

Douglas S. Galvao

List of Publications by Year in descending order

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216
papers

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citations

46918

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9923
citing authors

#	ARTICLE	IF	CITATIONS
1	Electrically, Chemically, and Photonically Powered Torsional and Tensile Actuation of Hybrid Carbon Nanotube Yarn Muscles. <i>Science</i> , 2012, 338, 928-932.	6.0	585
2	Hierarchically buckled sheath-core fibers for superelastic electronics, sensors, and muscles. <i>Science</i> , 2015, 349, 400-404.	6.0	447
3	Molecular-Dynamics Simulations of Carbon Nanotubes as Gigahertz Oscillators. <i>Physical Review Letters</i> , 2003, 90, 055504.	2.9	342
4	Structure and Dynamics of Carbon Nanoscrolls. <i>Nano Letters</i> , 2004, 4, 881-884.	4.5	296
5	Exfoliation of a non-van der Waals material from iron ore hematite. <i>Nature Nanotechnology</i> , 2018, 13, 602-609.	15.6	295
6	Sign Change of Poisson's Ratio for Carbon Nanotube Sheets. <i>Science</i> , 2008, 320, 504-507.	6.0	245
7	Crystalline networks with unusual predicted mechanical and thermal properties. <i>Nature</i> , 1993, 365, 735-737.	13.7	224
8	Graphene to graphane: a theoretical study. <i>Nanotechnology</i> , 2009, 20, 465704.	1.3	219
9	Chemical Vapor Deposition of Monolayer Rhenium Disulfide (ReS ₂). <i>Advanced Materials</i> , 2015, 27, 4640-4648.	11.1	203
10	Surface functionalization of two-dimensional metal chalcogenides by Lewis acid-base chemistry. <i>Nature Nanotechnology</i> , 2016, 11, 465-471.	15.6	197
11	Families of carbon nanotubes: Graphyne-based nanotubes. <i>Physical Review B</i> , 2003, 68, .	1.1	185
12	Nonzero Gap Two-Dimensional Carbon Allotrope from Porous Graphene. <i>Journal of Physical Chemistry C</i> , 2012, 116, 12810-12813.	1.5	152
13	Torsional refrigeration by twisted, coiled, and supercoiled fibers. <i>Science</i> , 2019, 366, 216-221.	6.0	133
14	Lock-and-key effect in the surface diffusion of large organic molecules probed by STM. <i>Nature Materials</i> , 2004, 3, 779-782.	13.3	116
15	New families of carbon nanotubes based on graphyne motifs. <i>Nanotechnology</i> , 2004, 15, S142-S149.	1.3	116
16	Gigahertz nanomechanical oscillators based on carbon nanotubes. <i>Nanotechnology</i> , 2004, 15, S184-S189.	1.3	112
17	On the Structural and Stability Features of Linear Atomic Suspended Chains Formed from Gold Nanowires Stretching. <i>Nano Letters</i> , 2004, 4, 1187-1191.	4.5	106
18	Indication of Unusual Pentagonal Structures in Atomic-Size Cu Nanowires. <i>Physical Review Letters</i> , 2004, 93, 126103.	2.9	105

