K P Katin

List of Publications by Year
in descending order

84 papers	1,273 citations	361413 20 h-index	477307 29 g-index
84 all docs	84 docs citations	84 times ranked	574 citing authors

#	Article	IF	Citations
1	Novel gossypolâ€“indole modification as a green corrosion inhibitor for lowâ€“carbon steel in aggressive alkalineâ€“saline solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 637, 128207.	4.7	70
2	Nonorthogonal tight-binding model with Hâ€“Câ€“Nâ€“O parameterisation. Molecular Simulation, 2016, 42, 305-311.	2.0	51
3	Novel bromideâ€“cucurbit[7]uril supramolecular ionic liquid as a green corrosion inhibitor for the oil and gas industry. Journal of Electroanalytical Chemistry, 2021, 901, 115794.	3.8	51
4	Morse parameters for the interaction of metals with graphene and silicene. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 252-258.	2.1	44
5	Fast Switching Properties and Ion Diffusion Behavior of Polytriphenylamine Derivative with Pendent Ionic Liquid Unit. ACS Applied Materials & Interfaces, 2018, 10, 32404-32412.	8.0	38
6	Novel cucurbit[6]uril-based [3]rotaxane supramolecular ionic liquid as a green and excellent corrosion inhibitor for the chemical industry. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 633, 127837.	4.7	36
7	AA-Stacked Borophene-Graphene Bilayer with Covalent Bonding: Ab Initio Investigation of Structural, Electronic and Elastic properties. Journal of Physical Chemistry Letters, 2020, 11, 5668-5673.	4.6	34
8	Experimental and theoretical investigation for the spectrophotometric determination of thiabendazole in fruit samples. Microchemical Journal, 2021, 168, 106488.	4.5	33
9	Chemisorption of hydrogen atoms and hydroxyl groups on stretched graphene: A coupled QM/QM study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 2686-2690.	2.1	32
10	Toward CL-20 crystalline covalent solids: On the dependence of energy and electronic properties on the effective size of CL-20 chains. Journal of Physics and Chemistry of Solids, 2017, 108, 82-87.	4.0	28
11	Influence of methyl functional groups on the stability of cubane carbon cage. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 81, 1-6.	2.7	27
12	Molecular dynamics simulation of nickelâ€coated graphene bending. Micro and Nano Letters, 2018, 13, 160-164.	1.3	27
13	Thermal stability of nitro derivatives of hydrocarbon cubane. Russian Journal of Physical Chemistry B, 2011, 5, 770-779.	1.3	26
14	Computer Test of a Modified Silicene/Graphite Anode for Lithium-Ion Batteries. ACS Omega, 2020, 5, 13207-13218.	3.5	25
15	Efficient cleaning of graphene from residual lithographic polymers by ozone treatment. Carbon, 2016, 109, 221-226.	10.3	24
16	On the thermal stability of tetrahedrane: Tight-binding molecular dynamics study. Chemical Physics, 2011, 387, 66-68.	1.9	23
17	High kinetic stability of hypercubane: Tight-binding molecular dynamics study. Chemical Physics Letters, 2016, 644, 280-283.	2.6	23
18	Hole mobility in thieno[3,2-b]thiophene oligomers. Mendeleev Communications, 2019, 29, 218-219.	1.6	23

