Douglas S. Galvao

List of Publications by Year
in descending order

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216	8,097	46984 47	53190 85
papers	citations	h-index	g-index

216	216	216	9923
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanical properties of 3D printed macroscopic models of schwarzites. Nano Select, 2022, 3, 450-458.	1.9	7
2	Revisiting Quasicrystals for the Synthesis of 2D Metals. Transactions of the Indian Institute of Metals, 2022, 75, 1093.	0.7	2
3	Mechanical response of pentadiamond: A DFT and molecular dynamics study. Physica B: Condensed Matter, 2022, 629, 413576.	1.3	9
4	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
5	Two-dimensional cobalt telluride as a piezo-tribogenerator. Nanoscale, 2022, 14, 7788-7797.	2.8	18
6	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
7	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
8	Synthesis and Characterization of Biotene: A New 2DÂNatural Oxide From Biotite. Small, 2022, 18, .	5.2	7
9	On the mechanical properties of atomic and 3D printed zeolite-templated carbon nanotube networks. Additive Manufacturing, 2021, 37, 101628.	1.7	14
10	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
11	On the Mechanical Properties of Popgrapheneâ€Based Nanotubes: a Reactive Molecular Dynamics Study. ChemPhysChem, 2021, 22, 701-707.	1.0	5
12	Scalable Synthesis of Atomically Thin Gallium Telluride Nanosheets for Supercapacitor Applications. ACS Applied Nano Materials, 2021, 4, 4829-4838.	2.4	38
13	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
14	Oxygenation of Diamond Surfaces via Hummerâ€™s Method. Chemistry of Materials, 2021, 33, 4977-4987.	3.2	4
15	Controlling Movement at Nanoscale: Curvature Driven Mechanotaxis. Small, 2021, 17, 2100909.	5.2	3
16	Apparent Ferromagnetism in Exfoliated Ultrathin Pyrite Sheets. Journal of Physical Chemistry C, 2021, 125, 18927-18935.	1.5	30
17	A reactive molecular dynamics study of the hydrogenation of diamond surfaces. Computational Materials Science, 2021, 200, 110859.	1.4	2
18	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

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19	Gasâ€Phase Fluorination of Hexagonal Boron Nitride. Advanced Materials, 2021, 33, e2106084.	11.1	10
20	Mechanical and energy-absorption properties of schwarzites. Carbon, 2020, 157, 670-680.	5.4	17
21	Few-Wall Carbon Nanotube Coils. Nano Letters, 2020, 20, 953-962.	4.5	14
22	New Zero Poisson's Ratio Structures. Physica Status Solidi - Rapid Research Letters, 2020, 14, 1900564.	1.2	14
23	On the elastic properties of single-walled phagraphene nanotubes. Chemical Physics Letters, 2020, 756, 137830.	1.2	6
24	Temperature Effects on the Fracture Dynamics and Elastic Properties of Popgraphene Membranes. ChemPhysChem, 2020, 21, 1918-1924.	1.0	5
25	Schwarzites to schwarzynes: A new class of superdeformable materials. MRS Advances, 2020, 5, 1947-1954.	0.5	1
26	Three-dimensional carbon nanotube networks from beta zeolite templates: Thermal stability and mechanical properties. Computational Materials Science, 2020, 182, 109781.	1.4	6
27	Mechanical Properties of Diamond Schwarzites: From Atomistic Models to 3D-Printed Structures. MRS Advances, 2020, 5, 1775-1781.	0.5	9
28	Extraction of Two-Dimensional Aluminum Alloys from Decagonal Quasicrystals. ACS Nano, 2020, 14, 7435-7443.	7.3	19
29	Zeolite-templated Carbon Network: A Beta Zeolite Case Study. MRS Advances, 2020, 5, 751-756.	0.5	2
30	On the sulfur doping of Î³-graphdiyne: A Molecular Dynamics and DFT study. MRS Advances, 2020, 5, 2701-2706.	0.5	1
31	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
32	Structural and electronic properties of defective AlN/GaN hybrid nanostructures. Computational Materials Science, 2020, 183, 109860.	1.4	4
33	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
34	Graphene Supported MoS₂ Structures with High Defect Density for an Efficient HER Electrocatalysts. ACS Applied Materials & Interfaces, 2020, 12, 12629-12638.	4.0	101
35	Bioinspired Aluminum Composite Reinforced with Soft Polymers with Enhanced Strength and Plasticity. Advanced Engineering Materials, 2020, 22, 1901116.	1.6	2
36	Carbon Nanotube Peapods Under High-Strain Rate Conditions: A Molecular Dynamics Investigation. MRS Advances, 2020, 5, 1723-1730.	0.5	3