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19	Excitation and relaxation energies of trans-stilbene: Confined singlet, triplet, and charged bipolarons. <i>Physical Review B</i> , 1993, 47, 1742-1753.	1.1	101
20	Graphene Supported MoS ₂ Structures with High Defect Density for an Efficient HER Electrocatalysts. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 12629-12638.	4.0	101
21	Strong, Twist-Stable Carbon Nanotube Yarns and Muscles by Tension Annealing at Extreme Temperatures. <i>Advanced Materials</i> , 2016, 28, 6598-6605.	11.1	100
22	Prediction of the hydrogen storage capacity of carbon nanoscrolls. <i>Physical Review B</i> , 2007, 75, .	1.1	98
23	Experimental realization of suspended atomic chains composed of different atomic species. <i>Nature Nanotechnology</i> , 2006, 1, 182-185.	15.6	95
24	Low-density three-dimensional foam using self-reinforced hybrid two-dimensional atomic layers. <i>Nature Communications</i> , 2014, 5, 4541.	5.8	91
25	Prediction of Ordered Phases of Encapsulated C ₆₀ , C ₇₀ , and C ₇₈ Inside Carbon Nanotubes. <i>Nano Letters</i> , 2005, 5, 349-355.	4.5	85
26	Mechanical Properties of Nanosprings. <i>Physical Review Letters</i> , 2004, 92, 175502.	2.9	82
27	Synthesis of Low-Density, Carbon-Doped, Porous Hexagonal Boron Nitride Solids. <i>ACS Nano</i> , 2015, 9, 12088-12095.	7.3	81
28	Inorganic Graphenylene: A Porous Two-Dimensional Material With Tunable Band Gap. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23670-23674.	1.5	76
29	Multiscale Geometric Design Principles Applied to 3D Printed Schwarzites. <i>Advanced Materials</i> , 2018, 30, 1704820.	11.1	76
30	Geometric and electronic structure of carbon nanotube networks: $\sqrt{3}$ -carbon nanotubes. <i>Nanotechnology</i> , 2006, 17, 617-621.	1.3	74
31	Theoretical investigation of electromechanical effects for graphyne carbon nanotubes. <i>Journal of Chemical Physics</i> , 2004, 121, 3228-3237.	1.2	72
32	Atomistic simulations of the mechanical properties of $\sqrt{3}$ carbon nanotubes. <i>Nanotechnology</i> , 2007, 18, 335702.	1.3	72
33	Graphene to fluorographene and fluorographane: a theoretical study. <i>Nanotechnology</i> , 2013, 24, 035706.	1.3	69
34	Fullerenynes: a new family of porous fullerenes. <i>Chemical Physics Letters</i> , 1993, 204, 8-14.	1.2	67
35	Designing nanoscaled hybrids from atomic layered boron nitride with silver nanoparticle deposition. <i>Journal of Materials Chemistry A</i> , 2014, 2, 3148.	5.2	65
36	Prediction of giant electroactuation for papyruslike carbon nanoscroll structures: First-principles calculations. <i>Physical Review B</i> , 2006, 74, .	1.1	63

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37	Unzipping Carbon Nanotubes at High Impact. Nano Letters, 2014, 14, 4131-4137.	4.5	63
38	Curved graphene nanoribbons: structure and dynamics of carbon nanobelts. Nanotechnology, 2010, 21, 075710.	1.3	59
39	Mechanical properties and fracture dynamics of silicene membranes. Physical Chemistry Chemical Physics, 2014, 16, 19417-19423.	1.3	56
40	Lightweight Hexagonal Boron Nitride Foam for CO ₂ Absorption. ACS Nano, 2017, 11, 8944-8952.	7.3	56
41	Möbius and twisted graphene nanoribbons: Stability, geometry, and electronic properties. Journal of Chemical Physics, 2008, 128, 164719.	1.2	54
42	Deformation Mechanisms of Vertically Stacked WS ₂ /MoS ₂ Heterostructures: The Role of Interfaces. ACS Nano, 2018, 12, 4036-4044.	7.3	54
43	3D Porous Graphene by Low-Temperature Plasma Welding for Bone Implants. Advanced Materials, 2016, 28, 8959-8967.	11.1	52
44	Molecular dynamics simulations of C60 nanobearings. Chemical Physics Letters, 2004, 386, 425-429.	1.2	51
45	The structure and dynamics of boron nitride nanoscrolls. Nanotechnology, 2009, 20, 335702.	1.3	51
46	Gas Adsorption and Separation by the Al-Based Metal-Organic Framework MIL-160. Journal of Physical Chemistry C, 2017, 121, 26822-26832.	1.5	51
47	Observation of the smallest metal nanotube with a square cross-section. Nature Nanotechnology, 2009, 4, 149-152.	15.6	50
48	Mechanical properties of carbon nanotube networks by molecular mechanics and impact molecular dynamics calculations. Physical Review B, 2007, 75, .	1.1	49
49	Linear Carbon Chains under High-Pressure Conditions. Journal of Physical Chemistry C, 2015, 119, 10669-10676.	1.5	46
50	Scale Effects on the Ballistic Penetration of Graphene Sheets. Scientific Reports, 2018, 8, 6750.	1.6	46
51	Synthesis and porous h-BN 3D architectures for effective humidity and gas sensors. RSC Advances, 2016, 6, 87888-87896.	1.7	43
52	Modeling the auxetic transition for carbon nanotube sheets. Physical Review B, 2008, 78, .	1.1	42
53	Entanglement and the Nonlinear Elastic Behavior of Forests of Coiled Carbon Nanotubes. Physical Review Letters, 2008, 100, 086807.	2.9	42
54	Synthetic melanin films: Assembling mechanisms, scaling behavior, and structural properties. Journal of Applied Physics, 2006, 99, 113511.	1.1	41

