Letters</i> , 2021, 114, 143-149.	1.4	6
22	Novel bromide-cucurbit[7]uril supramolecular ionic liquid as a green corrosion inhibitor for the oil and gas industry. <i>Journal of Electroanalytical Chemistry</i> , 2021, 901, 115794.	3.8	51
23	Comparison of traditional and fullerene-based adsorbents for extraction of 1,4-dioxane and 2-methyl-1,3-dioxolane from milk. <i>Letters on Materials</i> , 2021, 11, 442-446.	0.7	0
24	Carbon vs silicon polyprismanes: a comparative study of metallic sp^3 -hybridized allotropes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2020, 28, 97-103.	2.1	18
25	Silicon rebirth: Ab initio prediction of metallic sp^3 -hybridized silicon allotropes. <i>Computational Materials Science</i> , 2020, 174, 109480.	3.0	12
26	Kinetic stability of nitrogen cubane inside the fullerene cage: Molecular dynamics study. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2020, 28, 304-308.	2.1	4
27	Spectrophotometric determination of aflatoxin B1 in food sample: Chemometric optimization and theoretical supports for reaction mechanisms and binding regions. <i>Journal of Food Composition and Analysis</i> , 2020, 94, 103646.	3.9	13
28	All-Nitrogen Cages and Molecular Crystals: Topological Rules, Stability, and Pyrolysis Paths. <i>Computation</i> , 2020, 8, 91.	2.0	7
29	On the Impact of Substrate Uniform Mechanical Tension on the Graphene Electronic Structure. <i>Materials</i> , 2020, 13, 4683.	2.9	5
30	Ultrasonic-assisted supramolecular solvent liquid-liquid microextraction for determination of manganese and zinc at trace levels in vegetables: Experimental and theoretical studies. <i>Journal of Molecular Liquids</i> , 2020, 310, 113192.	4.9	23
31	The study of thiazole adsorption upon BC ₂ N nanotube: DFT/TD-DFT investigation. <i>Structural Chemistry</i> , 2020, 31, 1959-1967.	2.0	7
32	Computer Test of a Modified Silicene/Graphite Anode for Lithium-Ion Batteries. <i>ACS Omega</i> , 2020, 5, 13207-13218.	3.5	25
33	Molecular Hyperdynamics Coupled with the Nonorthogonal Tight-Binding Approach: Implementation and Validation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2065-2070.	5.3	14
34	AA-Stacked Borophene-Graphene Bilayer with Covalent Bonding: Ab Initio Investigation of Structural, Electronic and Elastic properties. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5668-5673.	4.6	34
35	Interaction of dopants and functional groups adsorbed on the carbon fullerenes: Computational study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 124, 114319.	2.7	8
36	The Effects of Doping on the Electronic Characteristics and Adsorption Behavior of Silicon Polyprismanes. <i>Computation</i> , 2020, 8, 25.	2.0	0

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37	Theoretical and experimental studies aimed at the development of vortex-assisted supramolecular solvent microextraction for determination of nickel in plant samples by FAAS. <i>Microchemical Journal</i> , 2020, 159, 105491.	4.5	7
38	Effect of an Electric Field on a Lithium Ion in a Channel of the Doped Siliceneâ€“Graphite System. <i>Russian Journal of Physical Chemistry B</i> , 2020, 14, 1055-1062.	1.3	5
39	Kinetic Stability and Reactivity of Silicon and Fluorineâ€“Containing CLâ€“20 Derivatives. <i>ChemistrySelect</i> , 2019, 4, 9659-9665.	1.5	6
40	Tuning the supercritical effective charge in gapless graphene via Fermi velocity modifying through the mechanical stretching. <i>Diamond and Related Materials</i> , 2019, 100, 107566.	3.9	4
41	Hole mobility in thieno[3,2-b]thiophene oligomers. <i>Mendeleev Communications</i> , 2019, 29, 218-219.	1.6	23