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37	Nature inspired solidâ€“liquid phase amphibious adhesive. Soft Matter, 2020, 16, 5854-5860.	1.2	3
38	Tuning Penta-Graphene Electronic Properties Through Engineered Line Defects. Scientific Reports, 2020, 10, 8014.	1.6	15
39	Structural and Thermal Stability of Graphyne and Graphdiyne Nanoscroll Structures. ACS Applied Materials & Interfaces, 2019, 11, 2670-2676.	4.0	36
40	Mixing the immiscible through high-velocity mechanical impacts: an experimental and theoretical study. Journal Physics D: Applied Physics, 2019, 52, 445304.	1.3	0
41	Torsional refrigeration by twisted, coiled, and supercoiled fibers. Science, 2019, 366, 216-221.	6.0	133
42	3D Printed Tubulanes as Lightweight Hypervelocity Impact Resistant Structures. Small, 2019, 15, e1904747.	5.2	24
43	Strainâ€Induced Structural Deformation Study of 2D Mo_xW_{(1â€“}_x₎ S₂. Advanced Materials Interfaces, 2019, 6, 1801262.	1.9	13
44	On the mechanical properties of protomene: A theoretical investigation. Computational Materials Science, 2019, 161, 190-198.	1.4	11
45	3D Printing: 3D Printed Tubulanes as Lightweight Hypervelocity Impact Resistant Structures (Small) Tj ETQq1 1 0.784314 rgBT /Overl	5.2	2
46	Mechanical Properties of Protomene: A Molecular Dynamics Investigation. MRS Advances, 2019, 4, 191-196.	0.5	2
47	Idealized Carbon-Based Materials Exhibiting Record Deliverable Capacities for Vehicular Methane Storage. Journal of Physical Chemistry C, 2019, 123, 1050-1058.	1.5	11
48	Schwarzites for Natural Gas Storage: A Grand-Canonical Monte Carlo Study. MRS Advances, 2018, 3, 115-120.	0.5	8
49	Silver Hardening via Hypersonic Impacts. MRS Advances, 2018, 3, 493-498.	0.5	1
50	Efficient prediction of suitable functional monomers for molecular imprintingvialocal density of states calculations. Physical Chemistry Chemical Physics, 2018, 20, 13153-13158.	1.3	9
51	Virtually imprinted polymers (VIPs): understanding molecularly templated materialsviamolecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 13145-13152.	1.3	19
52	Differences in the Mechanical Properties of Monolayer and Multilayer WSe2/MoSe2. MRS Advances, 2018, 3, 373-378.	0.5	2
53	Mechanical Properties of Schwarzites - A Fully Atomistic Reactive Molecular Dynamics Investigation. MRS Advances, 2018, 3, 451-456.	0.5	7
54	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

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55	Liquid Exfoliation of Icosahedral Quasicrystals. Advanced Functional Materials, 2018, 28, 1801181.	7.8	21
56	Deformation Mechanisms of Vertically Stacked WS₂ /MoS₂ Heterostructures: The Role of Interfaces. ACS Nano, 2018, 12, 4036-4044.	7.3	54
57	Mechanical Properties of Pentagraphene-based Nanotubes: A Molecular Dynamics Study. MRS Advances, 2018, 3, 97-102.	0.5	10
58	Water/Alcohol Separation in Graphene Oxide Membranes: Insights from Molecular Dynamics and Monte Carlo Simulations. MRS Advances, 2018, 3, 109-114.	0.5	5
59	Self-Driven Graphene Tearing and Peeling: A Fully Atomistic Molecular Dynamics Investigation. MRS Advances, 2018, 3, 463-468.	0.5	1
60	Improving Graphene-metal Contacts: Thermal Induced Polishing. MRS Advances, 2018, 3, 73-78.	0.5	4
61	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
62	Mechanical Properties of Ultralow Density Graphene Oxide/Polydimethylsiloxane Foams. MRS Advances, 2018, 3, 61-66.	0.5	2
63	Mechanical Properties of Phagraphene Membranes: A Fully Atomistic Molecular Dynamics Investigation. MRS Advances, 2018, 3, 67-72.	0.5	6
64	Structural transformations of carbon and boron nitride nanoscrolls at high impact collisions. Physical Chemistry Chemical Physics, 2018, 20, 4911-4916.	1.3	15
65	Scale Effects on the Ballistic Penetration of Graphene Sheets. Scientific Reports, 2018, 8, 6750.	1.6	46
66	Molecular dynamics simulations of ballistic penetration of penta-graphene sheets. MRS Advances, 2018, 3, 433-437.	0.5	4
67	Multiscale Geometric Design Principles Applied to 3D Printed Schwarzites. Advanced Materials, 2018, 30, 1704820.	11.1	76
68	On the mechanical properties of novamene: A fully atomistic molecular dynamics and DFT investigation. Carbon, 2018, 139, 782-788.	5.4	18
69	Exfoliation of a non-van der Waals material from iron ore hematite. Nature Nanotechnology, 2018, 13, 602-609.	15.6	295
70	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
71	Mechanical and Thermal Stability of Graphyne and Graphdiyne Nanoscrolls. MRS Advances, 2017, 2, 129-134.	0.5	3
72	High Toughness in Ultralow Density Graphene Oxide Foam. Advanced Materials Interfaces, 2017, 4, 1700030.	1.9	20

