Douglas S. Galvao

List of Publications by Year
in descending order

216 papers	8,097 citations	46984 47 h-index	53190 85 g-index
216 all docs	216 docs citations	216 times ranked	9923 citing authors

#	Article	IF	Citations
1	Electrically, Chemically, and Photonically Powered Torsional and Tensile Actuation of Hybrid Carbon Nanotube Yarn Muscles. Science, 2012, 338, 928-932.	6.0	585
2	Hierarchically buckled sheath-core fibers for superelastic electronics, sensors, and muscles. Science, 2015, 349, 400-404.	6.0	447
3	Molecular-Dynamics Simulations of Carbon Nanotubes as Gigahertz Oscillators. Physical Review Letters, 2003, 90, 055504.	2.9	342
4	Structure and Dynamics of Carbon Nanoscrolls. Nano Letters, 2004, 4, 881-884.	4.5	296
5	Exfoliation of a non-van der Waals material from iron ore hematite. Nature Nanotechnology, 2018, 13, 602-609.	15.6	295
6	Sign Change of Poisson's Ratio for Carbon Nanotube Sheets. Science, 2008, 320, 504-507.	6.0	245
7	Crystalline networks with unusual predicted mechanical and thermal properties. Nature, 1993, 365, 735-737.	13.7	224
8	Graphene to graphane: a theoretical study. Nanotechnology, 2009, 20, 465704.	1.3	219
9	Chemical Vapor Deposition of Monolayer Rhenium Disulfide (ReS₂). Advanced Materials, 2015, 27, 4640-4648.	11.1	203
10	Surface functionalization of two-dimensional metal chalcogenides by Lewis acidâ€“base chemistry. Nature Nanotechnology, 2016, 11, 465-471.	15.6	197
11	Families of carbon nanotubes: Graphyne-based nanotubes. Physical Review B, 2003, 68, .	1.1	185
12	Nonzero Gap Two-Dimensional Carbon Allotrope from Porous Graphene. Journal of Physical Chemistry C, 2012, 116, 12810-12813.	1.5	152
13	Torsional refrigeration by twisted, coiled, and supercoiled fibers. Science, 2019, 366, 216-221.	6.0	133
14	Lock-and-key effect in the surface diffusion of large organic molecules probed by STM. Nature Materials, 2004, 3, 779-782.	13.3	116
15	New families of carbon nanotubes based on graphyne motifs. Nanotechnology, 2004, 15, S142-S149.	1.3	116
16	Gigahertz nanomechanical oscillators based on carbon nanotubes. Nanotechnology, 2004, 15, S184-S189.	1.3	112
17	On the Structural and Stability Features of Linear Atomic Suspended Chains Formed from Gold Nanowires Stretching. Nano Letters, 2004, 4, 1187-1191.	4.5	106
18	Indication of Unusual Pentagonal Structures in Atomic-Size Cu Nanowires. Physical Review Letters, 2004, 93, 126103.	2.9	105

#	Article	IF	Citations
19	Excitation and relaxation energies oftrans-stilbene: Confined singlet, triplet, and charged bipolarons. Physical Review B, 1993, 47, 1742-1753.	1.1	101
20	Graphene Supported MoS₂ Structures with High Defect Density for an Efficient HER Electrocatalysts. ACS Applied Materials & Interfaces, 2020, 12, 12629-12638.	4.0	101
21	Strong, Twistâ€Stable Carbon Nanotube Yarns and Muscles by Tension Annealing at Extreme Temperatures. Advanced Materials, 2016, 28, 6598-6605.	11.1	100
22	Prediction of the hydrogen storage capacity of carbon nanoscrolls. Physical Review B, 2007, 75, .	1.1	98
23	Experimental realization of suspended atomic chains composed of different atomic species. Nature Nanotechnology, 2006, 1, 182-185.	15.6	95
24	Low-density three-dimensional foam using self-reinforced hybrid two-dimensional atomic layers. Nature Communications, 2014, 5, 4541.	5.8	91
25	Prediction of Ordered Phases of Encapsulated C60, C70, and C78Inside Carbon Nanotubes. Nano Letters, 2005, 5, 349-355.	4.5	85
26	Mechanical Properties of Nanosprings. Physical Review Letters, 2004, 92, 175502.	2.9	82
27	Synthesis of Low-Density, Carbon-Doped, Porous Hexagonal Boron Nitride Solids. ACS Nano, 2015, 9, 12088-12095.	7.3	81
28	Inorganic Graphenylene: A Porous Two-Dimensional Material With Tunable Band Gap. Journal of Physical Chemistry C, 2014, 118, 23670-23674.	1.5	76
29	Multiscale Geometric Design Principles Applied to 3D Printed Schwarzites. Advanced Materials, 2018, 30, 1704820.	11.1	76
30	Geometric and electronic structure of carbon nanotube networks: â€˜superâ€™-carbon nanotubes. Nanotechnology, 2006, 17, 617-621.	1.3	74
31	Theoretical investigation of electromechanical effects for graphyne carbon nanotubes. Journal of Chemical Physics, 2004, 121, 3228-3237.	1.2	72
32	Atomistic simulations of the mechanical properties of â€˜superâ€™ carbon nanotubes. Nanotechnology, 2007, 18, 335702.	1.3	72
33	Graphene to fluorographene and fluorographane: a theoretical study. Nanotechnology, 2013, 24, 035706.	1.3	69
34	Fullereneynes: a new family of porous fullerenes. Chemical Physics Letters, 1993, 204, 8-14.	1.2	67
35	Designing nanoscaled hybrids from atomic layered boron nitride with silver nanoparticle deposition. Journal of Materials Chemistry A, 2014, 2, 3148.	5.2	65
36	Prediction of giant electroactuation for papyruslike carbon nanoscroll structures: First-principles calculations. Physical Review B, 2006, 74, .	1.1	63