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55	On the unzipping of multiwalled carbon nanotubes. <i>Nanotechnology</i> , 2012, 23, 465702.	1.3	39
56	Controlled route to the fabrication of carbon and boron nitride nanoscrolls: A molecular dynamics investigation. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	38
57	Scalable Synthesis of Atomically Thin Gallium Telluride Nanosheets for Supercapacitor Applications. <i>ACS Applied Nano Materials</i> , 2021, 4, 4829-4838.	2.4	38
58	Structural and Thermal Stability of Graphyne and Graphdiyne Nanoscroll Structures. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 2670-2676.	4.0	36
59	Ambient solid-state mechano-chemical reactions between functionalized carbon nanotubes. <i>Nature Communications</i> , 2015, 6, 7291.	5.8	35
60	Enhanced supercapacitor performance of a 3D architecture tailored using atomically thin rGO@MoS ₂ 2D sheets. <i>RSC Advances</i> , 2016, 6, 93384-93393.	1.7	35
61	Chaotic signature in the motion of coupled carbon nanotube oscillators. <i>Nanotechnology</i> , 2005, 16, 583-589.	1.3	34
62	Contaminants in Suspended Gold Chains: An Ab Initio Molecular Dynamics Study. <i>Physical Review Letters</i> , 2004, 93, 216103.	2.9	32
63	A Brief Review on Syntheses, Structures, and Applications of Nanoscrolls. <i>Frontiers in Materials</i> , 2014, 1, .	1.2	31
64	Evaluation of carbon nanoscroll materials for post-combustion CO ₂ capture. <i>Carbon</i> , 2016, 101, 218-225.	5.4	31
65	Apparent Ferromagnetism in Exfoliated Ultrathin Pyrite Sheets. <i>Journal of Physical Chemistry C</i> , 2021, 125, 18927-18935.	1.5	30
66	Graphene healing mechanisms: A theoretical investigation. <i>Carbon</i> , 2016, 99, 302-309.	5.4	29
67	Mechanical Deformation of Nanoscale Metal Rods: When Size and Shape Matter. <i>Physical Review Letters</i> , 2011, 106, 055501.	2.9	28
68	Design of Porous Metal-Organic Frameworks for Adsorption Driven Thermal Batteries. <i>MRS Advances</i> , 2017, 2, 519-524.	0.5	28
69	Transmission electron microscopy and molecular dynamics study of the formation of suspended copper linear atomic chains. <i>Physical Review B</i> , 2006, 74, .	1.1	27
70	Defects in Graphene-Based Twisted Nanoribbons: Structural, Electronic, and Optical Properties. <i>Langmuir</i> , 2009, 25, 4751-4759.	1.6	26
71	Burning Graphene Layer-by-Layer. <i>Scientific Reports</i> , 2015, 5, 11546.	1.6	26
72	Controlled 3D Carbon Nanotube Structures by Plasma Welding. <i>Advanced Materials Interfaces</i> , 2016, 3, 1500755.	1.9	25