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73	Permeation of Water Nanodroplets on Carbon Nanotubes Forests. MRS Advances, 2017, 2, 123-128.	0.5	0
74	Design of Porous Metal-Organic Frameworks for Adsorption Driven Thermal Batteries. MRS Advances, 2017, 2, 519-524.	0.5	28
75	Nanodroplets Behavior on Graphdiyne Membranes. MRS Advances, 2017, 2, 1551-1556.	0.5	0
76	Multifunctional Hybrids Based on 2D Fluorinated Graphene Oxide and Superparamagnetic Iron Oxide Nanoparticles. Particle and Particle Systems Characterization, 2017, 34, 1700245.	1.2	7
77	Lightweight Hexagonal Boron Nitride Foam for CO₂ Absorption. ACS Nano, 2017, 11, 8944-8952.	7.3	56
78	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
79	The structural and dynamical aspects of boron nitride nanotubes under high velocity impacts. Physical Chemistry Chemical Physics, 2016, 18, 14776-14781.	1.3	15
80	Nanodroplets Impacting on Graphene. MRS Advances, 2016, 1, 675-680.	0.5	3
81	Synthesis and porous h-BN 3D architectures for effective humidity and gas sensors. RSC Advances, 2016, 6, 87888-87896.	1.7	43
82	Ballistic Fracturing of Carbon Nanotubes. ACS Applied Materials & Interfaces, 2016, 8, 24819-24825.	4.0	16
83	3D Porous Graphene by Lowâ€Temperature Plasma Welding for Bone Implants. Advanced Materials, 2016, 28, 8959-8967.	11.1	52
84	Enhanced supercapacitor performance of a 3D architecture tailored using atomically thin rGOâ€“MoS₂ 2D sheets. RSC Advances, 2016, 6, 93384-93393.	1.7	35
85	Strong, Twistâ€Stable Carbon Nanotube Yarns and Muscles by Tension Annealing at Extreme Temperatures. Advanced Materials, 2016, 28, 6598-6605.	11.1	100
86	Controlled 3D Carbon Nanotube Structures by Plasma Welding. Advanced Materials Interfaces, 2016, 3, 1500755.	1.9	25
87	Evaluation of carbon nanoscroll materials for post-combustion CO2 capture. Carbon, 2016, 101, 218-225.	5.4	31
88	Surface functionalization of two-dimensional metal chalcogenides by Lewis acidâ€“base chemistry. Nature Nanotechnology, 2016, 11, 465-471.	15.6	197
89	Graphene healing mechanisms: A theoretical investigation. Carbon, 2016, 99, 302-309.	5.4	29
90	Solidâ€“Liquid Self-Adaptive Polymeric Composite. ACS Applied Materials & Interfaces, 2016, 8, 2142-2147.	4.0	6