#	Article	IF	Citations
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 CO₂ Absorption. ACS Nano, 2017, 11, 8944-8952.	7.3	56
41	MÃ¶bius 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 WS₂ /MoS₂ Heterostructures: The Role of Interfaces. ACS Nano, 2018, 12, 4036-4044.	7.3	54
43	3D Porous Graphene by Lowâ€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 Metalâ€“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

#	Article	IF	Citations
55	On the unzipping of multiwalled carbon nanotubes. Nanotechnology, 2012, 23, 465702.	1.3	39
56	Controlled route to the fabrication of carbon and boron nitride nanoscrolls: A molecular dynamics investigation. Journal of Applied Physics, 2013, 113, .	1.1	38
57	Scalable Synthesis of Atomically Thin Gallium Telluride Nanosheets for Supercapacitor Applications. ACS Applied Nano Materials, 2021, 4, 4829-4838.	2.4	38
58	Structural and Thermal Stability of Graphyne and Graphdiyne Nanoscroll Structures. ACS Applied Materials & Interfaces, 2019, 11, 2670-2676.	4.0	36
59	Ambient solid-state mechano-chemical reactions between functionalized carbon nanotubes. Nature Communications, 2015, 6, 7291.	5.8	35
60	Enhanced supercapacitor performance of a 3D architecture tailored using atomically thin rGOâ€“MoS₂ 2D sheets. RSC Advances, 2016, 6, 93384-93393.	1.7	35
61	Chaotic signature in the motion of coupled carbon nanotube oscillators. Nanotechnology, 2005, 16, 583-589.	1.3	34
62	Contaminants in Suspended Gold Chains: AnAb InitioMolecular Dynamics Study. Physical Review Letters, 2004, 93, 216103.	2.9	32
63	A Brief Review on Syntheses, Structures, and Applications of Nanoscrolls. Frontiers in Materials, 2014, 1, .	1.2	31
64	Evaluation of carbon nanoscroll materials for post-combustion CO2 capture. Carbon, 2016, 101, 218-225.	5.4	31
65	Apparent Ferromagnetism in Exfoliated Ultrathin Pyrite Sheets. Journal of Physical Chemistry C, 2021, 125, 18927-18935.	1.5	30
66	Graphene healing mechanisms: A theoretical investigation. Carbon, 2016, 99, 302-309.	5.4	29
67	Mechanical Deformation of Nanoscale Metal Rods: When Size and Shape Matter. Physical Review Letters, 2011, 106, 055501.	2.9	28
68	Design of Porous Metal-Organic Frameworks for Adsorption Driven Thermal Batteries. MRS Advances, 2017, 2, 519-524.	0.5	28
69	Transmission electron microscopy and molecular dynamics study of the formation of suspended copper linear atomic chains. Physical Review B, 2006, 74, .	1.1	27
70	Defects in Graphene-Based Twisted Nanoribbons: Structural, Electronic, and Optical Properties. Langmuir, 2009, 25, 4751-4759.	1.6	26
71	Burning Graphene Layer-by-Layer. Scientific Reports, 2015, 5, 11546.	1.6	26
72	Controlled 3D Carbon Nanotube Structures by Plasma Welding. Advanced Materials Interfaces, 2016, 3, 1500755.	1.9	25