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73	On the Mechanical Properties and Thermal Stability of a Recently Synthesized Monolayer Amorphous Carbon. <i>Journal of Physical Chemistry C</i> , 2020, 124, 14855-14860.	1.5	25
74	Synthesis and 3D Interconnected Nanostructured h-BN-Based Biocomposites by Low-Temperature Plasma Sintering: Bone Regeneration Applications. <i>ACS Omega</i> , 2018, 3, 6013-6021.	1.6	24
75	3D Printed Tubulanes as Lightweight Hypervelocity Impact Resistant Structures. <i>Small</i> , 2019, 15, e1904747.	5.2	24
76	Ordered phases of encapsulated diamondoids into carbon nanotubes. <i>Nanotechnology</i> , 2011, 22, 315708.	1.3	22
77	Carbon Nanotubes as Reinforcement Elements of Composite Nanotools. <i>Nano Letters</i> , 2008, 8, 842-847.	4.5	21
78	Intrinsic Stability of the Smallest Possible Silver Nanotube. <i>Physical Review Letters</i> , 2011, 106, 065501.	2.9	21
79	Enhanced Mechanical Stability of Gold Nanotips through Carbon Nanocone Encapsulation. <i>Scientific Reports</i> , 2015, 5, 10408.	1.6	21
80	Liquid Exfoliation of Icosahedral Quasicrystals. <i>Advanced Functional Materials</i> , 2018, 28, 1801181.	7.8	21
81	Thermophoretically driven carbon nanotube oscillators. <i>Applied Physics Letters</i> , 2009, 95, .	1.5	20
82	Defect-Free Carbon Nanotube Coils. <i>Nano Letters</i> , 2016, 16, 2152-2158.	4.5	20
83	High Toughness in Ultralow Density Graphene Oxide Foam. <i>Advanced Materials Interfaces</i> , 2017, 4, 1700030.	1.9	20
84	Virtually imprinted polymers (VIPs): understanding molecularly templated materials via molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13145-13152.	1.3	19
85	Extraction of Two-Dimensional Aluminum Alloys from Decagonal Quasicrystals. <i>ACS Nano</i> , 2020, 14, 7435-7443.	7.3	19
86	Identifying Relevant Molecular Descriptors Related to Carcinogenic Activity of Polycyclic Aromatic Hydrocarbons (PAHs) Using Pattern Recognition Methods. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 1479-1489.	2.8	18
87	Mechanical properties of amorphous nanosprings. <i>Nanotechnology</i> , 2006, 17, 5620-5626.	1.3	18
88	Temperature effects on the atomic arrangement and conductance of atomic-size gold nanowires generated by mechanical stretching. <i>Nanotechnology</i> , 2010, 21, 485702.	1.3	18
89	On the mechanical properties of novamene: A fully atomistic molecular dynamics and DFT investigation. <i>Carbon</i> , 2018, 139, 782-788.	5.4	18
90	Two-dimensional cobalt telluride as a piezo-tribogenerator. <i>Nanoscale</i> , 2022, 14, 7788-7797.	2.8	18

