Douglas S. Galvao

List of Publications by Year in Descending Order

212 papers	6,521 citations	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	Revisiting Quasicrystals for the Synthesis of 2D Metals. *Transactions of the Indian Institute of Metals*, **2022**, 75, 1093	1.2	1
211	Mechanical response of pentadiamond: A DFT and molecular dynamics study. *Physica B: Condensed Matter*, **2022**, 629, 413576	2.8	3
210	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	2.6	2
209	Gas-Phase Fluorination of Hexagonal Boron Nitride. *Advanced Materials*, **2021**, e2106084	24	2
208	On the Mechanical Properties of Popgraphene-Based Nanotubes: a Reactive Molecular Dynamics Study. *ChemPhysChem*, **2021**, 22, 701-707	3.2	1
207	Scalable Synthesis of Atomically Thin Gallium Telluride Nanosheets for Supercapacitor Applications. *ACS Applied Nano Materials*, **2021**, 4, 4829-4838	5.6	15
206	Thiophene-Tetrathia-Annulene monolayer (TTA-2D): A new 2D semiconductor material with indirect bandgap. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 129, 114586	3	2
205	Oxygenation of Diamond Surfaces via Hummers Method. *Chemistry of Materials*, **2021**, 33, 4977-4987	9.6	1
204	Controlling Movement at Nanoscale: Curvature Driven Mechanotaxis. *Small*, **2021**, 17, e2100909	11	1
203	On the mechanical properties of atomic and 3D printed zeolite-templated carbon nanotube networks. *Additive Manufacturing*, **2021**, 37, 101628	6.1	2
202	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	3.8	
201	Apparent Ferromagnetism in Exfoliated Ultrathin Pyrite Sheets. *Journal of Physical Chemistry C*, **2021**, 125, 18927-18935	3.8	8
200	A reactive molecular dynamics study of the hydrogenation of diamond surfaces. *Computational Materials Science*, **2021**, 200, 110859	3.2	0
199	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	3.6	3
198	Three-dimensional carbon nanotube networks from beta zeolite templates: Thermal stability and mechanical properties. *Computational Materials Science*, **2020**, 182, 109781	3.2	3
197	Mechanical Properties of Diamond Schwarzites: From Atomistic Models to 3D-Printed Structures. *MRS Advances*, **2020**, 5, 1775-1781	0.7	2
196	Extraction of Two-Dimensional Aluminum Alloys from Decagonal Quasicrystals. *ACS Nano*, **2020**, 14, 7435-7443	16.7	11

195	Zeolite-templated Carbon Network: A Beta Zeolite Case Study. *MRS Advances*, **2020**, 5, 751-756	0.7	1
194	On the sulfur doping of graphdiyne: A Molecular Dynamics and DFT study. *MRS Advances*, **2020**, 5, 2701-2706	0.7	1
193	On the Mechanical Properties and Thermal Stability of a Recently Synthesized Monolayer Amorphous Carbon. *Journal of Physical Chemistry C*, **2020**, 124, 14855-14860	3.8	7
192	Structural and electronic properties of defective AlN/GaN hybrid nanostructures. *Computational Materials Science*, **2020**, 183, 109860	3.2	2
191	On the structural stability and optical properties of germanium-based schwarzites: a density functional theory investigation. *Physical Chemistry Chemical Physics*, **2020**, 22, 16286-16293	3.6	
190	Graphene Supported MoS Structures with High Defect Density for an Efficient HER Electrocatalysts. *ACS Applied Materials & Interfaces*, **2020**, 12, 12629-12638	9.5	49
189	Bioinspired Aluminum Composite Reinforced with Soft Polymers with Enhanced Strength and Plasticity. *Advanced Engineering Materials*, **2020**, 22, 1901116	3.5	1
188	Carbon Nanotube Peapods Under High-Strain Rate Conditions: A Molecular Dynamics Investigation. *MRS Advances*, **2020**, 5, 1723-1730	0.7	0
187	Tuning Penta-Graphene Electronic Properties Through Engineered Line Defects. *Scientific Reports*, **2020**, 10, 8014	4.9	5
