

Douglas S. Galvao

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212
papers

6,521
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44
h-index

76
g-index

216
ext. papers

7,301
ext. citations

6.6
avg, IF

5.64
L-index

#	Paper	IF	Citations
212	Electrically, chemically, and photonically powered torsional and tensile actuation of hybrid carbon nanotube yarn muscles. <i>Science</i> , 2012 , 338, 928-32	33.3	462
211	STRETCHY ELECTRONICS. Hierarchically buckled sheath-core fibers for superelastic electronics, sensors, and muscles. <i>Science</i> , 2015 , 349, 400-4	33.3	346
210	Molecular-dynamics simulations of carbon nanotubes as gigahertz oscillators. <i>Physical Review Letters</i> , 2003 , 90, 055504	7.4	310
209	Structure and Dynamics of Carbon Nanoscrolls. <i>Nano Letters</i> , 2004 , 4, 881-884	11.5	271
208	Sign Change of Poisson's Ratio for Carbon Nanotube Sheets. <i>Science</i> , 2008 , 320, 504-7	33.3	208
207	Graphene to graphane: a theoretical study. <i>Nanotechnology</i> , 2009 , 20, 465704	3.4	199
206	Crystalline networks with unusual predicted mechanical and thermal properties. <i>Nature</i> , 1993 , 365, 735-737	33.4	190
205	Exfoliation of a non-van der Waals material from iron ore hematite. <i>Nature Nanotechnology</i> , 2018 , 13, 602-609	28.7	179
204	Chemical Vapor Deposition of Monolayer Rhenium Disulfide (ReS ₂). <i>Advanced Materials</i> , 2015 , 27, 4640-44	8.4	177
203	Families of carbon nanotubes: Graphyne-based nanotubes. <i>Physical Review B</i> , 2003 , 68,	3.3	169
202	Surface functionalization of two-dimensional metal chalcogenides by Lewis acid-base chemistry. <i>Nature Nanotechnology</i> , 2016 , 11, 465-71	28.7	150
201	Nonzero Gap Two-Dimensional Carbon Allotrope from Porous Graphene. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 12810-12813	3.8	120
200	Gigahertz nanomechanical oscillators based on carbon nanotubes. <i>Nanotechnology</i> , 2004 , 15, S184-S189	3.4	110
199	New families of carbon nanotubes based on graphyne motifs. <i>Nanotechnology</i> , 2004 , 15, S142-S149	3.4	107
198	Lock-and-key effect in the surface diffusion of large organic molecules probed by STM. <i>Nature Materials</i> , 2004 , 3, 779-82	27	106
197	Excitation and relaxation energies of trans-stilbene: Confined singlet, triplet, and charged bipolarons. <i>Physical Review B</i> , 1993 , 47, 1742-1753	3.3	100
196	On the Structural and Stability Features of Linear Atomic Suspended Chains Formed from Gold Nanowires Stretching. <i>Nano Letters</i> , 2004 , 4, 1187-1191	11.5	98

195	Indication of unusual pentagonal structures in atomic-size Cu nanowires. <i>Physical Review Letters</i> , 2004 , 93, 126103	7.4	98
194	Prediction of the hydrogen storage capacity of carbon nanoscrolls. <i>Physical Review B</i> , 2007 , 75,	3.3	90
193	Experimental realization of suspended atomic chains composed of different atomic species. <i>Nature Nanotechnology</i> , 2006 , 1, 182-5	28.7	84
192	Low-density three-dimensional foam using self-reinforced hybrid two-dimensional atomic layers. <i>Nature Communications</i> , 2014 , 5, 4541	17.4	82
191	Prediction of ordered phases of encapsulated C60, C70, and C78 inside carbon nanotubes. <i>Nano Letters</i> , 2005 , 5, 349-55	11.5	80
190	Mechanical properties of nanosprings. <i>Physical Review Letters</i> , 2004 , 92, 175502	7.4	73
189	Strong, Twist-Stable Carbon Nanotube Yarns and Muscles by Tension Annealing at Extreme Temperatures. <i>Advanced Materials</i> , 2016 , 28, 6598-605	24	72
188	Geometric and electronic structure of carbon nanotube networks: SuperCarbon nanotubes. <i>Nanotechnology</i> , 2006 , 17, 617-621	3.4	70
187	Torsional refrigeration by twisted, coiled, and supercoiled fibers. <i>Science</i> , 2019 , 366, 216-221	33.3	65
186	Atomistic simulations of the mechanical properties of SuperCarbon nanotubes. <i>Nanotechnology</i> , 2007 , 18, 335702	3.4	65
185	Graphene to fluorographene and fluorographane: a theoretical study. <i>Nanotechnology</i> , 2013 , 24, 035706	3.4	64
184	Theoretical investigation of electromechanical effects for graphyne carbon nanotubes. <i>Journal of Chemical Physics</i> , 2004 , 121, 3228-37	3.9	64
183	Synthesis of Low-Density, Carbon-Doped, Porous Hexagonal Boron Nitride Solids. <i>ACS Nano</i> , 2015 , 9, 12088-95	16.7	61
182	Fullerenynes: a new family of porous fullerenes. <i>Chemical Physics Letters</i> , 1993 , 204, 8-14	2.5	61
181	Prediction of giant electroactuation for papyruslike carbon nanoscroll structures: First-principles calculations. <i>Physical Review B</i> , 2006 , 74,	3.3	60
180	Inorganic Graphenylene: A Porous Two-Dimensional Material With Tunable Band Gap. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 23670-23674	3.8	56
179	Unzipping carbon nanotubes at high impact. <i>Nano Letters</i> , 2014 , 14, 4131-7	11.5	55
178	Curved graphene nanoribbons: structure and dynamics of carbon nanobelts. <i>Nanotechnology</i> , 2010 , 21, 75710	3.4	54

