Emmanuel N. Koukaras

List of Publications by Year
in descending order

101 papers	2,136 citations	257450 24 h-index	265206 42 g-index
102 all docs	102 docs citations	102 times ranked	3214 citing authors

#	Article	IF	Citations
1	Insight on the Formation of Chitosan Nanoparticles through Ionotropic Gelation with Tripolyphosphate. Molecular Pharmaceutics, 2012, 9, 2856-2862.	4.6	177
2	Phonon properties of graphene derived from molecular dynamics simulations. Scientific Reports, 2015, 5, 12923.	3.3	113
3	Stress Transfer Mechanisms at the Submicron Level for Graphene/Polymer Systems. ACS Applied Materials & Interfaces, 2015, 7, 4216-4223.	8.0	105
4	Tunable macroscale structural superlubricity in two-layer graphene via strain engineering. Nature Communications, 2020, 11, 1595.	12.8	88
5	Graphene flakes under controlled biaxial deformation. Scientific Reports, 2016, 5, 18219.	3.3	84
6	Graphene Mechanics: Current Status and Perspectives. Annual Review of Chemical and Biomolecular Engineering, 2015, 6, 121-140.	6.8	76
7	Chitosan derivatives as effective nanocarriers for ocular release of timolol drug. International Journal of Pharmaceutics, 2015, 495, 249-264.	5.2	76
8	Failure Processes in Embedded Monolayer Graphene under Axial Compression. Scientific Reports, 2014, 4, 5271.	3.3	65
9	New conjugated alternating benzodithiophene-containing copolymers with different acceptor units: synthesis and photovoltaic application. Journal of Materials Chemistry A, 2014, 2, 155-171.	10.3	55
10	Suspended monolayer graphene under true uniaxial deformation. Nanoscale, 2015, 7, 13033-13042.	5.6	52
11	Ab Initio Study of Magnesium and Magnesium Hydride Nanoclusters and Nanocrystals: Examining Optimal Structures and Compositions for Efficient Hydrogen Storage. Journal of the American Chemical Society, 2012, 134, 15914-15922.	13.7	51
12	Strained hexagonal boron nitride: Phonon shift and GrÃ¼neisen parameter. Physical Review B, 2018, 97, .	3.2	51
13	Synthesis, optical and electrochemical properties of the Aâ€"Ï€-Dâ€"Ï€-A porphyrin and its application as an electron donor in efficient solution processed bulk heterojunction solar cells. Nanoscale, 2015, 7, 179-189.	5.6	48
14	Aâ€"Ï€â€"Dâ€"Ï€â€"A based porphyrin for solution processed small molecule bulk heterojunction solar cells. Journal of Materials Chemistry A, 2015, 3, 16287-16301.	10.3	47
15	Wrinkled Few-Layer Graphene as Highly Efficient Load Bearer. ACS Applied Materials & Interfaces, 2017, 9, 26593-26601.	8.0	46
16	BODIPYâ€"diketopyrrolopyrroleâ€"porphyrin conjugate small molecules for use in bulk heterojunction solar cells. Journal of Materials Chemistry A, 2018, 6, 8449-8461.	10.3	45
17	Structure and properties of theNi@Si12cluster from all-electronab initiocalculations. Physical Review B, 2006, 73, .	3.2	43
18	Toward Efficient Drug Delivery through Suitably Prepared Metalâ€"Organic Frameworks: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 8885-8890.	3.1	37

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19	Synthesis and characterization of a low band gap quinoxaline based Dâ€“A copolymer and its application as a donor for bulk heterojunction polymer solar cells. Polymer Chemistry, 2013, 4, 4033.	3.9	33
20	Wrinkling formation in simply-supported graphenes under tension and compression loadings. Nanoscale, 2017, 9, 18180-18188.	5.6	31
21	Effect of Poly(vinyl alcohol) on Nanoencapsulation of Budesonide in Chitosan Nanoparticles via Ionic Gelation and Its Improved Bioavailability. Polymers, 2020, 12, 1101.	4.5	31
22	Study of an indolineâ€“phenothiazine based organic dye for Dye-Sensitized Solar Cells. Theoretical calculations and experimental data. Organic Electronics, 2015, 25, 66-73.	2.6	29
