

Emmanuel N. Koukaras

List of Publications by Year in descending order

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papers

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257450

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102
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102
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#	ARTICLE	IF	CITATIONS
1	CF ₄ Capture and Separation of CF ₄ and SF ₆ and CF ₄ and N ₂ Fluid Mixtures Using Selected Carbon Nanoporous Materials and Metal-Organic Frameworks: A Computational Study. ACS Omega, 2022, 7, 6691-6699.	3.5	1
2	Properties of Medium Hydrogenated Beryllium Nanoparticles. Journal of Nuclear Materials, 2022, , 153782.	2.7	0
3	A Computational Study on Phenylidiboronic Acid-Pillared Graphene Oxide Frameworks for Gas Storage and Separation. ACS Applied Nano Materials, 2022, 5, 9286-9297.	5.0	2
4	Impact of prolonged environmental exposure on stress transfer efficiency in poly(p-phenylene) Tj ETQq0 0 0 rgBT/Overlock_10 Tf 50 6	4.6	2
5	The Impact of Ionic Liquid Loading in Three-Dimensional Carbon Nanotube Networks on the Separation of CO ₂ /CH ₄ Fluid Mixtures: Insights from Molecular Simulations. Journal of Physical Chemistry C, 2021, 125, 13508-13522.	3.1	2
6	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
7	Synthesis and Photovoltaic Investigation of 8,10-Bis(2-octyldodecyl)-8,10-dihydro-9H-bistieno[2,3:7,8;3,2:5,6] naphtho[2,3-d]imidazol-9-one Based Conjugated Polymers Using a Nonfullerene Acceptor. ACS Applied Energy Materials, 2020, 3, 495-505.	5.1	10
8	Hierarchy of nanoscale graphene wrinkles on compliant substrate: Theory and experiment. Extreme Mechanics Letters, 2020, 40, 100948.	4.1	2
9	Indole-based DA 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
10	Doping-Induced Stacking Transition in Trilayer Graphene: Implications for Layer Stacking Manipulation. ACS Applied Nano Materials, 2020, 3, 11861-11868.	5.0	9
11	Porous carbon nanotube networks and pillared graphene materials exhibiting high SF ₆ adsorption uptake and separation selectivity of SF ₆ /N ₂ fluid mixtures: A comparative molecular simulation study. Microporous and Mesoporous Materials, 2020, 307, 110464.	4.4	16
12	Enhancement of photovoltaic efficiency through fine adjustment of indacene based nonfullerene acceptor by minimal chlorination for polymer solar cells. Nano Select, 2020, 1, 320-333.	3.7	11
13	New High-Bandgap 8,10-Dihydro-9H-bistieno[2,3:7,8;3,2:5,6]Naphtho[2,3-d]imidazole-9-one Based Donor-Acceptor Copolymers for Nonfullerene Polymer Solar Cells. Energy Technology, 2020, 8, 2000611.	3.8	2
14	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
15	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
16	DA type 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
17	Thermomechanical Response of Supported Hexagonal Boron Nitride Sheets of Various Thicknesses. Journal of Physical Chemistry C, 2020, 124, 12134-12143.	3.1	7
18	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