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19	Ultrasonic-assisted supramolecular solvent liquid-liquid microextraction for determination of manganese and zinc at trace levels in vegetables: Experimental and theoretical studies. Journal of Molecular Liquids, 2020, 310, 113192.	4.9	23
20	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. International Journal of Biological Macromolecules, 2022, 209, 1234-1247.	7.5	22
21	Geometry, Energy, and Some Electronic Properties of Carbon Polyprismanes: Ab Initio and Tight-Binding Study. Advances in Physical Chemistry, 2015, 2015, 1-6.	2.0	21
22	MoirÃ© diamanes based on the hydrogenated or fluorinated twisted bigraphene: The features of atomic and electronic structures, Raman and infrared spectra. Applied Surface Science, 2021, 537, 148011.	6.1	21
23	Dynamic modeling of cyclotetracubyl thermal decomposition. Russian Journal of Physical Chemistry B, 2014, 8, 152-157.	1.3	20
24	Electrochemical polymerization process and excellent electrochromic properties of ferrocene-functionalized polytriphenylamine derivative. Dyes and Pigments, 2019, 163, 433-440.	3.7	20
25	Relative stabilities of various fully functionalized graphene polymorphs under mechanical strain and electric field. Applied Surface Science, 2019, 463, 1051-1057.	6.1	19
26	Optimization of vortex-assisted ionic liquid dispersive liquidâ€“liquid microextraction by experimental design prior to hydride generation atomic absorption spectrometry for determination of selenium species in food, beverage and water samples. Journal of Food Composition and Analysis, 2021, 99, 103871.	3.9	19
27	On the dependence of the lifetime of an atomic cluster on the intensity of its heat exchange with the environment. JETP Letters, 2010, 92, 52-56.	1.4	18
28	Simulation of metastable CL-20 cluster structures. Physics of the Solid State, 2014, 56, 1467-1471.	0.6	18
29	Thermal stability of hexaprismane C12H12 and octaprismane C16H16. Physics of the Solid State, 2015, 57, 1023-1027.	0.6	18
30	Carbon vs silicon polyprismanes: a comparative study of metallic sp³-hybridized allotropes. Fullerenes Nanotubes and Carbon Nanostructures, 2020, 28, 97-103.	2.1	18
31	Specific features of the stone-wales transformation in the C20 and C36 fullerenes. Physics of the Solid State, 2011, 53, 215-220.	0.6	17
32	Enhanced properties of covalently coupled borophene-graphene layers through fluorination and hydrogenation. Applied Surface Science, 2021, 562, 150150.	6.1	17
33	Dynamic characteristics of the low-temperature decomposition of the C20 fullerene. Physics of the Solid State, 2010, 52, 436-438.	0.6	16
34	Electronic and reactivity characteristics of CL-20 covalent chains and networks: a density functional theory study. CrystEngComm, 2018, 20, 4336-4344.	2.6	16
35	Thermal stability of carbon [n,5] prismanes (n = 2â€“4): a molecular dynamics study. Molecular Simulation, 2018, 44, 703-707.	2.0	15
36	Stone-Wales defects in nitrogen-doped C 20 fullerenes: Insight from ab initio calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2018, 96, 6-10.	2.7	15