186	Mechanical and energy-absorption properties of schwarzites. *Carbon*, **2020**, 157, 670-680	10.4	11
185	Few-Wall Carbon Nanotube Coils. *Nano Letters*, **2020**, 20, 953-962	11.5	7
184	New Zero Poisson's Ratio Structures. *Physica Status Solidi - Rapid Research Letters*, **2020**, 14, 1900564	2.5	4
183	On the elastic properties of single-walled phagraphene nanotubes. *Chemical Physics Letters*, **2020**, 756, 137830	2.5	1
182	Temperature Effects on the Fracture Dynamics and Elastic Properties of Popgraphene Membranes. *ChemPhysChem*, **2020**, 21, 1918-1924	3.2	1
181	Schwarzites to schwarzynes: A new class of superdeformable materials. *MRS Advances*, **2020**, 5, 1947-1954	0.7	0
180	Nature inspired solid-liquid phase amphibious adhesive. *Soft Matter*, **2020**, 16, 5854-5860	3.6	2
179	Strain-Induced Structural Deformation Study of 2D MoxW(1-x) S2. *Advanced Materials Interfaces*, **2019**, 6, 1801262	4.6	9
178	On the mechanical properties of protomene: A theoretical investigation. *Computational Materials Science*, **2019**, 161, 190-198	3.2	10

177	Structural and Thermal Stability of Graphyne and Graphdiyne Nanoscroll Structures. *ACS Applied Materials & Interfaces*, **2019**, 11, 2670-2676	9.5	22
176	Mixing the immiscible through high-velocity mechanical impacts: an experimental and theoretical study. *Journal Physics D: Applied Physics*, **2019**, 52, 445304	3	
175	Torsional refrigeration by twisted, coiled, and supercoiled fibers. *Science*, **2019**, 366, 216-221	33.3	65
174	3D Printed Tubulanes as Lightweight Hypervelocity Impact Resistant Structures. *Small*, **2019**, 15, e1904747	11	13
173	3D Printing: 3D Printed Tubulanes as Lightweight Hypervelocity Impact Resistant Structures (Small 52/2019). *Small*, **2019**, 15, 1970284	11	1
172	Mechanical Properties of Protomene: A Molecular Dynamics Investigation. *MRS Advances*, **2019**, 4, 191-196	0.7	2
171	Idealized Carbon-Based Materials Exhibiting Record Deliverable Capacities for Vehicular Methane Storage. *Journal of Physical Chemistry C*, **2019**, 123, 1050-1058	3.8	6
170	Schwarzites for Natural Gas Storage: A Grand-Canonical Monte Carlo Study. *MRS Advances*, **2018**, 3, 115-120	0.7	4
169	Silver Hardening via Hypersonic Impacts. *MRS Advances*, **2018**, 3, 493-498	0.7	1
168	Efficient prediction of suitable functional monomers for molecular imprinting via local density of states calculations. *Physical Chemistry Chemical Physics*, **2018**, 20, 13153-13158	3.6	8
167	Virtually imprinted polymers (VIPs): understanding molecularly templated materials via molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2018**, 20, 13145-13152	3.6	15
166	Differences in the Mechanical Properties of Monolayer and Multilayer WSe2/MoSe2. *MRS Advances*, **2018**, 3, 373-378	0.7	2
165	Mechanical Properties of Schwarzites - A Fully Atomistic Reactive Molecular Dynamics Investigation. *MRS Advances*, **2018**, 3, 451-456	0.7	5
164	Experimental and computational investigation of reduced graphene oxide nanoplatelets stabilized in poly(styrene sulfonate) sodium salt. *Journal of Materials Science*, **2018**, 53, 10049-10058	4.3	13
163	Liquid Exfoliation of Icosahedral Quasicrystals. *Advanced Functional Materials*, **2018**, 28, 1801181	15.6	14
162	Deformation Mechanisms of Vertically Stacked WS /MoS Heterostructures: The Role of Interfaces. *ACS Nano*, **2018**, 12, 4036-4044	16.7	35
161	Mechanical Properties of Pentagraphene-based Nanotubes: A Molecular Dynamics Study. *MRS Advances*, **2018**, 3, 97-102	0.7	9