177	Designing nanoscaled hybrids from atomic layered boron nitride with silver nanoparticle deposition. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 3148	13	52
176	Graphene Supported MoS Structures with High Defect Density for an Efficient HER Electrocatalysts. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 12629-12638	9.5	49
175	Mechanical properties and fracture dynamics of silicene membranes. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 19417-23	3.6	49
174	Molecular dynamics simulations of C60 nanobearings. <i>Chemical Physics Letters</i> , 2004 , 386, 425-429	2.5	49
173	MBius and twisted graphene nanoribbons: stability, geometry, and electronic properties. <i>Journal of Chemical Physics</i> , 2008 , 128, 164719	3.9	47
172	Observation of the smallest metal nanotube with a square cross-section. <i>Nature Nanotechnology</i> , 2009 , 4, 149-52	28.7	46
171	Mechanical properties of carbon nanotube networks by molecular mechanics and impact molecular dynamics calculations. <i>Physical Review B</i> , 2007 , 75,	3.3	45
170	The structure and dynamics of boron nitride nanoscrolls. <i>Nanotechnology</i> , 2009 , 20, 335702	3.4	44
169	Multiscale Geometric Design Principles Applied to 3D Printed Schwarzites. <i>Advanced Materials</i> , 2018 , 30, 1704820	24	44
168	3D Porous Graphene by Low-Temperature Plasma Welding for Bone Implants. <i>Advanced Materials</i> , 2016 , 28, 8959-8967	24	43
167	Lightweight Hexagonal Boron Nitride Foam for CO Absorption. <i>ACS Nano</i> , 2017 , 11, 8944-8952	16.7	42
166	Modeling the auxetic transition for carbon nanotube sheets. <i>Physical Review B</i> , 2008 , 78,	3.3	42
165	Synthetic melanin films: Assembling mechanisms, scaling behavior, and structural properties. <i>Journal of Applied Physics</i> , 2006 , 99, 113511	2.5	38
164	Linear Carbon Chains under High-Pressure Conditions. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 10669-10676	3.8	37
163	Controlled route to the fabrication of carbon and boron nitride nanoscrolls: A molecular dynamics investigation. <i>Journal of Applied Physics</i> , 2013 , 113, 054306	2.5	37
162	Deformation Mechanisms of Vertically Stacked WS /MoS Heterostructures: The Role of Interfaces. <i>ACS Nano</i> , 2018 , 12, 4036-4044	16.7	35
161	Entanglement and the nonlinear elastic behavior of forests of coiled carbon nanotubes. <i>Physical Review Letters</i> , 2008 , 100, 086807	7.4	35
160	On the unzipping of multiwalled carbon nanotubes. <i>Nanotechnology</i> , 2012 , 23, 465702	3.4	33