#	Article	IF	Citations
73	On the Mechanical Properties and Thermal Stability of a Recently Synthesized Monolayer Amorphous Carbon. Journal of Physical Chemistry C, 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. ACS Omega, 2018, 3, 6013-6021.	1.6	24
75	3D Printed Tubulanes as Lightweight Hypervelocity Impact Resistant Structures. Small, 2019, 15, e1904747.	5.2	24
76	Ordered phases of encapsulated diamondoids into carbon nanotubes. Nanotechnology, 2011, 22, 315708.	1.3	22
77	Carbon Nanotubes as Reinforcement Elements of Composite Nanotools. Nano Letters, 2008, 8, 842-847.	4.5	21
78	Intrinsic Stability of the Smallest Possible Silver Nanotube. Physical Review Letters, 2011, 106, 065501.	2.9	21
79	Enhanced Mechanical Stability of Gold Nanotips through Carbon Nanocone Encapsulation. Scientific Reports, 2015, 5, 10408.	1.6	21
80	Liquid Exfoliation of Icosahedral Quasicrystals. Advanced Functional Materials, 2018, 28, 1801181.	7.8	21
81	Thermophoretically driven carbon nanotube oscillators. Applied Physics Letters, 2009, 95, .	1.5	20
82	Defect-Free Carbon Nanotube Coils. Nano Letters, 2016, 16, 2152-2158.	4.5	20
83	High Toughness in Ultralow Density Graphene Oxide Foam. Advanced Materials Interfaces, 2017, 4, 1700030.	1.9	20
84	Virtually imprinted polymers (VIPs): understanding molecularly templated materialsviamolecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 13145-13152.	1.3	19
85	Extraction of Two-Dimensional Aluminum Alloys from Decagonal Quasicrystals. ACS Nano, 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. Journal of Chemical Information and Computer Sciences, 2002, 42, 1479-1489.	2.8	18
87	Mechanical properties of amorphous nanosprings. Nanotechnology, 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. Nanotechnology, 2010, 21, 485702.	1.3	18
89	On the mechanical properties of novamene: A fully atomistic molecular dynamics and DFT investigation. Carbon, 2018, 139, 782-788.	5.4	18
90	Two-dimensional cobalt telluride as a piezo-tribogenerator. Nanoscale, 2022, 14, 7788-7797.	2.8	18

#	Article	IF	Citations
91	A Structureâ^'Activity Study of Taxol, Taxotere, and Derivatives Using the Electronic Indices Methodology (EIM). Journal of Chemical Information and Computer Sciences, 2003, 43, 699-706.	2.8	17
92	Carbon nanotube with square cross-section: An ab initio investigation. Journal of Chemical Physics, 2010, 133, 124513.	1.2	17
93	Mechanical and energy-absorption properties of schwarzites. Carbon, 2020, 157, 670-680.	5.4	17
94	Size Limit of Defect Formation in Pyramidal Pt Nanocontacts. Physical Review Letters, 2007, 99, 255501.	2.9	16
95	Ballistic Fracturing of Carbon Nanotubes. ACS Applied Materials & Interfaces, 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. International Journal of Quantum Chemistry, 2005, 103, 588-596.	1.0	15
97	Elastic properties of nanowires. Journal of Applied Physics, 2006, 99, 094310.	1.1	15
98	Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes. Journal of Physics Condensed Matter, 2007, 19, 236222.	0.7	15
99	The structural and dynamical aspects of boron nitride nanotubes under high velocity impacts. Physical Chemistry Chemical Physics, 2016, 18, 14776-14781.	1.3	15
100	Structural transformations of carbon and boron nitride nanoscrolls at high impact collisions. Physical Chemistry Chemical Physics, 2018, 20, 4911-4916.	1.3	15
101	Tuning Penta-Graphene Electronic Properties Through Engineered Line Defects. Scientific Reports, 2020, 10, 8014.	1.6	15
102	Experimental and computational investigation of reduced graphene oxide nanoplatelets stabilized in poly(styrene sulfonate) sodium salt. Journal of Materials Science, 2018, 53, 10049-10058.	1.7	14
103	Few-Wall Carbon Nanotube Coils. Nano Letters, 2020, 20, 953-962.	4.5	14
104	New Zero Poisson's Ratio Structures. Physica Status Solidi - Rapid Research Letters, 2020, 14, 1900564.	1.2	14
105	On the mechanical properties of atomic and 3D printed zeolite-templated carbon nanotube networks. Additive Manufacturing, 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. Nanoscale, 2022, 14, 3200-3211.	2.8	14
107	Molecular dynamics simulation of single wall carbon nanotubes polymerization under compression. Journal of Computational Chemistry, 2007, 28, 1724-1734.	1.5	13
108	Strainâ€Induced Structural Deformation Study of 2D Mo_xW<sub>(1â€_x₎ S₂. Advanced Materials Interfaces, 2019, 6, 1801262.	1.9	13