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19	New Donor-Acceptor polymers with a wide absorption range for photovoltaic applications. <i>Solar Energy</i> , 2020, 205, 211-220.	6.1	11
20	Tunable macroscale structural superlubricity in two-layer graphene via strain engineering. <i>Nature Communications</i> , 2020, 11, 1595.	12.8	88
21	Cardanol- and Guaiacol-Sourced Solution-Processable Green Small Molecule-Based Organic Solar Cells. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 5891-5902.	6.7	14
22	Synthesis and Photovoltaic Properties of New Conjugated D π A Polymers Based on the Same Fluoro π Benzothiadiazole Acceptor Unit and Different Donor Units. <i>ChemistrySelect</i> , 2020, 5, 853-863.	1.5	6
23	Absorption spectrum of magnesium and aluminum hydride nanoparticles. <i>Materials Chemistry and Physics</i> , 2019, 228, 244-253.	4.0	3
24	Sculpturing graphene wrinkle patterns into compliant substrates. <i>Carbon</i> , 2019, 146, 772-778.	10.3	18
25	Stress-transfer from polymer substrates to monolayer and few-layer graphenes. <i>Nanoscale Advances</i> , 2019, 1, 4972-4980.	4.6	14
26	Synthesis and photovoltaic properties of new D π A copolymers based on 5,6-bis(2-ethylhexyl)naphtha[2,1-b:3,4-b π 2]dithiophene π 2,9-diyl donor and fluorine substituted 6,7-bis(9,9-didodecyl π 9-h π fluorena π 2-yl)[1,2,5]thiadiazolo[3,4-cg]quinoxaline acceptor units. <i>Journal of Polymer Science Part A</i> , 2018, 56, 1297-1307.	2.3	2
27	BODIPY π -diketopyrrolopyrrole π porphyrin conjugate small molecules for use in bulk heterojunction solar cells. <i>Journal of Materials Chemistry A</i> , 2018, 6, 8449-8461.	10.3	45
28	Dithienosilole π -phenylquinoxaline π based copolymers with A π D π A π D and A π D structures for polymer solar cells. <i>Journal of Polymer Science Part A</i> , 2018, 56, 376-386.	2.3	6
29	Strained hexagonal boron nitride: Phonon shift and Gr π 4neisen parameter. <i>Physical Review B</i> , 2018, 97, .	3.2	51
30	Non-Eulerian behavior of graphitic materials under compression. <i>Carbon</i> , 2018, 138, 227-233.	10.3	13
31	<i>Ab initio</i> study of medium sized boron-doped silicon clusters Si π _n B π _m , π _n = 11 π 13, π _m = 1 π 3. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18556-18570.	2.8	12
32	Computational Study of the Excitation Energies of CdSe Nanoparticles With Defects. <i>IEEE Journal of Selected Topics in Quantum Electronics</i> , 2017, 23, 1-5.	2.9	4
33	Polymer solar cells based low bandgap A1-D-A2-D terpolymer based on fluorinated thiadiazoloquinoxaline and benzothiadiazole acceptors with energy loss less than 0.5 eV. <i>Organic Electronics</i> , 2017, 46, 192-202.	2.6	11
34	Wrinkled Few-Layer Graphene as Highly Efficient Load Bearer. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 26593-26601.	8.0	46
35	Wrinkling formation in simply-supported graphenes under tension and compression loadings. <i>Nanoscale</i> , 2017, 9, 18180-18188.	5.6	31
36	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. <i>Dyes and Pigments</i> , 2016, 132, 387-397.	3.7	7