160	Water/Alcohol Separation in Graphene Oxide Membranes: Insights from Molecular Dynamics and Monte Carlo Simulations. *MRS Advances*, **2018**, 3, 109-114	0.7	2

159	Self-Driven Graphene Tearing and Peeling: A Fully Atomistic Molecular Dynamics Investigation. *MRS Advances*, **2018**, 3, 463-468	0.7	1
158	Improving Graphene-metal Contacts: Thermal Induced Polishing. *MRS Advances*, **2018**, 3, 73-78	0.7	4
157	On hardening silver nanocubes by high-velocity impacts: a fully atomistic molecular dynamics investigation. *Journal of Materials Science*, **2018**, 53, 7486-7492	4.3	4
156	Mechanical Properties of Ultralow Density Graphene Oxide/Polydimethylsiloxane Foams. *MRS Advances*, **2018**, 3, 61-66	0.7	0
155	Mechanical Properties of Phagraphene Membranes: A Fully Atomistic Molecular Dynamics Investigation. *MRS Advances*, **2018**, 3, 67-72	0.7	4
154	Structural transformations of carbon and boron nitride nanoscrolls at high impact collisions. *Physical Chemistry Chemical Physics*, **2018**, 20, 4911-4916	3.6	11
153	Scale Effects on the Ballistic Penetration of Graphene Sheets. *Scientific Reports*, **2018**, 8, 6750	4.9	25
152	Molecular dynamics simulations of ballistic penetration of penta-graphene sheets. *MRS Advances*, **2018**, 3, 433-437	0.7	4
151	On the mechanical properties of novamene: A fully atomistic molecular dynamics and DFT investigation. *Carbon*, **2018**, 139, 782-788	10.4	16
150	Exfoliation of a non-van der Waals material from iron ore hematite. *Nature Nanotechnology*, **2018**, 13, 602-609	28.7	179
149	Synthesis and 3D Interconnected Nanostructured h-BN-Based Biocomposites by Low-Temperature Plasma Sintering: Bone Regeneration Applications. *ACS Omega*, **2018**, 3, 6013-6021	3.9	18
148	Multiscale Geometric Design Principles Applied to 3D Printed Schwarzites. *Advanced Materials*, **2018**, 30, 1704820	24	44
147	Mechanical and Thermal Stability of Graphyne and Graphdiyne Nanoscrolls. *MRS Advances*, **2017**, 2, 129-134	0.7	3
146	High Toughness in Ultralow Density Graphene Oxide Foam. *Advanced Materials Interfaces*, **2017**, 4, 1700030	4.6	15
145	Permeation of Water Nanodroplets on Carbon Nanotubes Forests. *MRS Advances*, **2017**, 2, 123-128	0.7	
144	Design of Porous Metal-Organic Frameworks for Adsorption Driven Thermal Batteries. *MRS Advances*, **2017**, 2, 519-524	0.7	22
143	Nanodroplets Behavior on Graphdiyne Membranes. *MRS Advances*, **2017**, 2, 1551-1556	0.7	
142	Multifunctional Hybrids Based on 2D Fluorinated Graphene Oxide and Superparamagnetic Iron Oxide Nanoparticles. *Particle and Particle Systems Characterization*, **2017**, 34, 1700245	3.1	5

141	Lightweight Hexagonal Boron Nitride Foam for CO Absorption. *ACS Nano*, **2017**, 11, 8944-8952	16.7	42
140	Gas Adsorption and Separation by the Al-Based Metal Organic Framework MIL-160. *Journal of Physical Chemistry C*, **2017**, 121, 26822-26832	3.8	32
139	Ballistic Fracturing of Carbon Nanotubes. *ACS Applied Materials & Interfaces*, **2016**, 8, 24819-25	9.5	13
138	3D Porous Graphene by Low-Temperature Plasma Welding for Bone Implants. *Advanced Materials*, **2016**, 28, 8959-8967	24	43
137	Enhanced supercapacitor performance of a 3D architecture tailored using atomically thin rGO MoS2 2D sheets. *RSC Advances*, **2016**, 6, 93384-93393	3.7	27
136	Strong, Twist-Stable Carbon Nanotube Yarns and Muscles by Tension Annealing at Extreme Temperatures. *Advanced Materials*, **2016**, 28, 6598-605	24	72
135	Controlled 3D Carbon Nanotube Structures by Plasma Welding. *Advanced Materials Interfaces*, **2016**, 3, 1500755	4.6	21
134	Evaluation of carbon nanoscroll materials for post-combustion CO2 capture. *Carbon*, **2016**, 101, 218-225	10.4	23