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91	A Structure-Activity Study of Taxol, Taxotere, and Derivatives Using the Electronic Indices Methodology (EIM). <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 699-706.	2.8	17
92	Carbon nanotube with square cross-section: An <i>ab initio</i> investigation. <i>Journal of Chemical Physics</i> , 2010, 133, 124513.	1.2	17
93	Mechanical and energy-absorption properties of schwarzites. <i>Carbon</i> , 2020, 157, 670-680.	5.4	17
94	Size Limit of Defect Formation in Pyramidal Pt Nanocontacts. <i>Physical Review Letters</i> , 2007, 99, 255501.	2.9	16
95	Ballistic Fracturing of Carbon Nanotubes. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 24819-24825.	4.0	16
96	Band gap engineering for poly(p-phenylene) and poly(p-phenylene vinylene) copolymers using the tight-binding approach. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 588-596.	1.0	15
97	Elastic properties of nanowires. <i>Journal of Applied Physics</i> , 2006, 99, 094310.	1.1	15
98	Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 236222.	0.7	15
99	The structural and dynamical aspects of boron nitride nanotubes under high velocity impacts. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14776-14781.	1.3	15
100	Structural transformations of carbon and boron nitride nanoscrolls at high impact collisions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4911-4916.	1.3	15
101	Tuning Penta-Graphene Electronic Properties Through Engineered Line Defects. <i>Scientific Reports</i> , 2020, 10, 8014.	1.6	15
102	Experimental and computational investigation of reduced graphene oxide nanoplatelets stabilized in poly(styrene sulfonate) sodium salt. <i>Journal of Materials Science</i> , 2018, 53, 10049-10058.	1.7	14
103	Few-Wall Carbon Nanotube Coils. <i>Nano Letters</i> , 2020, 20, 953-962.	4.5	14
104	New Zero Poisson's Ratio Structures. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020, 14, 1900564.	1.2	14
105	On the mechanical properties of atomic and 3D printed zeolite-templated carbon nanotube networks. <i>Additive Manufacturing</i> , 2021, 37, 101628.	1.7	14
106	On the mechanical properties and fracture patterns of the nonbenzenoid carbon allotrope (biphenylene network): a reactive molecular dynamics study. <i>Nanoscale</i> , 2022, 14, 3200-3211.	2.8	14
107	Molecular dynamics simulation of single wall carbon nanotubes polymerization under compression. <i>Journal of Computational Chemistry</i> , 2007, 28, 1724-1734.	1.5	13
108	Strain-Induced Structural Deformation Study of 2D Mo ₂ W ₂ (1-x) ₂ S ₂ . <i>Advanced Materials Interfaces</i> , 2019, 6, 1801262.	1.9	13

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109	Correlation between quantum conductance and atomic arrangement of atomic-size silver nanowires. <i>Journal of Applied Physics</i> , 2012, 111, 124316.	1.1	12
110	Structural and optical properties of plasma-deposited amorphous hydrogenated oxygenated carbon films. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1997, 15, 1334-1339.	0.9	11
111	Novel Nanoscroll Structures from Carbon Nitride Layers. <i>ChemPhysChem</i> , 2014, 15, 2367-2371.	1.0	11
112	On the mechanical properties of protomene: A theoretical investigation. <i>Computational Materials Science</i> , 2019, 161, 190-198.	1.4	11
113	Idealized Carbon-Based Materials Exhibiting Record Deliverable Capacities for Vehicular Methane Storage. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1050-1058.	1.5	11
114	Emergence of Prime Numbers as the Result of Evolutionary Strategy. <i>Physical Review Letters</i> , 2004, 93, 098107.	2.9	10
115	Rotational dynamics and polymerization of C ₆₀ in C ₆₀ -cubane crystals: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2008, 129, 064506.	1.2	10
116	Dynamics of the Formation of Carbon Nanotube Serpentine. <i>Physical Review Letters</i> , 2013, 110, 105502.	2.9	10
117	Mechanical Properties of Pentagraphene-based Nanotubes: A Molecular Dynamics Study. <i>MRS Advances</i> , 2018, 3, 97-102.	0.5	10
118	Gas-Phase Fluorination of Hexagonal Boron Nitride. <i>Advanced Materials</i> , 2021, 33, e2106084.	11.1	10
119	Some electronic properties of saturated and unsaturated cubane oligomers using DFT-based calculations. <i>Computational and Theoretical Chemistry</i> , 2008, 868, 37-41.	1.5	9
120	Efficient prediction of suitable functional monomers for molecular imprinting via local density of states calculations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13153-13158.	1.3	9
121	Mechanical Properties of Diamond Schwarzites: From Atomistic Models to 3D-Printed Structures. <i>MRS Advances</i> , 2020, 5, 1775-1781.	0.5	9
122	Mechanical response of pentadiamond: A DFT and molecular dynamics study. <i>Physica B: Condensed Matter</i> , 2022, 629, 413576.	1.3	9
123	Spatially variable reaction in the formation of anodically grown porous silicon structures. <i>Journal of Applied Physics</i> , 1995, 78, 590-592.	1.1	8
124	C ₆₀ -derived nanobaskets: stability, vibrational signatures, and molecular trapping. <i>Nanotechnology</i> , 2009, 20, 395701.	1.3	8
125	Temperature effects on the occurrence of long interatomic distances in atomic chains formed from stretched gold nanowires. <i>Nanotechnology</i> , 2011, 22, 095705.	1.3	8
126	One-dimensional silicon and germanium nanostructures with no carbon analogues. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24570-24574.	1.3	8