159	Gas Adsorption and Separation by the Al-Based Metal-Organic Framework MIL-160. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 26822-26832	3.8	32
158	Contaminants in suspended gold chains: an ab initio molecular dynamics study. <i>Physical Review Letters</i> , 2004 , 93, 216103	7.4	30
157	Chaotic signature in the motion of coupled carbon nanotube oscillators. <i>Nanotechnology</i> , 2005 , 16, 583-589	5.8	30
156	Ambient solid-state mechano-chemical reactions between functionalized carbon nanotubes. <i>Nature Communications</i> , 2015 , 6, 7291	17.4	28
155	Enhanced supercapacitor performance of a 3D architecture tailored using atomically thin rGO/MoS ₂ 2D sheets. <i>RSC Advances</i> , 2016 , 6, 93384-93393	3.7	27
154	Synthesis and porous h-BN 3D architectures for effective humidity and gas sensors. <i>RSC Advances</i> , 2016 , 6, 87888-87896	3.7	26
153	Scale Effects on the Ballistic Penetration of Graphene Sheets. <i>Scientific Reports</i> , 2018 , 8, 6750	4.9	25
152	Graphene healing mechanisms: A theoretical investigation. <i>Carbon</i> , 2016 , 99, 302-309	10.4	25
151	A Brief Review on Syntheses, Structures, and Applications of Nanoscrolls. <i>Frontiers in Materials</i> , 2014 , 1,	4	24
150	Mechanical deformation of nanoscale metal rods: when size and shape matter. <i>Physical Review Letters</i> , 2011 , 106, 055501	7.4	24
149	Defects in graphene-based twisted nanoribbons: structural, electronic, and optical properties. <i>Langmuir</i> , 2009 , 25, 4751-9	4	24
148	Transmission electron microscopy and molecular dynamics study of the formation of suspended copper linear atomic chains. <i>Physical Review B</i> , 2006 , 74,	3.3	24
147	Evaluation of carbon nanoscroll materials for post-combustion CO ₂ capture. <i>Carbon</i> , 2016 , 101, 218-225	10.4	23
146	Design of Porous Metal-Organic Frameworks for Adsorption Driven Thermal Batteries. <i>MRS Advances</i> , 2017 , 2, 519-524	0.7	22
145	Structural and Thermal Stability of Graphyne and Graphdiyne Nanoscroll Structures. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 2670-2676	9.5	22
144	Controlled 3D Carbon Nanotube Structures by Plasma Welding. <i>Advanced Materials Interfaces</i> , 2016 , 3, 1500755	4.6	21
143	Ordered phases of encapsulated diamondoids into carbon nanotubes. <i>Nanotechnology</i> , 2011 , 22, 315708	9.4	21
142	Intrinsic stability of the smallest possible silver nanotube. <i>Physical Review Letters</i> , 2011 , 106, 065501	7.4	21

141	Burning Graphene Layer-by-Layer. <i>Scientific Reports</i> , 2015 , 5, 11546	4.9	20
140	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	3.9	18
139	Carbon nanotubes as reinforcement elements of composite nanotools. <i>Nano Letters</i> , 2008 , 8, 842-7	11.5	18
138	Mechanical properties of amorphous nanosprings. <i>Nanotechnology</i> , 2006 , 17, 5620-6	3.4	18
137	On the mechanical properties of novamene: A fully atomistic molecular dynamics and DFT investigation. <i>Carbon</i> , 2018 , 139, 782-788	10.4	16
136	Temperature effects on the atomic arrangement and conductance of atomic-size gold nanowires generated by mechanical stretching. <i>Nanotechnology</i> , 2010 , 21, 485702	3.4	16
135	Carbon nanotube with square cross-section: an ab initio investigation. <i>Journal of Chemical Physics</i> , 2010 , 133, 124513	3.9	16
134	Size limit of defect formation in pyramidal Pt nanocontacts. <i>Physical Review Letters</i> , 2007 , 99, 255501	7.4	16
133	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, 1479-89		16
132	High Toughness in Ultralow Density Graphene Oxide Foam. <i>Advanced Materials Interfaces</i> , 2017 , 4, 1700030	13.0	15
131	Virtually imprinted polymers (VIPs): understanding molecularly templated materials via molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 13145-13152	3.6	15
130	Defect-Free Carbon Nanotube Coils. <i>Nano Letters</i> , 2016 , 16, 2152-8	11.5	15
129	Scalable Synthesis of Atomically Thin Gallium Telluride Nanosheets for Supercapacitor Applications. <i>ACS Applied Nano Materials</i> , 2021 , 4, 4829-4838	5.6	15
128	Liquid Exfoliation of Icosahedral Quasicrystals. <i>Advanced Functional Materials</i> , 2018 , 28, 1801181	15.6	14
127	Thermophoretically driven carbon nanotube oscillators. <i>Applied Physics Letters</i> , 2009 , 95, 253103	3.4	14
126	Enhanced Mechanical Stability of Gold Nanotips through Carbon Nanocone Encapsulation. <i>Scientific Reports</i> , 2015 , 5, 10408	4.9	13
125	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	4.3	13
124	Ballistic Fracturing of Carbon Nanotubes. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 24819-25	9.5	13