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37	Computational Study of Lithium Intercalation in Silicene Channels on a Carbon Substrate after Nuclear Transmutation Doping. Computation, 2019, 7, 60.	2.0	14
38	Molecular Hyperdynamics Coupled with the Nonorthogonal Tight-Binding Approach: Implementation and Validation. Journal of Chemical Theory and Computation, 2020, 16, 2065-2070.	5.3	14
39	Improved lithium-ion batteries and their communication with hydrogen power. International Journal of Hydrogen Energy, 2021, 46, 17019-17036.	7.1	14
40	Covalent and van der Waals interactions in a vertical heterostructure composed of boron and carbon. Physical Review B, 2022, 105, .	3.2	14
41	Chemical Functionalization Effects on Cubane-Based Chain Electronic Transport. Advances in Condensed Matter Physics, 2015, 2015, 1-6.	1.1	13
42	Spectrophotometric determination of aflatoxin B1 in food sample: Chemometric optimization and theoretical supports for reaction mechanisms and binding regions. Journal of Food Composition and Analysis, 2020, 94, 103646.	3.9	13
43	Strain-induced semiconductor-to-metal transitions in C36-based carbon peapods: Ab initio study. Diamond and Related Materials, 2018, 84, 112-118.	3.9	12
44	Silicon rebirth: Ab initio prediction of metallic sp3-hybridized silicon allotropes. Computational Materials Science, 2020, 174, 109480.	3.0	12
45	Probing of Neural Networks as a Bridge from Ab Initio Relevant Characteristics to Differential Scanning Calorimetry Measurements of Highâ€Energy Compounds. Physica Status Solidi - Rapid Research Letters, 2022, 16, 2100191.	2.4	11
46	Theoretical Studies of the Stone-Wales Defect in C₃₆ Fullerene Embedded inside Zigzag Carbon Nanotube. Advances in Physical Chemistry, 2016, 2016, 1-4.	2.0	10
47	Effect of the embedded atom on the electronic, optical properties and kinetic stability of [3,6]silaprismane. Chemical Physics, 2017, 487, 59-66.	1.9	10
48	Influence of Mechanical Stretching on Adsorption Properties of Nitrogen-Doped Graphene. Physics of the Solid State, 2018, 60, 821-825.	0.6	9
49	Silicon buckyballs versus prismanes: Influence of spatial confinement on the structural properties and optical spectra of the Si₁₈H₁₂ and Si₁₉H₁₂ clusters. International Journal of Quantum Chemistry, 2018, 118, e25609.	2.0	9
50	Development of sensitive and accurate solid-phase microextraction procedure for preconcentration of As(III) ions in real samples. Scientific Reports, 2021, 11, 5481.	3.3	9
51	Stability and energy characteristics of extended nitrogen nanotubes: density functional theory study. Letters on Materials, 2019, 9, 366-369.	0.7	9
52	Fluorinated carbon and boron nitride fullerenes for drug Delivery: Computational study of structure and adsorption. Journal of Molecular Liquids, 2022, 353, 118773.	4.9	9
53	Electronic coupling in fullerene-doped semiconducting carbon nanotubes probed by Raman spectroscopy and electronic transport. Carbon, 2013, 57, 498-506.	10.3	8
54	Interaction of dopants and functional groups adsorbed on the carbon fullerenes: Computational study. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114319.	2.7	8

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55	Ab initio Study of Hydrogen Adsorption on Metal-Decorated Borophene-Graphene Bilayer. Energies, 2021, 14, 2473.	3.1	8
56	A bottom-up approach for controlled deformation of carbon nanotubes through blistering of supporting substrate surface. Nanotechnology, 2018, 29, 365304.	2.6	7
57	All-Nitrogen Cages and Molecular Crystals: Topological Rules, Stability, and Pyrolysis Paths. Computation, 2020, 8, 91.	2.0	7
58	The study of thiazole adsorption upon BC2N nanotube: DFT/TD-DFT investigation. Structural Chemistry, 2020, 31, 1959-1967.	2.0	7
59	Interlayer Heat Conductivity and Thermal Stability of Distorted Bilayer Graphene. JETP Letters, 2021, 113, 169-175.	1.4	7
60	Theoretical and experimental studies aimed at the development of vortex-assisted supramolecular solvent microextraction for determination of nickel in plant samples by FAAS. Microchemical Journal, 2020, 159, 105491.	4.5	7
61	Effect of DFT-functional on the energy and electronic characteristics of carbon compounds with the unconventional geometry of the framework. Letters on Materials, 2017, 7, 433-436.	0.7	7
62	Energy and electronic characteristics of silicon polyprismanes: density functional theory study. Letters on Materials, 2018, 8, 454-457.	0.7	7
63	Graphene nanoflakes and fullerenes doped with aluminum: features of Al-C interaction and adsorption characteristics of carbon shell. Letters on Materials, 2022, 12, 148-152.	0.7	7
64	Schottky-to-Ohmic Behavior in Annealed Ti/Si/Ti/Al/Ni/Au on AlGaN/GaN. Physics Procedia, 2015, 72, 419-424.	1.2	6
65	Kinetic Stability and Reactivity of Silicon and Fluorineâ€Containing CLâ€20 Derivatives. ChemistrySelect, 2019, 4, 9659-9665.	1.5	6
66	Stoneâ€“Wales Bilayer Graphene: Structure, Stability, and Interlayer Heat Transfer. JETP Letters, 2021, 114, 143-149.	1.4	6
67	Ab Initio Insight into the Interaction of Metal-Decorated Fluorinated Carbon Fullerenes with Anti-COVID Drugs. International Journal of Molecular Sciences, 2022, 23, 2345.	4.1	6
68	On the Impact of Substrate Uniform Mechanical Tension on the Graphene Electronic Structure. Materials, 2020, 13, 4683.	2.9	5
69	Effect of an Electric Field on a Lithium Ion in a Channel of the Doped Siliceneâ€“Graphite System. Russian Journal of Physical Chemistry B, 2020, 14, 1055-1062.	1.3	5
70	Headspace Âµâ€“solid phase extraction of 1,4â€“dioxane and 2â€“methylâ€“1,3â€“dioxolane from shampoo samples in a homeâ€“mode device and large volume injection of deep eutectic solvent: Theoretical and experimental studies. Microchemical Journal, 2022, 173, 107040.	4.5	5
71	Tuning the supercritical effective charge in gapless graphene via Fermi velocity modifying through the mechanical stretching. Diamond and Related Materials, 2019, 100, 107566.	3.9	4
72	Kinetic stability of nitrogen cubane inside the fullerene cage: Molecular dynamics study. Fullerenes Nanotubes and Carbon Nanostructures, 2020, 28, 304-308.	2.1	4