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127	Schwarzites for Natural Gas Storage: A Grand-Canonical Monte Carlo Study. MRS Advances, 2018, 3, 115-120.	0.5	8
128	A reactive molecular dynamics study on the mechanical properties of a recently synthesized amorphous carbon monolayer converted into a nanotube/nanoscroll. Physical Chemistry Chemical Physics, 2021, 23, 9089-9095.	1.3	8
129	Enhancement in magnetization of two-dimensional cobalt telluride and its magnetic field-assisted photocatalytic activity. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	1.1	8
130	A semiempirical study on the electronic structure of 10-deacetylbaocatin-III. Journal of Molecular Graphics and Modelling, 2002, 21, 57-70.	1.3	7
131	Comparative parametric method 6 (PM6) and Recife model 1 (RM1) study of <i>trans</i> -stilbene. Molecular Simulation, 2012, 38, 1-7.	0.9	7
132	Multifunctional Hybrids Based on 2D Fluorinated Graphene Oxide and Superparamagnetic Iron Oxide Nanoparticles. Particle and Particle Systems Characterization, 2017, 34, 1700245.	1.2	7
133	Mechanical Properties of Schwarzites - A Fully Atomistic Reactive Molecular Dynamics Investigation. MRS Advances, 2018, 3, 451-456.	0.5	7
134	Thiophene-Tetrathia-Annulene monolayer (TTA-2D): A new 2D semiconductor material with indirect bandgap. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 129, 114586.	1.3	7
135	Mechanical properties of 3D printed macroscopic models of schwarzites. Nano Select, 2022, 3, 450-458.	1.9	7
136	Synthesis and Characterization of Biotene: A New 2D Natural Oxide From Biotite. Small, 2022, 18, .	5.2	7
137	Effects of chlorine gas exposure on the optical properties of rhodium phthalocyanine films. Solid State Communications, 2004, 131, 53-56.	0.9	6
138	Structural and electronic properties of radialenes and related systems. Computational and Theoretical Chemistry, 2005, 729, 203-210.	1.5	6
139	Dynamical aspects of the unzipping of multiwalled boron nitride nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 19147.	1.3	6
140	Graphyne Oxidation: Insights From a Reactive Molecular Dynamics Investigation. Materials Research Society Symposia Proceedings, 2013, 1549, 53-58.	0.1	6
141	Solid-Liquid Self-Adaptive Polymeric Composite. ACS Applied Materials & Interfaces, 2016, 8, 2142-2147.	4.0	6
142	Mechanical Properties of Phagraphene Membranes: A Fully Atomistic Molecular Dynamics Investigation. MRS Advances, 2018, 3, 67-72.	0.5	6
143	On the elastic properties of single-walled phagraphene nanotubes. Chemical Physics Letters, 2020, 756, 137830.	1.2	6
144	Three-dimensional carbon nanotube networks from beta zeolite templates: Thermal stability and mechanical properties. Computational Materials Science, 2020, 182, 109781.	1.4	6