23	Structural and static electric response properties of highly symmetric lithiated silicon cages: Theoretical predictions. Journal of Computational Chemistry, 2012, 33, 1068-1079.	3.3	26
24	Design and synthesis of new ultra-low band gap thiadiazoloquinoxaline-based polymers for near-infrared organic photovoltaic application. RSC Advances, 2016, 6, 14893-14908.	3.6	26
25	Donorâ€“acceptorâ€“acceptorâ€“donor small molecules for solution processed bulk heterojunction solar cells. Organic Electronics, 2015, 27, 72-83.	2.6	24
26	Solution processed organic solar cells based on Aâ€“Dâ€“Dâ€²â€“Dâ€“A small molecule with benzo[1,2-b:4,5-bâ€²]dithiophene donor (Dâ€²) unit, cyclopentadithiophene donor (D) and ethylrhodanine acceptor unit having 6% light to energy conversion efficiency. Journal of Materials Chemistry A, 2015, 3, 4892-4902.	10.3	23
27	Dye-sensitized solar cells based on triazine-linked porphyrin dyads containing one or two carboxylic acid anchoring groups. Inorganic Chemistry Frontiers, 2014, 1, 256-270.	6.0	21
28	Size dependence of the structural, electronic, and optical properties of (CdSe)_n, n = 6â€“60, nanocrystals. RSC Advances, 2014, 4, 14613-14623.	3.6	21
29	Ab initio theoretical investigation of beryllium and beryllium hydride nanoparticles and nanocrystals with implications for the corresponding infinite systems. Physical Chemistry Chemical Physics, 2014, 16, 14172-14182.	2.8	20
30	Design of diketopyrrolopyrrole chromophores applicable as sensitizers in dye-sensitized photovoltaic windows for green houses. Dyes and Pigments, 2016, 134, 472-479.	3.7	20
31	Long-lived discrete breathers in free-standing graphene. Chaos, Solitons and Fractals, 2016, 87, 262-267.	5.1	20
32	Properties and energetics for design and characterization of chitosan nanoparticles used for drug encapsulation. RSC Advances, 2014, 4, 12653.	3.6	18
33	Efficient bulk heterojunction solar cells based on solution processed small molecules based on the same benzo[1,2-b:4, 5-bâ€²]thiophene unit as core donor and different terminal units. Nanoscale, 2015, 7, 7692-7703.	5.6	18
34	New D-A1â€“D-A2-Type Regular Terpolymers Containing Benzothiadiazole and Benzotrithiophene Acceptor Units for Photovoltaic Application. ACS Applied Materials & Interfaces, 2016, 8, 32998-33009.	8.0	18
35	New low bandgap near-IR conjugated Dâ€“A copolymers for BHJ polymer solar cell applications. Physical Chemistry Chemical Physics, 2016, 18, 8389-8400.	2.8	18
36	Sculpturing graphene wrinkle patterns into compliant substrates. Carbon, 2019, 146, 772-778.	10.3	18

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37	Vanillin chitosan miscible hydrogel blends and their prospects for 3D printing biomedical applications. International Journal of Biological Macromolecules, 2021, 192, 1266-1275.	7.5	18
38	Efficient solution processed D1-A-D2-A-D1 small molecules bulk heterojunction solar cells based on alkoxy triphenylamine and benzo[1,2-b:4,5-bâ€²]thiophene units. Organic Electronics, 2015, 26, 36-47.	2.6	17
39	Compression behavior of simply-supported and fully embedded monolayer graphene: Theory and experiment. Extreme Mechanics Letters, 2016, 8, 191-200.	4.1	17
40	Dissolution Enhancement and Controlled Release of Paclitaxel Drug via a Hybrid Nanocarrier Based on mPEG-PCL Amphiphilic Copolymer and Fe-BTC Porous Metal-Organic Framework. Nanomaterials, 2020, 10, 2490.	4.1	17
41	Structural properties and magic structures in hydrogenated finite and infinite silicon nanowires. Applied Physics Letters, 2007, 91, 203112.	3.3	16