123	3D Printed Tubulanes as Lightweight Hypervelocity Impact Resistant Structures. <i>Small</i> , 2019 , 15, e1904747	13
122	Elastic properties of nanowires. <i>Journal of Applied Physics</i> , 2006 , 99, 094310	2.5 13
121	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	13
120	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	2.1 13
119	The structural and dynamical aspects of boron nitride nanotubes under high velocity impacts. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 14776-81	3.6 13
118	Molecular dynamics simulation of single wall carbon nanotubes polymerization under compression. <i>Journal of Computational Chemistry</i> , 2007 , 28, 1724-34	3.5 12
117	Extraction of Two-Dimensional Aluminum Alloys from Decagonal Quasicrystals. <i>ACS Nano</i> , 2020 , 14, 7435-7443	11
116	Structural transformations of carbon and boron nitride nanoscrolls at high impact collisions. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 4911-4916	3.6 11
115	Correlation between quantum conductance and atomic arrangement of atomic-size silver nanowires. <i>Journal of Applied Physics</i> , 2012 , 111, 124316	2.5 11
114	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	2.9 11
113	Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 236222	1.8 11
112	Mechanical and energy-absorption properties of schwarzites. <i>Carbon</i> , 2020 , 157, 670-680	10.4 11
111	On the mechanical properties of protomene: A theoretical investigation. <i>Computational Materials Science</i> , 2019 , 161, 190-198	3.2 10
110	Novel nanoscroll structures from carbon nitride layers. <i>ChemPhysChem</i> , 2014 , 15, 2367-71	3.2 10
109	Dynamics of the formation of carbon nanotube serpentines. <i>Physical Review Letters</i> , 2013 , 110, 105502	7.4 10
108	Rotational dynamics and polymerization of C60 in C60-cubane crystals: a molecular dynamics study. <i>Journal of Chemical Physics</i> , 2008 , 129, 064506	3.9 10
107	Strain-Induced Structural Deformation Study of 2D MoxW(1-x) S2. <i>Advanced Materials Interfaces</i> , 2019 , 6, 1801262	4.6 9
106	Mechanical Properties of Pentagraphene-based Nanotubes: A Molecular Dynamics Study. <i>MRS Advances</i> , 2018 , 3, 97-102	0.7 9

105	Some electronic properties of saturated and unsaturated cubane oligomers using DFT-based calculations. <i>Computational and Theoretical Chemistry</i> , 2008 , 868, 37-41		9
104	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	3.6	8
103	Temperature effects on the occurrence of long interatomic distances in atomic chains formed from stretched gold nanowires. <i>Nanotechnology</i> , 2011 , 22, 095705	3.4	8
102	Spatially variable reaction in the formation of anodically grown porous silicon structures. <i>Journal of Applied Physics</i> , 1995 , 78, 590-592	2.5	8
101	Apparent Ferromagnetism in Exfoliated Ultrathin Pyrite Sheets. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 18927-18935	3.8	8
100	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	3.8	7
99	C60-derived nanobaskets: stability, vibrational signatures, and molecular trapping. <i>Nanotechnology</i> , 2009 , 20, 395701	3.4	7
98	Emergence of prime numbers as the result of evolutionary strategy. <i>Physical Review Letters</i> , 2004 , 93, 098107	7.4	7
97	A semiempirical study on the electronic structure of 10-deacetylbaocatin-III. <i>Journal of Molecular Graphics and Modelling</i> , 2002 , 21, 57-70	2.8	7
96	Few-Wall Carbon Nanotube Coils. <i>Nano Letters</i> , 2020 , 20, 953-962	11.5	7
95	One-dimensional silicon and germanium nanostructures with no carbon analogues. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 24570-4	3.6	6
94	Comparative parametric method 6 (PM6) and Recife model 1 (RM1) study of trans-stilbene. <i>Molecular Simulation</i> , 2012 , 38, 1-7	2	6
93	Effects of chlorine gas exposure on the optical properties of rhodium phthalocyanine films. <i>Solid State Communications</i> , 2004 , 131, 53-56	1.6	6
92	Structural and electronic properties of radialenes and related systems. <i>Computational and Theoretical Chemistry</i> , 2005 , 729, 203-210		6
91	Idealized Carbon-Based Materials Exhibiting Record Deliverable Capacities for Vehicular Methane Storage. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 1050-1058	3.8	6
90	Multifunctional Hybrids Based on 2D Fluorinated Graphene Oxide and Superparamagnetic Iron Oxide Nanoparticles. <i>Particle and Particle Systems Characterization</i> , 2017 , 34, 1700245	3.1	5
89	Mechanical Properties of Schwarzites - A Fully Atomistic Reactive Molecular Dynamics Investigation. <i>MRS Advances</i> , 2018 , 3, 451-456	0.7	5
88	Solid-Liquid Self-Adaptive Polymeric Composite. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 2142-7	9.5	5