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145	Semiempirical studies of the electronic structure of polyphenylene sulfide phenyleneamine. International Journal of Quantum Chemistry, 2003, 95, 252-259.	1.0	5
146	Benzo[c]quinolizin-3-ones Theoretical Investigation: SAR Analysis and Application to Nontested Compounds. Journal of Chemical Information and Computer Sciences, 2004, 44, 1987-1997.	2.8	5
147	Water/Alcohol Separation in Graphene Oxide Membranes: Insights from Molecular Dynamics and Monte Carlo Simulations. MRS Advances, 2018, 3, 109-114.	0.5	5
148	On hardening silver nanocubes by high-velocity impacts: a fully atomistic molecular dynamics investigation. Journal of Materials Science, 2018, 53, 7486-7492.	1.7	5
149	Temperature Effects on the Fracture Dynamics and Elastic Properties of Popgraphene Membranes. ChemPhysChem, 2020, 21, 1918-1924.	1.0	5
150	On the Mechanical Properties of Popgraphene-Based Nanotubes: a Reactive Molecular Dynamics Study. ChemPhysChem, 2021, 22, 701-707.	1.0	5
151	A dual-mode photoswitching mechanism and charge transfer on chiroptical systems theoretical study. Synthetic Metals, 2001, 116, 275-279.	2.1	4
152	Is it possible to grow amorphous normal nanosprings?. Nanotechnology, 2007, 18, 435606.	1.3	4
153	Large electromechanical response in silicon nanowires predicted from first-principles electronic structure calculations. Physical Review B, 2008, 77, .	1.1	4
154	New Insights on the Growth of Anisotropic Nanoparticles from Total Energy Calculations. Journal of Physical Chemistry C, 2009, 113, 11976-11979.	1.5	4
155	Topologically Closed Macromolecules Made of Single Walled Carbon Nanotubes "Super'-Fullerenes. Journal of Nanoscience and Nanotechnology, 2010, 10, 4378-4383.	0.9	4
156	Electronic properties of Fibonacci and random Si-Ge chains. Journal of Physics Condensed Matter, 2011, 23, 405501.	0.7	4
157	On the Dynamics of Graphdiyne Hydrogenation. Materials Research Society Symposia Proceedings, 2013, 1549, 59-64.	0.1	4
158	Surface effects on the mechanical elongation of AuCu nanowires: De-alloying and the formation of mixed suspended atomic chains. Journal of Applied Physics, 2015, 117, .	1.1	4
159	Improving Graphene-metal Contacts: Thermal Induced Polishing. MRS Advances, 2018, 3, 73-78.	0.5	4
160	Molecular dynamics simulations of ballistic penetration of penta-graphene sheets. MRS Advances, 2018, 3, 433-437.	0.5	4
161	Structural and electronic properties of defective AlN/GaN hybrid nanostructures. Computational Materials Science, 2020, 183, 109860.	1.4	4
162	Oxygenation of Diamond Surfaces via Hummer's Method. Chemistry of Materials, 2021, 33, 4977-4987.	3.2	4

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163	Devising Bone Molecular Models at the Nanoscale: From Usual Mineralized Collagen Fibrils to the First Bone Fibers Including Hydroxyapatite in the Extra-Fibrillar Volume. <i>Materials</i> , 2022, 15, 2274.	1.3	4
164	Theoretical studies on Carter's soliton switch. <i>Synthetic Metals</i> , 1992, 51, 179-186.	2.1	3
165	Hysteresis-like Behavior in MBANP Crystals. <i>Crystal Growth and Design</i> , 2004, 4, 1079-1081.	1.4	3
166	Adsorption configuration effects on the surface diffusion of large organic molecules: The case of Violet Lander. <i>Journal of Chemical Physics</i> , 2010, 133, 224702.	1.2	3
167	Nanodroplets Impacting on Graphene. <i>MRS Advances</i> , 2016, 1, 675-680.	0.5	3
168	Mechanical and Thermal Stability of Graphyne and Graphdiyne Nanoscrolls. <i>MRS Advances</i> , 2017, 2, 129-134.	0.5	3
169	Carbon Nanotube Peapods Under High-Strain Rate Conditions: A Molecular Dynamics Investigation. <i>MRS Advances</i> , 2020, 5, 1723-1730.	0.5	3
170	Nature inspired solid-liquid phase amphibious adhesive. <i>Soft Matter</i> , 2020, 16, 5854-5860.	1.2	3
171	Controlling Movement at Nanoscale: Curvature Driven Mechanotaxis. <i>Small</i> , 2021, 17, 2100909.	5.2	3
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