42	Theoretical Study of Amino Acid Interaction with Metal Organic Frameworks. Journal of Physical Chemistry Letters, 2011, 2, 272-275.	4.6	16
43	Porous carbon nanotube networks and pillared graphene materials exhibiting high SF6 adsorption uptake and separation selectivity of SF6/N2 fluid mixtures: A comparative molecular simulation study. Microporous and Mesoporous Materials, 2020, 307, 110464.	4.4	16
44	Characterization of metal-free D-(Ï€-A)2 organic dye and its application as cosensitizer along with N719 dye for efficient dye-sensitized solar cells. Indian Journal of Physics, 2015, 89, 1041-1050.	1.8	14
45	Stress-transfer from polymer substrates to monolayer and few-layer graphenes. Nanoscale Advances, 2019, 1, 4972-4980.	4.6	14
46	Cardanol- and Guaiacol-Sourced Solution-Processable Green Small Molecule-Based Organic Solar Cells. ACS Sustainable Chemistry and Engineering, 2020, 8, 5891-5902.	6.7	14
47	Non-Eulerian behavior of graphitic materials under compression. Carbon, 2018, 138, 227-233.	10.3	13
48	<i>Ab initio</i> study of medium sized boron-doped silicon clusters Si_nB_m, <i>n</i> = 11â€“13, <i>m</i> = 1â€“3. Physical Chemistry Chemical Physics, 2018, 20, 18556-18570.	2.8	12
49	A parallel study of Ni@Si12 and Cu@Si12 nanoclusters. Journal of Mathematical Chemistry, 2009, 46, 971-980.	1.5	11
50	Multidecker Sandwiches of Siliconâˆ’Carbon Clusters. Organometallics, 2009, 28, 4308-4315.	2.3	11
51	Graphene as a hexagonal 2-lattice: Evaluation of the in-plane material constants for the linear theory. A multiscale approach. Journal of Applied Physics, 2015, 118, .	2.5	11
52	Alternative use of cross-linked polyallylamine (known as Sevelamer pharmaceutical compound) as biosorbent. Journal of Colloid and Interface Science, 2015, 442, 49-59.	9.4	11
53	Synthesis of alternating Dâ€“A1â€“Dâ€“A2 terpolymers comprising two electron-deficient moieties, quinoxaline and benzothiadiazole units for photovoltaic applications. Polymer Chemistry, 2016, 7, 4025-4035.	3.9	11
54	Synthesis and photophysical properties of regioregular low bandgap copolymers with controlled 5-fluorobenzotriazole orientation for photovoltaic application. Polymer Chemistry, 2016, 7, 5849-5861.	3.9	11

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55	Synthesis of new D-A1â€“D-A2 type low bandgap terpolymers based on different thiadiazoloquinoxaline acceptor units for efficient polymer solar cells. RSC Advances, 2016, 6, 71232-71244.	3.6	11
56	Polymer solar cells based low bandgap A1-D-A2-D terpolymer based on fluorinated thiadiazoloquinoxaline and benzothiadiazole acceptors with energy loss less than 0.5ÂeV. Organic Electronics, 2017, 46, 192-202.	2.6	11
57	Enhancement of photovoltaic efficiency through fine adjustment of indaceneâ€based nonâ€fullerene acceptor by minimal chlorination for polymer solar cells. Nano Select, 2020, 1, 320-333.	3.7	11
58	New Donor-Acceptor polymers with a wide absorption range for photovoltaic applications. Solar Energy, 2020, 205, 211-220.	6.1	11
59	New alternating Dâ€“A₁â€“Dâ€“A₂ copolymer containing two electronâ€deficient moieties based on benzothiadiazole and 9â€(2â€Octyldodecyl)â€8<i>H</i>â€pyrrolo[3,4â€<i>b</i>]bisthieno[2,3â€<i>f</i>:3',2'â€<i>h</i>]quinoxalineâ€8,10(9<i>H</i>)â€di for efficient polymer solar cells. Journal of Polymer Science Part A, 2016, 54, 155-168.	2.3	10
60	Synthesis and Photovoltaic Investigation of 8,10-Bis(2-octyldodecyl)-8,10-dihydro-9<i>H</i>-bisthieno[2â€²,3â€²:7,8;3â€³,2â€³:5,6] naphtho[2,3-<i>d</i>]imidazol-9-one Based Conjugated Polymers Using a Nonfullerene Acceptor. ACS Applied Energy Materials, 2020, 3, 495-505.	5.1	10