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73	Phenylamine/Amide Grafted in Silica as Sensing Nanocomposites for the Removal of Carbamazepine: A DFT Approach. Chemosensors, 2022, 10, 76.	3.6	3
74	A benzimidazolium salt as effective corrosion inhibitor against the corrosion of mild steel in acidic medium: experimental and theoretical studies. Journal of Adhesion Science and Technology, 0, , 1-23.	2.6	3
75	New mixedâ€ligand iron(III) complexes containing thiocarbohydrazones: Preparation, characterization, and chemical reactivity analysis through theoretical calculations. Applied Organometallic Chemistry, 2022, 36, .	3.5	3
76	Tight-binding Molecular Dynamics Simulation of the Endohedral Complex C4H4@C60. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 560-564.	2.1	2
77	Acoustical characteristics of single-walled noncarbon nanotubes: Longitudinal and torsional waves. Computational Condensed Matter, 2019, 18, e00350.	2.1	2
78	Theoretical Study of High-Frequency Response of InGaAs/AlAs Double-Barrier Nanostructures. Advances in Materials Science and Engineering, 2017, 2017, 1-7.	1.8	1
79	Temperature influence on process of Ti/Al/Ni/Au contact formation to heterostructure AlGaN/GaN. IOP Conference Series: Materials Science and Engineering, 2019, 498, 012019.	0.6	1
80	Raman and IR spectra of a 2D Thiophene-Tetrathia-Annulene monolayer calculated via density-functional theory. Materials Chemistry and Physics, 2022, 275, 125181.	4.0	1
81	Numerical simulation of Platonic hydrocarbons and fullerenes. Journal of Physics: Conference Series, 2010, 248, 012011.	0.4	0
82	Nitro Derivatives of Silaprismanes as High-Energy Compounds: Theoretical Study. International Journal of Nanoscience, 2019, 18, 1940047.	0.7	0
83	The Effects of Doping on the Electronic Characteristics and Adsorption Behavior of Silicon Polyprismanes. Computation, 2020, 8, 25.	2.0	0
84	Comparison of traditional and fullerene-based adsorbents for extraction of 1,4â€˘dioxane and 2â€˘methyl-1,3â€˘dioxolane from milk. Letters on Materials, 2021, 11, 442-446.	0.7	0