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37	New alternating D ¹ -A ² copolymer containing two electron-deficient moieties based on benzothiadiazole and 9-(2-octyldodecyl)pyrrolo[3,4-b]bisthieno[2,3-f':3',2'-h']quinoxaline for efficient polymer solar cells. <i>Journal of Polymer Science Part A</i> , 2016, 54, 155-168.	3.9	10
38	Synthesis of alternating D ¹ -A ² terpolymers comprising two electron-deficient moieties, quinoxaline and benzothiadiazole units for photovoltaic applications. <i>Polymer Chemistry</i> , 2016, 7, 4025-4035.	3.9	11
39	Design of diketopyrrolopyrrole chromophores applicable as sensitizers in dye-sensitized photovoltaic windows for green houses. <i>Dyes and Pigments</i> , 2016, 134, 472-479.	3.7	20
40	New ultra low bandgap thiadiazolequinoxaline-based D-A copolymers for photovoltaic applications. <i>Organic Electronics</i> , 2016, 37, 411-420.	2.6	2
41	Synthesis and photophysical properties of regioregular low bandgap copolymers with controlled 5-fluorobenzotriazole orientation for photovoltaic application. <i>Polymer Chemistry</i> , 2016, 7, 5849-5861.	3.9	11
42	New D-A ¹ -D-A ² -Type Regular Terpolymers Containing Benzothiadiazole and Benzotrithiophene Acceptor Units for Photovoltaic Application. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 32998-33009.	8.0	18
43	Synthesis of new D-A ¹ -D-A ² type low bandgap terpolymers based on different thiadiazoloquinoxaline acceptor units for efficient polymer solar cells. <i>RSC Advances</i> , 2016, 6, 71232-71244.	3.6	11
44	Systematic spatial and stoichiometric screening towards understanding the surface of ultrasmall oxygenated silicon nanocrystal. <i>Applied Surface Science</i> , 2016, 387, 771-778.	6.1	1
45	Graphene flakes under controlled biaxial deformation. <i>Scientific Reports</i> , 2016, 5, 18219.	3.3	84
46	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. <i>Organic Electronics</i> , 2016, 39, 361-370.	2.6	3
47	Long-lived discrete breathers in free-standing graphene. <i>Chaos, Solitons and Fractals</i> , 2016, 87, 262-267.	5.1	20
48	Design and synthesis of new ultra-low band gap thiadiazoloquinoxaline-based polymers for near-infrared organic photovoltaic application. <i>RSC Advances</i> , 2016, 6, 14893-14908.	3.6	26
49	Compression behavior of simply-supported and fully embedded monolayer graphene: Theory and experiment. <i>Extreme Mechanics Letters</i> , 2016, 8, 191-200.	4.1	17
50	New low bandgap near-IR conjugated D ¹ -A copolymers for BHJ polymer solar cell applications. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8389-8400.	2.8	18
51	Fully Hydrogenated Beryllium Nanoclusters. <i>Journal of the American Chemical Society</i> , 2016, 138, 3218-3227.	13.7	8
52	Phonon properties of graphene derived from molecular dynamics simulations. <i>Scientific Reports</i> , 2015, 5, 12923.	3.3	113
53	Study of an indoline-phenothiazine based organic dye for Dye-Sensitized Solar Cells. Theoretical calculations and experimental data. <i>Organic Electronics</i> , 2015, 25, 66-73.	2.6	29
54	Stress Transfer Mechanisms at the Submicron Level for Graphene/Polymer Systems. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 4216-4223.	8.0	105

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55	Solution processed organic solar cells based on Aâ€“Dâ€“Dâ€“A small molecule with benzo[1,2-b:4,5-bâ€“]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
56	Donor-â€“acceptor, triazine-linked porphyrin dyads as sensitizers for dye-sensitized solar cells. Journal of Porphyrins and Phthalocyanines, 2015, 19, 175-191.	0.8	5
57	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€“]thiophene units. Organic Electronics, 2015, 26, 36-47.	2.6	17
58	Suspended monolayer graphene under true uniaxial deformation. Nanoscale, 2015, 7, 13033-13042.	5.6	52
59	Aâ€“â€“Dâ€“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
60	Graphene Mechanics: Current Status and Perspectives. Annual Review of Chemical and Biomolecular Engineering, 2015, 6, 121-140.	6.8	76
61	Characterization of metal-free D-(â€“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
62	Efficient bulk heterojunction solar cells based on solution processed small molecules based on the same benzo[1,2-b:4,5-bâ€“]thiophene unit as core donor and different terminal units. Nanoscale, 2015, 7, 7692-7703.	5.6	18
63	Donor-â€“acceptor-â€“acceptor-â€“donor small molecules for solution processed bulk heterojunction solar cells. Organic Electronics, 2015, 27, 72-83.	2.6	24
64	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
65	Chitosan derivatives as effective nanocarriers for ocular release of timolol drug. International Journal of Pharmaceutics, 2015, 495, 249-264.	5.2	76
66	Synthesis, optical and electrochemical properties new donor-â€“acceptor (Dâ€“A) copolymers based on benzo[1,2-b:3,4-bâ€“: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
67	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
68	Synthesis, optical and electrochemical properties of the Aâ€“â€“Dâ€“â€“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
69	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
70	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
71	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
72	Synthesis and photovoltaic properties of new donor-â€“acceptor (Dâ€“A) copolymers based on benzo[1,2-b:3,4-bâ€“:6,5-bâ€“ ²] trithiophene donor and different acceptor units (P1 and P2). RSC Advances, 2014, 4, 53531-53542.	3.4	5