42	Nitro Derivatives of Silaprismanes as High-Energy Compounds: Theoretical Study. <i>International Journal of Nanoscience</i> , 2019, 18, 1940047.	0.7	0
43	Temperature influence on process of Ti/Al/Ni/Au contact formation to heterostructure AlGaIn/GaN. <i>IOP Conference Series: Materials Science and Engineering</i> , 2019, 498, 012019.	0.6	1
44	Computational Study of Lithium Intercalation in Silicene Channels on a Carbon Substrate after Nuclear Transmutation Doping. <i>Computation</i> , 2019, 7, 60.	2.0	14
45	Relative stabilities of various fully functionalized graphene polymorphs under mechanical strain and electric field. <i>Applied Surface Science</i> , 2019, 463, 1051-1057.	6.1	19
46	Electrochemical polymerization process and excellent electrochromic properties of ferrocene-functionalized polytriphenylamine derivative. <i>Dyes and Pigments</i> , 2019, 163, 433-440.	3.7	20
47	Morse parameters for the interaction of metals with graphene and silicene. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 252-258.	2.1	44
48	Acoustical characteristics of single-walled noncarbon nanotubes: Longitudinal and torsional waves. <i>Computational Condensed Matter</i> , 2019, 18, e00350.	2.1	2
49	Stability and energy characteristics of extended nitrogen nanotubes: density functional theory study. <i>Letters on Materials</i> , 2019, 9, 366-369.	0.7	9
50	Molecular dynamics simulation of nickelâ€“coated graphene bending. <i>Micro and Nano Letters</i> , 2018, 13, 160-164.	1.3	27
51	Influence of Mechanical Stretching on Adsorption Properties of Nitrogen-Doped Graphene. <i>Physics of the Solid State</i> , 2018, 60, 821-825.	0.6	9
52	Silicon buckyballs versus prismanes: Influence of spatial confinement on the structural properties and optical spectra of the Si₁₈H₁₂ and Si₁₉H₁₂ clusters. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25609.	2.0	9
53	Thermal stability of carbon [<i>n</i> ,5] prismanes (<i>n</i> = 2â€“4): a molecular dynamics study. <i>Molecular Simulation</i> , 2018, 44, 703-707.	2.0	15
54	Strain-induced semiconductor-to-metal transitions in C36-based carbon peapods: Ab initio study. <i>Diamond and Related Materials</i> , 2018, 84, 112-118.	3.9	12

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55	Stone-Wales defects in nitrogen-doped C ₂₀ fullerenes: Insight from ab initio calculations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 96, 6-10.	2.7	15
56	Fast Switching Properties and Ion Diffusion Behavior of Polytriphenylamine Derivative with Pendent Ionic Liquid Unit. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 32404-32412.	8.0	38
57	Electronic and reactivity characteristics of CL-20 covalent chains and networks: a density functional theory study. <i>CrystEngComm</i> , 2018, 20, 4336-4344.	2.6	16
58	A bottom-up approach for controlled deformation of carbon nanotubes through blistering of supporting substrate surface. <i>Nanotechnology</i> , 2018, 29, 365304.	2.6	7
59	Energy and electronic characteristics of silicon polyprismanes: density functional theory study. <i>Letters on Materials</i> , 2018, 8, 454-457.	0.7	7
60	Effect of the embedded atom on the electronic, optical properties and kinetic stability of [3,6]silaprismane. <i>Chemical Physics</i> , 2017, 487, 59-66.	1.9	10
61	Toward CL-20 crystalline covalent solids: On the dependence of energy and electronic properties on the effective size of CL-20 chains. <i>Journal of Physics and Chemistry of Solids</i> , 2017, 108, 82-87.	4.0	28