133	Surface functionalization of two-dimensional metal chalcogenides by Lewis acid-base chemistry. *Nature Nanotechnology*, **2016**, 11, 465-71	28.7	150
132	Graphene healing mechanisms: A theoretical investigation. *Carbon*, **2016**, 99, 302-309	10.4	25
131	Solid-Liquid Self-Adaptive Polymeric Composite. *ACS Applied Materials & Interfaces*, **2016**, 8, 2142-7	9.5	5
130	Defect-Free Carbon Nanotube Coils. *Nano Letters*, **2016**, 16, 2152-8	11.5	15
129	The structural and dynamical aspects of boron nitride nanotubes under high velocity impacts. *Physical Chemistry Chemical Physics*, **2016**, 18, 14776-81	3.6	13
128	Nanodroplets Impacting on Graphene. *MRS Advances*, **2016**, 1, 675-680	0.7	3
127	Synthesis and porous h-BN 3D architectures for effective humidity and gas sensors. *RSC Advances*, **2016**, 6, 87888-87896	3.7	26
126	High Pressure Induced Binding Between Linear Carbon Chains and Nanotubes. *Materials Research Society Symposia Proceedings*, **2015**, 1752, 53-58		
125	Ambient solid-state mechano-chemical reactions between functionalized carbon nanotubes. *Nature Communications*, **2015**, 6, 7291	17.4	28
124	Enhanced Mechanical Stability of Gold Nanotips through Carbon Nanocone Encapsulation. *Scientific Reports*, **2015**, 5, 10408	4.9	13

123	STRETCHY ELECTRONICS. Hierarchically buckled sheath-core fibers for superelastic electronics, sensors, and muscles. *Science*, **2015**, 349, 400-4	33.3	346
122	Linear Carbon Chains under High-Pressure Conditions. *Journal of Physical Chemistry C*, **2015**, 119, 10669-10676	4.8	37
121	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, 094301	2.5	3
120	Synthesis of Low-Density, Carbon-Doped, Porous Hexagonal Boron Nitride Solids. *ACS Nano*, **2015**, 9, 12088-95	16.7	61
119	The Influence of Morphology on the Charge Transport in Two-Phase Disordered Organic Systems. *Materials Research Society Symposia Proceedings*, **2015**, 1737, 13		
118	Burning Graphene Layer-by-Layer. *Scientific Reports*, **2015**, 5, 11546	4.9	20
117	Chemical Vapor Deposition of Monolayer Rhenium Disulfide (ReS2). *Advanced Materials*, **2015**, 27, 4640-8	14	177
116	Designing nanoscaled hybrids from atomic layered boron nitride with silver nanoparticle deposition. *Journal of Materials Chemistry A*, **2014**, 2, 3148	13	52
115	Mechanical properties and fracture dynamics of silicene membranes. *Physical Chemistry Chemical Physics*, **2014**, 16, 19417-23	3.6	49
114	Inorganic Graphenylene: A Porous Two-Dimensional Material With Tunable Band Gap. *Journal of Physical Chemistry C*, **2014**, 118, 23670-23674	3.8	56
113	Low-density three-dimensional foam using self-reinforced hybrid two-dimensional atomic layers. *Nature Communications*, **2014**, 5, 4541	17.4	82
112	Unzipping carbon nanotubes at high impact. *Nano Letters*, **2014**, 14, 4131-7	11.5	55
111	Novel nanoscroll structures from carbon nitride layers. *ChemPhysChem*, **2014**, 15, 2367-71	3.2	10
110	A Brief Review on Syntheses, Structures, and Applications of Nanoscrolls. *Frontiers in Materials*, **2014**, 1,	4	24
109	One-dimensional silicon and germanium nanostructures with no carbon analogues. *Physical Chemistry Chemical Physics*, **2014**, 16, 24570-4	3.6	6
108	Species fractionation in atomic chains from mechanically stretched alloys. *Journal of Physics Condensed Matter*, **2014**, 26, 435304	1.8	1
107	Violation of the universal behavior of membranes inside cylindrical tubes at nanoscale. *Europhysics Letters*, **2014**, 105, 56002	1.6	2
106	Mechanical Properties of Graphene Nanowiggles. *Materials Research Society Symposia Proceedings*, **2014**, 1658, 14		