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91	Defect-Free Carbon Nanotube Coils. Nano Letters, 2016, 16, 2152-2158.	4.5	20
92	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
93	Burning Graphene Layer-by-Layer. Scientific Reports, 2015, 5, 11546.	1.6	26
94	Chemical Vapor Deposition of Monolayer Rhenium Disulfide (ReS₂). Advanced Materials, 2015, 27, 4640-4648.	11.1	203
95	High Pressure Induced Binding Between Linear Carbon Chains and Nanotubes. Materials Research Society Symposia Proceedings, 2015, 1752, 53-58.	0.1	0
96	Ambient solid-state mechano-chemical reactions between functionalized carbon nanotubes. Nature Communications, 2015, 6, 7291.	5.8	35
97	Enhanced Mechanical Stability of Gold Nanotips through Carbon Nanocone Encapsulation. Scientific Reports, 2015, 5, 10408.	1.6	21
98	Hierarchically buckled sheath-core fibers for superelastic electronics, sensors, and muscles. Science, 2015, 349, 400-404.	6.0	447
99	Linear Carbon Chains under High-Pressure Conditions. Journal of Physical Chemistry C, 2015, 119, 10669-10676.	1.5	46
100	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
101	Synthesis of Low-Density, Carbon-Doped, Porous Hexagonal Boron Nitride Solids. ACS Nano, 2015, 9, 12088-12095.	7.3	81
102	A Brief Review on Syntheses, Structures, and Applications of Nanoscrolls. Frontiers in Materials, 2014, 1, .	1.2	31
103	One-dimensional silicon and germanium nanostructures with no carbon analogues. Physical Chemistry Chemical Physics, 2014, 16, 24570-24574.	1.3	8
104	Species fractionation in atomic chains from mechanically stretched alloys. Journal of Physics Condensed Matter, 2014, 26, 435304.	0.7	0
105	Violation of the universal behavior of membranes inside cylindrical tubes at nanoscale. Europhysics Letters, 2014, 105, 56002.	0.7	2
106	Mechanical Properties of Graphene Nanowiggles. Materials Research Society Symposia Proceedings, 2014, 1658, 14.	0.1	0
107	Graphene-like Membranes: From Impermeable to Selective Sieves. Materials Research Society Symposia Proceedings, 2014, 1658, 8.	0.1	1
108	Designing nanoscaled hybrids from atomic layered boron nitride with silver nanoparticle deposition. Journal of Materials Chemistry A, 2014, 2, 3148.	5.2	65

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109	Mechanical properties and fracture dynamics of silicene membranes. Physical Chemistry Chemical Physics, 2014, 16, 19417-19423.	1.3	56
110	Inorganic Graphenylene: A Porous Two-Dimensional Material With Tunable Band Gap. Journal of Physical Chemistry C, 2014, 118, 23670-23674.	1.5	76
111	Low-density three-dimensional foam using self-reinforced hybrid two-dimensional atomic layers. Nature Communications, 2014, 5, 4541.	5.8	91
112	Unzipping Carbon Nanotubes at High Impact. Nano Letters, 2014, 14, 4131-4137.	4.5	63
113	Novel Nanoscroll Structures from Carbon Nitride Layers. ChemPhysChem, 2014, 15, 2367-2371.	1.0	11
114	Dynamical aspects of the unzipping of multiwalled boron nitride nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 19147.	1.3	6
115	Controlled route to the fabrication of carbon and boron nitride nanoscrolls: A molecular dynamics investigation. Journal of Applied Physics, 2013, 113, .	1.1	38
116	Dynamics of the Formation of Carbon Nanotube Serpentines. Physical Review Letters, 2013, 110, 105502.	2.9	10
117	Graphene to fluorographene and fluorographane: a theoretical study. Nanotechnology, 2013, 24, 035706.	1.3	69
118	The Hydrogenation Dynamics of h-BN Sheets. Materials Research Society Symposia Proceedings, 2013, 1549, 91-98.	0.1	1
119	Mechanical Properties and Fracture Dynamics of Silicene Membranes. Materials Research Society Symposia Proceedings, 2013, 1549, 99-107.	0.1	1
120	Graphyne Oxidation: Insights From a Reactive Molecular Dynamics Investigation. Materials Research Society Symposia Proceedings, 2013, 1549, 53-58.	0.1	6
121	Fracture Patterns of Boron Nitride Nanotubes. Materials Research Society Symposia Proceedings, 2013, 1526, 1.	0.1	0
122	On the Dynamics of Graphdiyne Hydrogenation. Materials Research Society Symposia Proceedings, 2013, 1549, 59-64.	0.1	4
123	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
124	A Nonzero Gap Two-dimensional Carbon Allotrope from Porous Graphene. Materials Research Society Symposia Proceedings, 2012, 1407, 199.	0.1	2
125	When Small is Different: The Case of Membranes Inside Tubes. Materials Research Society Symposia Proceedings, 2012, 1451, 15-20.	0.1	0
126	Correlation Between Quantum Conductance and Atomic Arrangement of Silver Atomic-Size Nanocontacts. Materials Research Society Symposia Proceedings, 2012, 1429, 7.	0.1	1