62	Chemisorption of hydrogen atoms and hydroxyl groups on stretched graphene: A coupled QM/QM study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 2686-2690.	2.1	32
63	Theoretical Study of High-Frequency Response of InGaAs/AlAs Double-Barrier Nanostructures. <i>Advances in Materials Science and Engineering</i> , 2017, 2017, 1-7.	1.8	1
64	Effect of DFT-functional on the energy and electronic characteristics of carbon compounds with the unconventional geometry of the framework. <i>Letters on Materials</i> , 2017, 7, 433-436.	0.7	7
65	Theoretical Studies of the Stone-Wales Defect in C ₃₆ Fullerene Embedded inside Zigzag Carbon Nanotube. <i>Advances in Physical Chemistry</i> , 2016, 2016, 1-4.	2.0	10
66	Efficient cleaning of graphene from residual lithographic polymers by ozone treatment. <i>Carbon</i> , 2016, 109, 221-226.	10.3	24
67	High kinetic stability of hypercubane: Tight-binding molecular dynamics study. <i>Chemical Physics Letters</i> , 2016, 644, 280-283.	2.6	23
68	Influence of methyl functional groups on the stability of cubane carbon cage. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2016, 81, 1-6.	2.7	27
69	Nonorthogonal tight-binding model with $\text{H}\hat{=}\text{C}\hat{=}\text{O}$ parameterisation. <i>Molecular Simulation</i> , 2016, 42, 305-311.	2.0	51
70	Geometry, Energy, and Some Electronic Properties of Carbon Polyprismanes: <i>Ab Initio</i> and Tight-Binding Study. <i>Advances in Physical Chemistry</i> , 2015, 2015, 1-6.	2.0	21
71	Chemical Functionalization Effects on Cubane-Based Chain Electronic Transport. <i>Advances in Condensed Matter Physics</i> , 2015, 2015, 1-6.	1.1	13
72	Schottky-to-Ohmic Behavior in Annealed Ti/Si/Ti/Al/Ni/Au on AlGaIn/GaN. <i>Physics Procedia</i> , 2015, 72, 419-424.	1.2	6

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73	Thermal stability of hexaprismane C ₁₂ H ₁₂ and octaprismane C ₁₆ H ₁₆ . <i>Physics of the Solid State</i> , 2015, 57, 1023-1027.	0.6	18
74	Tight-binding Molecular Dynamics Simulation of the Endohedral Complex C ₄ H ₄ @C ₆₀ . <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2014, 22, 560-564.	2.1	2
75	Simulation of metastable CL-20 cluster structures. <i>Physics of the Solid State</i> , 2014, 56, 1467-1471.	0.6	18
76	Dynamic modeling of cyclotetracubyl thermal decomposition. <i>Russian Journal of Physical Chemistry B</i> , 2014, 8, 152-157.	1.3	20
77	Electronic coupling in fullerene-doped semiconducting carbon nanotubes probed by Raman spectroscopy and electronic transport. <i>Carbon</i> , 2013, 57, 498-506.	10.3	8
78	On the thermal stability of tetrahedrane: Tight-binding molecular dynamics study. <i>Chemical Physics</i> , 2011, 387, 66-68.	1.9	23
79	Thermal stability of nitro derivatives of hydrocarbon cubane. <i>Russian Journal of Physical Chemistry B</i> , 2011, 5, 770-779.	1.3	26
80	Specific features of the stone-wales transformation in the C ₂₀ and C ₃₆ fullerenes. <i>Physics of the Solid State</i> , 2011, 53, 215-220.	0.6	17
81	Numerical simulation of Platonic hydrocarbons and fullerenes. <i>Journal of Physics: Conference Series</i> , 2010, 248, 012011.	0.4	0
82	Dynamic characteristics of the low-temperature decomposition of the C ₂₀ fullerene. <i>Physics of the Solid State</i> , 2010, 52, 436-438.	0.6	16
83	On the dependence of the lifetime of an atomic cluster on the intensity of its heat exchange with the environment. <i>JETP Letters</i> , 2010, 92, 52-56.	1.4	18
84	A benzimidazolium salt as effective corrosion inhibitor against the corrosion of mild steel in acidic medium: experimental and theoretical studies. <i>Journal of Adhesion Science and Technology</i> , 0, , 1-23.	2.6	3