105	Graphene-like Membranes: From Impermeable to Selective Sieves. *Materials Research Society Symposia Proceedings*, **2014**, 1658, 8		1
104	Dynamical aspects of the unzipping of multiwalled boron nitride nanotubes. *Physical Chemistry Chemical Physics*, **2013**, 15, 19147-50	3.6	4
103	Controlled route to the fabrication of carbon and boron nitride nanoscrolls: A molecular dynamics investigation. *Journal of Applied Physics*, **2013**, 113, 054306	2.5	37
102	Dynamics of the formation of carbon nanotube serpentines. *Physical Review Letters*, **2013**, 110, 105502	7.4	10
101	Graphene to fluorographene and fluorographane: a theoretical study. *Nanotechnology*, **2013**, 24, 035706	3.4	64
100	The Hydrogenation Dynamics of h-BN Sheets. *Materials Research Society Symposia Proceedings*, **2013**, 1549, 91-98		1
99	Mechanical Properties and Fracture Dynamics of Silicene Membranes. *Materials Research Society Symposia Proceedings*, **2013**, 1549, 99-107		1
98	Graphyne Oxidation: Insights From a Reactive Molecular Dynamics Investigation. *Materials Research Society Symposia Proceedings*, **2013**, 1549, 53-58		5
97	Fracture Patterns of Boron Nitride Nanotubes. *Materials Research Society Symposia Proceedings*, **2013**, 1526, 1		
96	On the Dynamics of Graphdiyne Hydrogenation. *Materials Research Society Symposia Proceedings*, **2013**, 1549, 59-64		2
95	Electrically, chemically, and photonically powered torsional and tensile actuation of hybrid carbon nanotube yarn muscles. *Science*, **2012**, 338, 928-32	33.3	462
94	Nonzero Gap Two-Dimensional Carbon Allotrope from Porous Graphene. *Journal of Physical Chemistry C*, **2012**, 116, 12810-12813	3.8	120
93	On the unzipping of multiwalled carbon nanotubes. *Nanotechnology*, **2012**, 23, 465702	3.4	33
92	Comparative parametric method 6 (PM6) and Recife model 1 (RM1) study of trans-stilbene. *Molecular Simulation*, **2012**, 38, 1-7	2	6
91	Correlation between quantum conductance and atomic arrangement of atomic-size silver nanowires. *Journal of Applied Physics*, **2012**, 111, 124316	2.5	11
90	Tribological Properties of Graphene and Boron-Nitride Layers: A Fully Atomistic Molecular Dynamics Study. *Materials Research Society Symposia Proceedings*, **2012**, 1407, 181		
89	A Nonzero Gap Two-dimensional Carbon Allotrope from Porous Graphene. *Materials Research Society Symposia Proceedings*, **2012**, 1407, 199		1
88	When Small is Different: The Case of Membranes Inside Tubes. *Materials Research Society Symposia Proceedings*, **2012**, 1451, 15-20		

87	Correlation Between Quantum Conductance and Atomic Arrangement of Silver Atomic-Size Nanocontacts. *Materials Research Society Symposia Proceedings*, **2012**, 1429, 7		1
86	Multi-Million Fully Atomistic Molecular Dynamics Simulations of Yarn Formation from Carbon Nanotube Forests. *Materials Research Society Symposia Proceedings*, **2012**, 1407, 205		1
85	On the Unzipping Mechanisms of Carbon Nanotubes: Insights from Reactive Molecular Dynamics Simulations. *Materials Research Society Symposia Proceedings*, **2012**, 1451, 3-8		
84	On the Existence of Ordered Phases of Encapsulated Diamondoids into Carbon Nanotubes. *Materials Research Society Symposia Proceedings*, **2012**, 1407, 26		
83	Electronic properties of Fibonacci and random Si-Ge chains. *Journal of Physics Condensed Matter*, **2011**, 23, 405501	1.8	2
82	Ordered phases of encapsulated diamondoids into carbon nanotubes. *Nanotechnology*, **2011**, 22, 315708	3.4	21
81	Intrinsic stability of the smallest possible silver nanotube. *Physical Review Letters*, **2011**, 106, 065501	7.4	21