61	Synthesis, optical and electrochemical properties new donorâ€“acceptor (Dâ€“A) copolymers based on benzo[1,2-b:3,4-bâ€²:6,5-bâ€³] trithiophene donor and different acceptor units: Application as donor for photovoltaic devices. Organic Electronics, 2015, 17, 167-177.	2.6	9
62	Doping-Induced Stacking Transition in Trilayer Graphene: Implications for Layer Stacking Manipulation. ACS Applied Nano Materials, 2020, 3, 11861-11868.	5.0	9
63	Size dependence of the optical gap of â€œsmallâ€• silicon quantum dots: Ab initio and empirical correlation schemes. Microelectronic Engineering, 2013, 112, 231-234.	2.4	8
64	Fully Hydrogenated Beryllium Nanoclusters. Journal of the American Chemical Society, 2016, 138, 3218-3227.	13.7	8
65	Indole-based Aâ€“DAâ€²Dâ€“A type acceptor-based organic solar cells achieve efficiency over 15 % with low energy loss. Sustainable Energy and Fuels, 2020, 4, 6203-6211.	4.9	8
66	Aâ€“DAâ€²Dâ€“A Nonfullerene Acceptor Obtained by Fine-Tuning Side Chains on Pyrroles Enables PBDB-T-Based Organic Solar Cells with over 14% Efficiency. ACS Applied Energy Materials, 2020, 3, 11981-11991.	5.1	8
67	Design, synthesis and photophysical properties of D1-A-D2-A-D1-type small molecules based on fluorobenzotriazole acceptor and dithienosilole core donor for solution processed organic solar cells. Dyes and Pigments, 2016, 132, 387-397.	3.7	7
68	Thermomechanical Response of Supported Hexagonal Boron Nitride Sheets of Various Thicknesses. Journal of Physical Chemistry C, 2020, 124, 12134-12143.	3.1	7
69	Phononic bandgaps in graphene-based materials. Applied Physics Letters, 2012, 100, .	3.3	6
70	Dithienosiloleâ€“phenylquinoxalineâ€based copolymers with Aâ€Dâ€Aâ€D and Aâ€D structures for polymer solar cells. Journal of Polymer Science Part A, 2018, 56, 376-386.	2.3	6
71	Synthesis and Photovoltaic Properties of New Conjugated Dâ€A Polymers Based on the Same Fluoroâ€Benzothiadiazole Acceptor Unit and Different Donor Units. ChemistrySelect, 2020, 5, 853-863.	1.5	6
72	Mixed siliconâ€“germanium nanocrystals: a detailed study of Si x Ge47â^'x :H. Journal of Mathematical Chemistry, 2009, 46, 942-951.	1.5	5

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73	Synthesis and characterization of two carbazole-based alternating copolymers with 4-nitrophenylcyanovinylene pendant groups and their use as electron donors for bulk heterojunction solar cells. RSC Advances, 2013, 3, 18821.	3.6	5
74	Synthesis and photovoltaic properties of new donorâ€“acceptor (Dâ€“A) copolymers based on benzo[1,2-b:3,4-bâ€²:6,5-bâ€²â€²] trithiophene donor and different acceptor units (P1 and P2). RSC Advances, 2014, 4, 53531-53542.	3.6	5
75	Donor-Ï€-acceptor, triazine-linked porphyrin dyads as sensitizers for dye-sensitized solar cells. Journal of Porphyrins and Phthalocyanines, 2015, 19, 175-191.	0.8	5
76	Variation and adjustment of the optical gap of small Si nanocrystals by partial substitution of Si with Ge. Journal of Physics: Conference Series, 2005, 10, 101-104.	0.4	4
77	Theoretical study of oxygen contaminated silicon quantum dots: A case study for Si29H29âˆ'xO29âˆ'y. Microelectronic Engineering, 2013, 112, 227-230.	2.4	4
78	Computational Study of the Excitation Energies of CdSe Nanoparticles With Defects. IEEE Journal of Selected Topics in Quantum Electronics, 2017, 23, 1-5.	2.9	4
79	Confinement Effects on the Properties of Polar Hydrogen-Bonded Fluids: A Showcase on Methanol Adsorbed in Three-Dimensional Pillared Graphene and Carbon Nanotube Networks. Journal of Physical Chemistry C, 2020, 124, 22959-22971.	3.1	4