#	Article	IF	Citations
109	Correlation between quantum conductance and atomic arrangement of atomic-size silver nanowires. Journal of Applied Physics, 2012, 111, 124316.	1.1	12
110	Structural and optical properties of plasma-deposited amorphous hydrogenated oxygenated carbon films. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1997, 15, 1334-1339.	0.9	11
111	Novel Nanoscroll Structures from Carbon Nitride Layers. ChemPhysChem, 2014, 15, 2367-2371.	1.0	11
112	On the mechanical properties of protomene: A theoretical investigation. Computational Materials Science, 2019, 161, 190-198.	1.4	11
113	Idealized Carbon-Based Materials Exhibiting Record Deliverable Capacities for Vehicular Methane Storage. Journal of Physical Chemistry C, 2019, 123, 1050-1058.	1.5	11
114	Emergence of Prime Numbers as the Result of Evolutionary Strategy. Physical Review Letters, 2004, 93, 098107.	2.9	10
115	Rotational dynamics and polymerization of C60 in C60-cubane crystals: A molecular dynamics study. Journal of Chemical Physics, 2008, 129, 064506.	1.2	10
116	Dynamics of the Formation of Carbon Nanotube Serpentines. Physical Review Letters, 2013, 110, 105502.	2.9	10
117	Mechanical Properties of Pentagraphene-based Nanotubes: A Molecular Dynamics Study. MRS Advances, 2018, 3, 97-102.	0.5	10
118	Gasâ€Phase Fluorination of Hexagonal Boron Nitride. Advanced Materials, 2021, 33, e2106084.	11.1	10
119	Some electronic properties of saturated and unsaturated cubane oligomers using DFT-based calculations. Computational and Theoretical Chemistry, 2008, 868, 37-41.	1.5	9
120	Efficient prediction of suitable functional monomers for molecular imprintingvialocal density of states calculations. Physical Chemistry Chemical Physics, 2018, 20, 13153-13158.	1.3	9
121	Mechanical Properties of Diamond Schwarzites: From Atomistic Models to 3D-Printed Structures. MRS Advances, 2020, 5, 1775-1781.	0.5	9
122	Mechanical response of pentadiamond: A DFT and molecular dynamics study. Physica B: Condensed Matter, 2022, 629, 413576.	1.3	9
123	Spatially variable reaction in the formation of anodically grown porous silicon structures. Journal of Applied Physics, 1995, 78, 590-592.	1.1	8
124	C₆₀-derived nanobaskets: stability, vibrational signatures, and molecular trapping. Nanotechnology, 2009, 20, 395701.	1.3	8
125	Temperature effects on the occurrence of long interatomic distances in atomic chains formed from stretched gold nanowires. Nanotechnology, 2011, 22, 095705.	1.3	8
126	One-dimensional silicon and germanium nanostructures with no carbon analogues. Physical Chemistry Chemical Physics, 2014, 16, 24570-24574.	1.3	8

#	Article	IF	Citations
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-deacetylbaccatin-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 oftrans-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 2DÂNatural 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	Solidâ€“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

#	Article	IF	Citations
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:â€‰ 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 Popgrapheneâ€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 â€” 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 Nanotubesâ€"'Super'-Fullerenes. Journal of Nanoscience and Nanotechnology, 2010, 10, 4378-4383.	0.9	4
156	Electronic properties of Fibonacci and random Siâ€“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 Hummerâ€™s Method. Chemistry of Materials, 2021, 33, 4977-4987.	3.2	4