80	van der Waals potential barrier for cobaltocene encapsulation into single-walled carbon nanotubes: classical molecular dynamics and ab initio study. *Molecular Simulation*, **2011**, 37, 746-751	2	1
79	The First Molecular Wheel: A Theoretical Investigation. *Materials Research Society Symposia Proceedings*, **2011**, 1286, 44		
78	Temperature effects on the occurrence of long interatomic distances in atomic chains formed from stretched gold nanowires. *Nanotechnology*, **2011**, 22, 095705	3.4	8
77	Mechanical deformation of nanoscale metal rods: when size and shape matter. *Physical Review Letters*, **2011**, 106, 055501	7.4	24
76	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		
75	On the Formation of Carbon Nanotube Serpentines: Insights from Multi-Million Atom Molecular Dynamics Simulation. *Materials Research Society Symposia Proceedings*, **2011**, 1284, 79		1
74	Dynamics of Graphene Nanodrums. *Materials Research Society Symposia Proceedings*, **2011**, 1284, 173		
73	Stability and Dynamics of Boron Nitride Nanoscrolls. *Materials Research Society Symposia Proceedings*, **2011**, 1307, 1		1
72	The Dynamics of Formation of Graphane-like Fluorinated Graphene Membranes (Fluorographene): A Reactive Molecular Dynamics Study. *Materials Research Society Symposia Proceedings*, **2011**, 1344, 1		
71	A Fully Atomistic Reactive Molecular Dynamics Study on the Formation of Graphane from Graphene Hydrogenated Membranes. *Materials Research Society Symposia Proceedings*, **2011**, 1284, 31		
70	Temperature effects on the atomic arrangement and conductance of atomic-size gold nanowires generated by mechanical stretching. *Nanotechnology*, **2010**, 21, 485702	3.4	16

69	Curved graphene nanoribbons: structure and dynamics of carbon nanobelts. *Nanotechnology*, **2010**, 21, 75710	3.4	54
68	Neon atoms oscillating inside carbon and boron nitride nanotubes: a fully atomistic molecular dynamics investigation. *Molecular Simulation*, **2010**, 36, 639-643	2	2
67	Carbon nanotube with square cross-section: an ab initio investigation. *Journal of Chemical Physics*, **2010**, 133, 124513	3.9	16
66	Topologically closed macromolecules made of single walled carbon nanotubes-'super'-fullerenes. *Journal of Nanoscience and Nanotechnology*, **2010**, 10, 4378-83	1.3	4
65	Adsorption configuration effects on the surface diffusion of large organic molecules: the case of Violet Lander. *Journal of Chemical Physics*, **2010**, 133, 224702	3.9	1
64	Thermophoretically driven carbon nanotube oscillators. *Applied Physics Letters*, **2009**, 95, 253103	3.4	14
63	Observation of the smallest metal nanotube with a square cross-section. *Nature Nanotechnology*, **2009**, 4, 149-52	28.7	46
62	New Insights on the Growth of Anisotropic Nanoparticles from Total Energy Calculations. *Journal of Physical Chemistry C*, **2009**, 113, 11976-11979	3.8	4
61	Graphene to graphane: a theoretical study. *Nanotechnology*, **2009**, 20, 465704	3.4	199
60	Defects in graphene-based twisted nanoribbons: structural, electronic, and optical properties. *Langmuir*, **2009**, 25, 4751-9	4	24
59	The structure and dynamics of boron nitride nanoscrolls. *Nanotechnology*, **2009**, 20, 335702	3.4	44
58	C60-derived nanobaskets: stability, vibrational signatures, and molecular trapping. *Nanotechnology*, **2009**, 20, 395701	3.4	7
57	MBius and twisted graphene nanoribbons: stability, geometry, and electronic properties. *Journal of Chemical Physics*, **2008**, 128, 164719	3.9	47
56	Carbon nanotubes as reinforcement elements of composite nanotools. *Nano Letters*, **2008**, 8, 842-7	11.5	18