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73	Size dependence of the structural, electronic, and optical properties of (CdSe) _n , n = 6–60, nanocrystals. RSC Advances, 2014, 4, 14613-14623.	3.6	21
74	Toward Efficient Drug Delivery through Suitably Prepared Metal–Organic Frameworks: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 8885-8890.	3.1	37
75	Properties and energetics for design and characterization of chitosan nanoparticles used for drug encapsulation. RSC Advances, 2014, 4, 12653.	3.6	18
76	Failure Processes in Embedded Monolayer Graphene under Axial Compression. Scientific Reports, 2014, 4, 5271.	3.3	65
77	Size dependence of the optical gap of silicon quantum dots: Ab initio and empirical correlation schemes. Microelectronic Engineering, 2013, 112, 231-234.	2.4	8
78	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
79	Theoretical study of oxygen contaminated silicon quantum dots: A case study for Si ₂₉ H ₂₉ xO ₂₉ y. Microelectronic Engineering, 2013, 112, 227-230.	2.4	4
80	Synthesis and characterization of a low band gap quinoxaline based D–A copolymer and its application as a donor for bulk heterojunction polymer solar cells. Polymer Chemistry, 2013, 4, 4033.	3.9	33
81	Theoretical study of Si ₂₀ Li ₂₀ cage cluster. , 2012, , .		0
82	Phononic bandgaps in graphene-based materials. Applied Physics Letters, 2012, 100, .	3.3	6
83	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
84	Insight on the Formation of Chitosan Nanoparticles through Ionotropic Gelation with Tripolyphosphate. Molecular Pharmaceutics, 2012, 9, 2856-2862.	4.6	177
85	Theoretical study of the elasticity of ultra-thin finite silicon nanowires. I. Semiempirical model considerations. Microelectronic Engineering, 2012, 90, 88-91.	2.4	3
86	Ab initio study of the silicon–bismuth interface: Bismuth nanolines and bismuth-covered silicon nanoparticles. Microelectronic Engineering, 2012, 90, 99-103.	2.4	1
87	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
88	Theoretical Study of Amino Acid Interaction with Metal Organic Frameworks. Journal of Physical Chemistry Letters, 2011, 2, 272-275.	4.6	16
89	Elastic Properties of Ultra-Thin Hydrogenated Silicon Nanowires Based on all Electron Mixed ab initio and Semiempirical Calculations. , 2009, , .		0
90	A Systematic Way for Obtaining the Structural and Electronic Properties of Silicon-Carbon Clusters of the Form Si _n C ₂ , n = 5. , 2009, , .		1

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91	A parallel study of Ni@Si ₁₂ and Cu@Si ₁₂ nanoclusters. Journal of Mathematical Chemistry, 2009, 46, 971-980.	1.5	11
92	Mixed silicon-germanium nanocrystals: a detailed study of Si _x Ge _{47-x} H. Journal of Mathematical Chemistry, 2009, 46, 942-951.	1.5	5
93	Multidecker Sandwiches of Silicon-Carbon Clusters. Organometallics, 2009, 28, 4308-4315.	2.3	11
94	Multidecker Stacking and Cluster Fusion of Silicon-Carbon Clusters. , 2009, , .		1
95	Novel effects in finite-length silicon nanowires. Physica Status Solidi (A) Applications and Materials Science, 2008, 205, 2625-2629.	1.8	2
96	Structural properties and magic structures in hydrogenated finite and infinite silicon nanowires. Applied Physics Letters, 2007, 91, 203112.	3.3	16
97	High-stability Finite-Length Silicon Nanowires: A Real Space Theoretical Study. AIP Conference Proceedings, 2007, , .	0.4	0
98	Electronic and Structural Properties of M@Si ₁₂ and M@Si ₁₂ H ₁₂ Clusters, M=Ni, Zn. AIP Conference Proceedings, 2007, , .	0.4	0
99	Structure and properties of the Ni@Si ₁₂ cluster from all-electron ab initio calculations. Physical Review B, 2006, 73, .	3.2	43
100	Ab initio Study of Optical and Electronic Properties of Silicon and Germanium Nanowires. , 2006, , 1174-1177.		0
101	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