#	Article	IF	Citations
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. Materials, 2022, 15, 2274.	1.3	4
164	Theoretical studies on Carter's soliton switch. Synthetic Metals, 1992, 51, 179-186.	2.1	3
165	Hysteresis-like Behavior in MBANP Crystals. Crystal Growth and Design, 2004, 4, 1079-1081.	1.4	3
166	Adsorption configuration effects on the surface diffusion of large organic molecules: The case of Violet Lander. Journal of Chemical Physics, 2010, 133, 224702.	1.2	3
167	Nanodroplets Impacting on Graphene. MRS Advances, 2016, 1, 675-680.	0.5	3
168	Mechanical and Thermal Stability of Graphyne and Graphdiyne Nanoscrolls. MRS Advances, 2017, 2, 129-134.	0.5	3
169	Carbon Nanotube Peapods Under High-Strain Rate Conditions: A Molecular Dynamics Investigation. MRS Advances, 2020, 5, 1723-1730.	0.5	3
170	Nature inspired solidâ€“liquid phase amphibious adhesive. Soft Matter, 2020, 16, 5854-5860.	1.2	3
171	Controlling Movement at Nanoscale: Curvature Driven Mechanotaxis. Small, 2021, 17, 2100909.	5.2	3
172	Carcinogenic classification of polycyclic aromatic hydrocarbons through theoretical descriptors. International Journal of Quantum Chemistry, 2005, 103, 718-730.	1.0	2
173	Neon atoms oscillating inside carbon and boron nitride nanotubes: a fully atomistic molecular dynamics investigation. Molecular Simulation, 2010, 36, 639-643.	0.9	2
174	A Nonzero Gap Two-dimensional Carbon Allotrope from Porous Graphene. Materials Research Society Symposia Proceedings, 2012, 1407, 199.	0.1	2
175	Multi-Million Fully Atomistic Molecular Dynamics Simulations of Yarn Formation from Carbon Nanotube Forests. Materials Research Society Symposia Proceedings, 2012, 1407, 205.	0.1	2
176	Violation of the universal behavior of membranes inside cylindrical tubes at nanoscale. Europhysics Letters, 2014, 105, 56002.	0.7	2
177	Differences in the Mechanical Properties of Monolayer and Multilayer WSe2/MoSe2. MRS Advances, 2018, 3, 373-378.	0.5	2
178	Mechanical Properties of Ultralow Density Graphene Oxide/Polydimethylsiloxane Foams. MRS Advances, 2018, 3, 61-66.	0.5	2
179	3D Printing: 3D Printed Tubulanes as Lightweight Hypervelocity Impact Resistant Structures (Small) Tj ETQq1 1 0.784314 rgBT /Overl	5.2	2
180	Mechanical Properties of Protomene: A Molecular Dynamics Investigation. MRS Advances, 2019, 4, 191-196.	0.5	2

#	Article	IF	Citations
181	Zeolite-templated Carbon Network: A Beta Zeolite Case Study. MRS Advances, 2020, 5, 751-756.	0.5	2
182	Bioinspired Aluminum Composite Reinforced with Soft Polymers with Enhanced Strength and Plasticity. Advanced Engineering Materials, 2020, 22, 1901116.	1.6	2
183	A reactive molecular dynamics study of the hydrogenation of diamond surfaces. Computational Materials Science, 2021, 200, 110859.	1.4	2
184	Revisiting Quasicrystals for the Synthesis of 2D Metals. Transactions of the Indian Institute of Metals, 2022, 75, 1093.	0.7	2
185	A Theoretical Investigation on the Dual-Mode Photoswitching Mechanism of Some Chiroptical Systems. Journal of Physical Chemistry B, 2001, 105, 8334-8338.	1.2	1
186	van der Waals potential barrier for cobaltocene encapsulation into single-walled carbon nanotubes: classical molecular dynamics andab initiostudy. Molecular Simulation, 2011, 37, 746-751.	0.9	1
187	On the Formation of Carbon Nanotube Serpentines: Insights from Multi-Million Atom Molecular Dynamics Simulation. Materials Research Society Symposia Proceedings, 2011, 1284, 79.	0.1	1
188	Stability and Dynamics of Boron Nitride Nanoscrolls. Materials Research Society Symposia Proceedings, 2011, 1307, 1.	0.1	1
189	Correlation Between Quantum Conductance and Atomic Arrangement of Silver Atomic-Size Nanocontacts. Materials Research Society Symposia Proceedings, 2012, 1429, 7.	0.1	1
190	The Hydrogenation Dynamics of h-BN Sheets. Materials Research Society Symposia Proceedings, 2013, 1549, 91-98.	0.1	1
191	Mechanical Properties and Fracture Dynamics of Silicene Membranes. Materials Research Society Symposia Proceedings, 2013, 1549, 99-107.	0.1	1
192	Graphene-like Membranes: From Impermeable to Selective Sieves. Materials Research Society Symposia Proceedings, 2014, 1658, 8.	0.1	1
193	Silver Hardening via Hypersonic Impacts. MRS Advances, 2018, 3, 493-498.	0.5	1
194	Self-Driven Graphene Tearing and Peeling: A Fully Atomistic Molecular Dynamics Investigation. MRS Advances, 2018, 3, 463-468.	0.5	1
195	Schwarzites to schwarzynes: A new class of superdeformable materials. MRS Advances, 2020, 5, 1947-1954.	0.5	1
196	On the sulfur doping of Î³-graphdiyne: A Molecular Dynamics and DFT study. MRS Advances, 2020, 5, 2701-2706.	0.5	1
197	On the structural stability and optical properties of germanium-based schwarzites: a density functional theory investigation. Physical Chemistry Chemical Physics, 2020, 22, 16286-16293.	1.3	1
198	Effect of Oxygen and Aluminum Incorporation on the Local Structure of GaN Nanowires: Insight from Extended X-ray Absorption Fine Structure Analysis. Journal of Physical Chemistry C, 2021, 125, 3225-3234.	1.5	1