55	Rotational dynamics and polymerization of C60 in C60-cubane crystals: a molecular dynamics study. *Journal of Chemical Physics*, **2008**, 129, 064506	3.9	10
54	Large electromechanical response in silicon nanowires predicted from first-principles electronic structure calculations. *Physical Review B*, **2008**, 77,	3.3	4
53	Entanglement and the nonlinear elastic behavior of forests of coiled carbon nanotubes. *Physical Review Letters*, **2008**, 100, 086807	7.4	35
52	Some electronic properties of saturated and unsaturated cubane oligomers using DFT-based calculations. *Computational and Theoretical Chemistry*, **2008**, 868, 37-41		9

51	Modeling the auxetic transition for carbon nanotube sheets. *Physical Review B*, **2008**, 78,	3.3	42
50	Sign Change of Poisson's Ratio for Carbon Nanotube Sheets. *Science*, **2008**, 320, 504-7	33.3	208
49	Atomistic simulations of the mechanical properties of Superlcarbon nanotubes. *Nanotechnology*, **2007**, 18, 335702	3.4	65
48	Molecular dynamics simulation of single wall carbon nanotubes polymerization under compression. *Journal of Computational Chemistry*, **2007**, 28, 1724-34	3.5	12
47	Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes. *Journal of Physics Condensed Matter*, **2007**, 19, 236222	1.8	11
46	Is it possible to grow amorphous normal nanosprings?. *Nanotechnology*, **2007**, 18, 435606	3.4	4
45	Prediction of the hydrogen storage capacity of carbon nanoscrolls. *Physical Review B*, **2007**, 75,	3.3	90
44	Size limit of defect formation in pyramidal Pt nanocontacts. *Physical Review Letters*, **2007**, 99, 255501	7.4	16
43	Mechanical properties of carbon nanotube networks by molecular mechanics and impact molecular dynamics calculations. *Physical Review B*, **2007**, 75,	3.3	45
42	Geometric and electronic structure of carbon nanotube networks: Superlcarbon nanotubes. *Nanotechnology*, **2006**, 17, 617-621	3.4	70
41	Mechanical properties of amorphous nanosprings. *Nanotechnology*, **2006**, 17, 5620-6	3.4	18
40	Prediction of giant electroactuation for papyruslike carbon nanoscroll structures: First-principles calculations. *Physical Review B*, **2006**, 74,	3.3	60
39	Transmission electron microscopy and molecular dynamics study of the formation of suspended copper linear atomic chains. *Physical Review B*, **2006**, 74,	3.3	24
38	Elastic properties of nanowires. *Journal of Applied Physics*, **2006**, 99, 094310	2.5	13
37	Synthetic melanin films: Assembling mechanisms, scaling behavior, and structural properties. *Journal of Applied Physics*, **2006**, 99, 113511	2.5	38
36	Experimental realization of suspended atomic chains composed of different atomic species. *Nature Nanotechnology*, **2006**, 1, 182-5	28.7	84
35	Carcinogenic classification of polycyclic aromatic hydrocarbons through theoretical descriptors. *International Journal of Quantum Chemistry*, **2005**, 103, 718-730	2.1	2
34	Prediction of ordered phases of encapsulated C60, C70, and C78 inside carbon nanotubes. *Nano Letters*, **2005**, 5, 349-55	11.5	80

33	Structural and electronic properties of radialenes and related systems. *Computational and Theoretical Chemistry*, **2005**, 729, 203-210		6
32	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	2.1	13
31	Chaotic signature in the motion of coupled carbon nanotube oscillators. *Nanotechnology*, **2005**, 16, 583-589	3.4	30
30	Contaminants in suspended gold chains: an ab initio molecular dynamics study. *Physical Review Letters*, **2004**, 93, 216103	7.4	30
29	Mechanical properties of nanosprings. *Physical Review Letters*, **2004**, 92, 175502	7.4	73