87	Graphyne Oxidation: Insights From a Reactive Molecular Dynamics Investigation. <i>Materials Research Society Symposia Proceedings</i> , 2013 , 1549, 53-58		5
86	Tuning Penta-Graphene Electronic Properties Through Engineered Line Defects. <i>Scientific Reports</i> , 2020 , 10, 8014	4.9	5
85	Schwarzites for Natural Gas Storage: A Grand-Canonical Monte Carlo Study. <i>MRS Advances</i> , 2018 , 3, 115-120	4	4
84	Improving Graphene-metal Contacts: Thermal Induced Polishing. <i>MRS Advances</i> , 2018 , 3, 73-78	0.7	4
83	On hardening silver nanocubes by high-velocity impacts: a fully atomistic molecular dynamics investigation. <i>Journal of Materials Science</i> , 2018 , 53, 7486-7492	4.3	4
82	Mechanical Properties of Phagraphene Membranes: A Fully Atomistic Molecular Dynamics Investigation. <i>MRS Advances</i> , 2018 , 3, 67-72	0.7	4
81	Molecular dynamics simulations of ballistic penetration of penta-graphene sheets. <i>MRS Advances</i> , 2018 , 3, 433-437	0.7	4
80	Dynamical aspects of the unzipping of multiwalled boron nitride nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 19147-50	3.6	4
79	New Insights on the Growth of Anisotropic Nanoparticles from Total Energy Calculations. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 11976-11979	3.8	4
78	Topologically closed macromolecules made of single walled carbon nanotubes-'super'-fullerenes. <i>Journal of Nanoscience and Nanotechnology</i> , 2010 , 10, 4378-83	1.3	4
77	Large electromechanical response in silicon nanowires predicted from first-principles electronic structure calculations. <i>Physical Review B</i> , 2008 , 77,	3.3	4
76	Is it possible to grow amorphous normal nanosprings?. <i>Nanotechnology</i> , 2007 , 18, 435606	3.4	4
75	Semiempirical studies of the electronic structure of polyphenylene sulfide phenyleneamine. <i>International Journal of Quantum Chemistry</i> , 2003 , 95, 252-259	2.1	4
74	A dual-mode photoswitching mechanism and charge transfer on chiroptical systems [theoretical study]. <i>Synthetic Metals</i> , 2001 , 116, 275-279	3.6	4
73	New Zero Poisson's Ratio Structures. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020 , 14, 1900564	2.5	4
72	Mechanical and Thermal Stability of Graphyne and Graphdiyne Nanoscrolls. <i>MRS Advances</i> , 2017 , 2, 129-134	3	3
71	Surface effects on the mechanical elongation of AuCu nanowires: De-alloying and the formation of mixed suspended atomic chains. <i>Journal of Applied Physics</i> , 2015 , 117, 094301	2.5	3
70	Three-dimensional carbon nanotube networks from beta zeolite templates: Thermal stability and mechanical properties. <i>Computational Materials Science</i> , 2020 , 182, 109781	3.2	3