80	Theoretical study of the elasticity of ultra-thin finite silicon nanowires. I. Semiempirical model considerations. Microelectronic Engineering, 2012, 90, 88-91.	2.4	3
81	Synthesis and photophysical properties of semiconductor molecules D1-A-D2-A-D1-type structure based on derivatives of quinoxaline and dithienosilole for organics solar cells. Organic Electronics, 2016, 39, 361-370.	2.6	3
82	Absorption spectrum of magnesium and aluminum hydride nanoparticles. Materials Chemistry and Physics, 2019, 228, 244-253.	4.0	3
83	Novel effects in finiteâ€length silicon nanowires. Physica Status Solidi (A) Applications and Materials Science, 2008, 205, 2625-2629.	1.8	2
84	New ultra low bandgap thiadiazolequinoxaline-based D-A copolymers for photovoltaic applications. Organic Electronics, 2016, 37, 411-420.	2.6	2
85	Synthesis and photovoltaic properties of new Dâ€A copolymers based on 5,6â€bis(2â€ethylhexyl)naphtha[2,1â€b:3,4â€bâ€²]dithiopheneâ€2,9â€diyl] donor and fluorine substituted 6,7â€bis(9,9â€didodecylâ€9hâ€fluorenâ€2â€yl) [1,2,5] thiadiazolo[3,4â€g]quinoxaline acceptor units. Journal of Polymer Science Part A, 2018, 56, 1297-1307.	2.3	2
86	Hierarchy of nanoscale graphene wrinkles on compliant substrate: Theory and experiment. Extreme Mechanics Letters, 2020, 40, 100948.	4.1	2
87	New Highâ€Bandgap 8,10â€Dihydroâ€9 H â€Bistieno[2â€²,3â€²:7.8;3â€³,2â€³:5.6]Naphtho[2,3â€d] Imidazoleâ€9â€Oneâ€Based Donorâ€“Acceptor Copolymers for Nonfullerene Polymer Solar Cells. Energy Technology, 2020, 8, 2000611.	3.8	2
88	Impact of prolonged environmental exposure on stress transfer efficiency in poly(pâ€phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 1	4.6	2
89	The Impact of Ionic Liquid Loading in Three-Dimensional Carbon Nanotube Networks on the Separation of CO2/CH4 Fluid Mixtures: Insights from Molecular Simulations. Journal of Physical Chemistry C, 2021, 125, 13508-13522.	3.1	2
90	A Computational Study on Phenyldiboronic Acid-Pillared Graphene Oxide Frameworks for Gas Storage and Separation. ACS Applied Nano Materials, 2022, 5, 9286-9297.	5.0	2

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91	A Systematic Way for Obtaining the Structural and Electronic Properties of Silicon-Carbon Clusters of the Form Si[sub n]C[sub 2], nâ€‰=â€‰1â€“5. , 2009, , .		1
92	Multidecker Stacking and Cluster Fusion of Silicon-Carbon Clusters. , 2009, , .		1
93	Ab initio study of the siliconâ€“bismuth interface: Bismuth nanolines and bismuth-covered silicon nanoparticles. Microelectronic Engineering, 2012, 90, 99-103.	2.4	1
94	Systematic spatial and stoichiometric screening towards understanding the surface of ultrasmall oxygenated silicon nanocrystal. Applied Surface Science, 2016, 387, 771-778.	6.1	1
95	CF₄ Capture and Separation of CF₄â€“SF₆ and CF₄â€“N₂ Fluid Mixtures Using Selected Carbon Nanoporous Materials and Metalâ€“Organic Frameworks: A Computational Study. ACS Omega, 2022, 7, 6691-6699.	3.5	1
96	High-stability Finite-Length Silicon Nanowires: A Real Space Theoretical Study. AIP Conference Proceedings, 2007, , .	0.4	0
97	Electronic and Structural Properties of M@Si[sub 12] and M@Si[sub 12]H[sub 12] Clusters, Mâ€‰=â€‰Ni, Zn. AIP Conference Proceedings, 2007, , .	0.4	0
98	Elastic Properties of Ultra-Thin Hydrogenated Silicon Nanowires Based on all Electron Mixed ab initio and Semiempirical Calculations. , 2009, , .		0
99	Theoretical study of Si[sub 20]Li[sub 20] cage cluster. , 2012, , .		0
100	Ab initio Study of Optical and Electronic Properties of Silicon and Germanium Nanowires. , 2006, , 1174-1177.		0
101	Properties of Medium Hydrogenated Beryllium Nanoparticles. Journal of Nuclear Materials, 2022, , 153782.	2.7	0