#	Article	IF	Citations
199	Electronic structure of polyacetylene with bonded oxygen. Synthetic Metals, 1992, 51, 175-178.	2.1	0
200	The First Molecular Wheel: A Theoretical Investigation. Materials Research Society Symposia Proceedings, 2011, 1286, 44.	0.1	0
201	Tuning Electronic and Structural Properties of Triple Layers of Intercalated Graphene and Hexagonal Boron Nitride: An Ab-initio Study.. Materials Research Society Symposia Proceedings, 2011, 1307, 1.	0.1	0
202	Dynamics of Graphene Nanodrums. Materials Research Society Symposia Proceedings, 2011, 1284, 173.	0.1	0
203	The Dynamics of Formation of Graphane-like Fluorinated Graphene Membranes (Fluorographene): A Reactive Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 2011, 1344, 1.	0.1	0
204	A Fully Atomistic Reactive Molecular Dynamics Study on the Formation of Graphane from Graphene Hydrogenated Membranes. Materials Research Society Symposia Proceedings, 2011, 1284, 31.	0.1	0
205	Tribological Properties of Graphene and Boron-Nitride Layers: A Fully Atomistic Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 2012, 1407, 181.	0.1	0
206	When Small is Different: The Case of Membranes Inside Tubes. Materials Research Society Symposia Proceedings, 2012, 1451, 15-20.	0.1	0
207	On the Unzipping Mechanisms of Carbon Nanotubes: Insights from Reactive Molecular Dynamics Simulations. Materials Research Society Symposia Proceedings, 2012, 1451, 3-8.	0.1	0
208	On the Existence of Ordered Phases of Encapsulated Diamondoids into Carbon Nanotubes. Materials Research Society Symposia Proceedings, 2012, 1407, 26.	0.1	0
209	Fracture Patterns of Boron Nitride Nanotubes. Materials Research Society Symposia Proceedings, 2013, 1526, 1.	0.1	0
210	Species fractionation in atomic chains from mechanically stretched alloys. Journal of Physics Condensed Matter, 2014, 26, 435304.	0.7	0
211	Mechanical Properties of Graphene Nanowiggles. Materials Research Society Symposia Proceedings, 2014, 1658, 14.	0.1	0
212	The Influence of Morphology on the Charge Transport in Two-Phase Disordered Organic Systems. Materials Research Society Symposia Proceedings, 2015, 1737, 13.	0.1	0
213	High Pressure Induced Binding Between Linear Carbon Chains and Nanotubes. Materials Research Society Symposia Proceedings, 2015, 1752, 53-58.	0.1	0
214	Permeation of Water Nanodroplets on Carbon Nanotubes Forests. MRS Advances, 2017, 2, 123-128.	0.5	0
215	Nanodroplets Behavior on Graphdiyne Membranes. MRS Advances, 2017, 2, 1551-1556.	0.5	0
216	Mixing the immiscible through high-velocity mechanical impacts: an experimental and theoretical study. Journal Physics D: Applied Physics, 2019, 52, 445304.	1.3	0