69	Hysteresis-like Behavior in MBANP Crystals. <i>Crystal Growth and Design</i> , 2004 , 4, 1079-1081	3.5	3
68	Benzo[c]quinolizin-3-ones theoretical investigation: SAR analysis and application to nontested compounds. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 1987-97		3
67	Theoretical studies on Carter's soliton switch. <i>Synthetic Metals</i> , 1992 , 51, 179-186	3.6	3
66	Mechanical response of pentadiamond: A DFT and molecular dynamics study. <i>Physica B: Condensed Matter</i> , 2022 , 629, 413576	2.8	3
65	Nanodroplets Impacting on Graphene. <i>MRS Advances</i> , 2016 , 1, 675-680	0.7	3
64	A reactive molecular dynamics study on the mechanical properties of a recently synthesized amorphous carbon monolayer converted into a nanotube/nanoscroll. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 9089-9095	3.6	3
63	Mechanical Properties of Diamond Schwarzites: From Atomistic Models to 3D-Printed Structures. <i>MRS Advances</i> , 2020 , 5, 1775-1781	0.7	2
62	Structural and electronic properties of defective AlN/GaN hybrid nanostructures. <i>Computational Materials Science</i> , 2020 , 183, 109860	3.2	2
61	Differences in the Mechanical Properties of Monolayer and Multilayer WSe ₂ /MoSe ₂ . <i>MRS Advances</i> , 2018 , 3, 373-378	0.7	2
60	Water/Alcohol Separation in Graphene Oxide Membranes: Insights from Molecular Dynamics and Monte Carlo Simulations. <i>MRS Advances</i> , 2018 , 3, 109-114	0.7	2
59	Violation of the universal behavior of membranes inside cylindrical tubes at nanoscale. <i>Europhysics Letters</i> , 2014 , 105, 56002	1.6	2
58	On the Dynamics of Graphdiyne Hydrogenation. <i>Materials Research Society Symposia Proceedings</i> , 2013 , 1549, 59-64		2
57	Electronic properties of Fibonacci and random Si-Ge chains. <i>Journal of Physics Condensed Matter</i> , 2011 , 23, 405501	1.8	2
56	Neon atoms oscillating inside carbon and boron nitride nanotubes: a fully atomistic molecular dynamics investigation. <i>Molecular Simulation</i> , 2010 , 36, 639-643	2	2
55	Carcinogenic classification of polycyclic aromatic hydrocarbons through theoretical descriptors. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 718-730	2.1	2
54	Gas-Phase Fluorination of Hexagonal Boron Nitride. <i>Advanced Materials</i> , 2021 , e2106084	24	2
53	Thiophene-Tetrathia-Annulene monolayer (TTA-2D): A new 2D semiconductor material with indirect bandgap. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 129, 114586	3	2
52	Mechanical Properties of Protomene: A Molecular Dynamics Investigation. <i>MRS Advances</i> , 2019 , 4, 191-196		2

51	Nature inspired solid-liquid phase amphibious adhesive. <i>Soft Matter</i> , 2020 , 16, 5854-5860	3.6	2
50	On the mechanical properties of atomic and 3D printed zeolite-templated carbon nanotube networks. <i>Additive Manufacturing</i> , 2021 , 37, 101628	6.1	2
49	Enhancement in magnetization of two-dimensional cobalt telluride and its magnetic field-assisted photocatalytic activity. <i>Applied Physics A: Materials Science and Processing</i> , 2022 , 128, 1	2.6	2
48	Zeolite-templated Carbon Network: A Beta Zeolite Case Study. <i>MRS Advances</i> , 2020 , 5, 751-756	0.7	1
47	On the sulfur doping of Graphdiyne: A Molecular Dynamics and DFT study. <i>MRS Advances</i> , 2020 , 5, 2701-2706	2.7	1
46	Bioinspired Aluminum Composite Reinforced with Soft Polymers with Enhanced Strength and Plasticity. <i>Advanced Engineering Materials</i> , 2020 , 22, 1901116	3.5	1
45	Silver Hardening via Hypersonic Impacts. <i>MRS Advances</i> , 2018 , 3, 493-498	0.7	1
44	Self-Driven Graphene Tearing and Peeling: A Fully Atomistic Molecular Dynamics Investigation. <i>MRS Advances</i> , 2018 , 3, 463-468	0.7	1
43	Species fractionation in atomic chains from mechanically stretched alloys. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 435304	1.8	1
42	Graphene-like Membranes: From Impermeable to Selective Sieves. <i>Materials Research Society Symposia Proceedings</i> , 2014 , 1658, 8		1
41	The Hydrogenation Dynamics of h-BN Sheets. <i>Materials Research Society Symposia Proceedings</i> , 2013 , 1549, 91-98		1
40	Mechanical Properties and Fracture Dynamics of Silicene Membranes. <i>Materials Research Society Symposia Proceedings</i> , 2013 , 1549, 99-107		1
39	van der Waals potential barrier for cobaltocene encapsulation into single-walled carbon nanotubes: classical molecular dynamics and ab initio study. <i>Molecular Simulation</i> , 2011 , 37, 746-751	2	1
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