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127	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
128	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
129	On the Existence of Ordered Phases of Encapsulated Diamondoids into Carbon Nanotubes. Materials Research Society Symposia Proceedings, 2012, 1407, 26.	0.1	0
130	Electrically, Chemically, and Photonically Powered Torsional and Tensile Actuation of Hybrid Carbon Nanotube Yarn Muscles. Science, 2012, 338, 928-932.	6.0	585
131	Nonzero Gap Two-Dimensional Carbon Allotrope from Porous Graphene. Journal of Physical Chemistry C, 2012, 116, 12810-12813.	1.5	152
132	On the unzipping of multiwalled carbon nanotubes. Nanotechnology, 2012, 23, 465702.	1.3	39
133	Comparative parametric method 6 (PM6) and Recife model 1 (RM1) study oftrans-stilbene. Molecular Simulation, 2012, 38, 1-7.	0.9	7
134	Correlation between quantum conductance and atomic arrangement of atomic-size silver nanowires. Journal of Applied Physics, 2012, 111, 124316.	1.1	12
135	Temperature effects on the occurrence of long interatomic distances in atomic chains formed from stretched gold nanowires. Nanotechnology, 2011, 22, 095705.	1.3	8
136	Electronic properties of Fibonacci and random Siâ€“Ge chains. Journal of Physics Condensed Matter, 2011, 23, 405501.	0.7	4
137	Ordered phases of encapsulated diamondoids into carbon nanotubes. Nanotechnology, 2011, 22, 315708.	1.3	22
138	Intrinsic Stability of the Smallest Possible Silver Nanotube. Physical Review Letters, 2011, 106, 065501.	2.9	21
139	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
140	The First Molecular Wheel: A Theoretical Investigation. Materials Research Society Symposia Proceedings, 2011, 1286, 44.	0.1	0
141	Mechanical Deformation of Nanoscale Metal Rods: When Size and Shape Matter. Physical Review Letters, 2011, 106, 055501.	2.9	28
142	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
143	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
144	Dynamics of Graphene Nanodrums. Materials Research Society Symposia Proceedings, 2011, 1284, 173.	0.1	0

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145	Stability and Dynamics of Boron Nitride Nanoscrolls. Materials Research Society Symposia Proceedings, 2011, 1307, 1.	0.1	1
146	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
147	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
148	Topologically Closed Macromolecules Made of Single Walled Carbon Nanotubesâ€"'Super'-Fullerenes. Journal of Nanoscience and Nanotechnology, 2010, 10, 4378-4383.	0.9	4
149	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
150	Temperature effects on the atomic arrangement and conductance of atomic-size gold nanowires generated by mechanical stretching. Nanotechnology, 2010, 21, 485702.	1.3	18
151	Curved graphene nanoribbons: structure and dynamics of carbon nanobelts. Nanotechnology, 2010, 21, 075710.	1.3	59
152	Neon atoms oscillating inside carbon and boron nitride nanotubes: a fully atomistic molecular dynamics investigation. Molecular Simulation, 2010, 36, 639-643.	0.9	2
153	Carbon nanotube with square cross-section: An ab initio investigation. Journal of Chemical Physics, 2010, 133, 124513.	1.2	17
154	Thermophoretically driven carbon nanotube oscillators. Applied Physics Letters, 2009, 95, .	1.5	20
155	Observation of the smallest metal nanotube with a square cross-section. Nature Nanotechnology, 2009, 4, 149-152.	15.6	50
156	New Insights on the Growth of Anisotropic Nanoparticles from Total Energy Calculations. Journal of Physical Chemistry C, 2009, 113, 11976-11979.	1.5	4
157	Graphene to graphane: a theoretical study. Nanotechnology, 2009, 20, 465704.	1.3	219
158	Defects in Graphene-Based Twisted Nanoribbons: Structural, Electronic, and Optical Properties. Langmuir, 2009, 25, 4751-4759.	1.6	26
159	The structure and dynamics of boron nitride nanoscrolls. Nanotechnology, 2009, 20, 335702.	1.3	51
160	C₆₀-derived nanobaskets: stability, vibrational signatures, and molecular trapping. Nanotechnology, 2009, 20, 395701.	1.3	8
161	Some electronic properties of saturated and unsaturated cubane oligomers using DFT-based calculations. Computational and Theoretical Chemistry, 2008, 868, 37-41.	1.5	9
162	Modeling the auxetic transition for carbon nanotube sheets. Physical Review B, 2008, 78, .	1.1	42