28	Emergence of prime numbers as the result of evolutionary strategy. *Physical Review Letters*, **2004**, 93, 098107	7.4	7
27	Lock-and-key effect in the surface diffusion of large organic molecules probed by STM. *Nature Materials*, **2004**, 3, 779-82	27	106
26	On the Structural and Stability Features of Linear Atomic Suspended Chains Formed from Gold Nanowires Stretching. *Nano Letters*, **2004**, 4, 1187-1191	11.5	98
25	Effects of chlorine gas exposure on the optical properties of rhodium phthalocyanine films. *Solid State Communications*, **2004**, 131, 53-56	1.6	6
24	Molecular dynamics simulations of C60 nanobearings. *Chemical Physics Letters*, **2004**, 386, 425-429	2.5	49
23	Hysteresis-like Behavior in MBANP Crystals. *Crystal Growth and Design*, **2004**, 4, 1079-1081	3.5	3
22	Benzo[c]quinolizin-3-ones theoretical investigation: SAR analysis and application to nontested compounds. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1987-97		3
21	New families of carbon nanotubes based on graphyne motifs. *Nanotechnology*, **2004**, 15, S142-S149	3.4	107
20	Indication of unusual pentagonal structures in atomic-size Cu nanowires. *Physical Review Letters*, **2004**, 93, 126103	7.4	98
19	Gigahertz nanomechanical oscillators based on carbon nanotubes. *Nanotechnology*, **2004**, 15, S184-S189	3.4	110
18	Structure and Dynamics of Carbon Nanoscrolls. *Nano Letters*, **2004**, 4, 881-884	11.5	271
17	Theoretical investigation of electromechanical effects for graphyne carbon nanotubes. *Journal of Chemical Physics*, **2004**, 121, 3228-37	3.9	64
16	Families of carbon nanotubes: Graphyne-based nanotubes. *Physical Review B*, **2003**, 68,	3.3	169

15	Semiempirical studies of the electronic structure of polyphenylene sulfide phenyleneamine. *International Journal of Quantum Chemistry*, **2003**, 95, 252-259	2.1	4
14	A structure-activity study of taxol, taxotere, and derivatives using the electronic indices methodology (EIM). *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 699-706		13
13	Molecular-dynamics simulations of carbon nanotubes as gigahertz oscillators. *Physical Review Letters*, **2003**, 90, 055504	7.4	310
12	A semiempirical study on the electronic structure of 10-deacetylbaccatin-III. *Journal of Molecular Graphics and Modelling*, **2002**, 21, 57-70	2.8	7
11	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, 1479-89		16
10	A dual-mode photoswitching mechanism and charge transfer on chiroptical systems □theoretical study. *Synthetic Metals*, **2001**, 116, 275-279	3.6	4
9	A Theoretical Investigation on the Dual-Mode Photoswitching Mechanism of Some Chiroptical Systems. *Journal of Physical Chemistry B*, **2001**, 105, 8334-8338	3.4	1
8	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	2.9	11
7	Spatially variable reaction in the formation of anodically grown porous silicon structures. *Journal of Applied Physics*, **1995**, 78, 590-592	2.5	8
6	Excitation and relaxation energies of trans-stilbene: Confined singlet, triplet, and charged bipolarons. *Physical Review B*, **1993**, 47, 1742-1753	3.3	100
5	Fullereneynes: a new family of porous fullerenes. *Chemical Physics Letters*, **1993**, 204, 8-14	2.5	61
4	Crystalline networks with unusual predicted mechanical and thermal properties. *Nature*, **1993**, 365, 735-737	38.1	190
3	Electronic structure of polyacetylene with bonded oxygen. *Synthetic Metals*, **1992**, 51, 175-178	3.6	
2	Theoretical studies on Carter's soliton switch. *Synthetic Metals*, **1992**, 51, 179-186	3.6	3
1	Synthesis and Characterization of Biotene: A New 2D□Natural Oxide From Biotite. *Small*,2201667	11	0