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163	Sign Change of Poisson's Ratio for Carbon Nanotube Sheets. Science, 2008, 320, 504-507.	6.0	245
164	MÃ¶bius and twisted graphene nanoribbons: Stability, geometry, and electronic properties. Journal of Chemical Physics, 2008, 128, 164719.	1.2	54
165	Carbon Nanotubes as Reinforcement Elements of Composite Nanotools. Nano Letters, 2008, 8, 842-847.	4.5	21
166	Rotational dynamics and polymerization of C60 in C60-cubane crystals: A molecular dynamics study. Journal of Chemical Physics, 2008, 129, 064506.	1.2	10
167	Large electromechanical response in silicon nanowires predicted from first-principles electronic structure calculations. Physical Review B, 2008, 77, .	1.1	4
168	Entanglement and the Nonlinear Elastic Behavior of Forests of Coiled Carbon Nanotubes. Physical Review Letters, 2008, 100, 086807.	2.9	42
169	Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes. Journal of Physics Condensed Matter, 2007, 19, 236222.	0.7	15
170	Is it possible to grow amorphous normal nanosprings?. Nanotechnology, 2007, 18, 435606.	1.3	4
171	Prediction of the hydrogen storage capacity of carbon nanoscrolls. Physical Review B, 2007, 75, .	1.1	98
172	Size Limit of Defect Formation in Pyramidal Pt Nanocontacts. Physical Review Letters, 2007, 99, 255501.	2.9	16
173	Mechanical properties of carbon nanotube networks by molecular mechanics and impact molecular dynamics calculations. Physical Review B, 2007, 75, .	1.1	49
174	Atomistic simulations of the mechanical properties of â€˜superâ€™ carbon nanotubes. Nanotechnology, 2007, 18, 335702.	1.3	72
175	Molecular dynamics simulation of single wall carbon nanotubes polymerization under compression. Journal of Computational Chemistry, 2007, 28, 1724-1734.	1.5	13
176	Transmission electron microscopy and molecular dynamics study of the formation of suspended copper linear atomic chains. Physical Review B, 2006, 74, .	1.1	27
177	Elastic properties of nanowires. Journal of Applied Physics, 2006, 99, 094310.	1.1	15
178	Synthetic melanin films: Assembling mechanisms, scaling behavior, and structural properties. Journal of Applied Physics, 2006, 99, 113511.	1.1	41
179	Experimental realization of suspended atomic chains composed of different atomic species. Nature Nanotechnology, 2006, 1, 182-185.	15.6	95
180	Geometric and electronic structure of carbon nanotube networks: â€˜superâ€™-carbon nanotubes. Nanotechnology, 2006, 17, 617-621.	1.3	74

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181	Mechanical properties of amorphous nanosprings. Nanotechnology, 2006, 17, 5620-5626.	1.3	18
182	Prediction of giant electroactuation for papyruslike carbon nanoscroll structures: First-principles calculations. Physical Review B, 2006, 74, .	1.1	63
183	Structural and electronic properties of radialenes and related systems. Computational and Theoretical Chemistry, 2005, 729, 203-210.	1.5	6
184	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
185	Chaotic signature in the motion of coupled carbon nanotube oscillators. Nanotechnology, 2005, 16, 583-589.	1.3	34
186	Carcinogenic classification of polycyclic aromatic hydrocarbons through theoretical descriptors. International Journal of Quantum Chemistry, 2005, 103, 718-730.	1.0	2
187	Prediction of Ordered Phases of Encapsulated C60, C70, and C78Inside Carbon Nanotubes. Nano Letters, 2005, 5, 349-355.	4.5	85
188	Contaminants in Suspended Gold Chains: AnAb InitioMolecular Dynamics Study. Physical Review Letters, 2004, 93, 216103.	2.9	32
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