

# David Tomanek

## List of Publications by Year in descending order

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243  
papers

32,366  
citations

9234

74  
h-index

3903

177  
g-index

247  
all docs

247  
docs citations

247  
times ranked

25554  
citing authors

#	ARTICLE	IF	CITATIONS
1	Thermal Decomposition of Hydrated Graphite Oxide: A Computational Study. <i>Physical Review Applied</i> , 2022, 17, .	1.5	0
2	Flow of polar and nonpolar liquids through nanotubes: A computational study. <i>Physical Review Materials</i> , 2021, 5, .	0.9	2
3	In-plane breathing and shear modes in low-dimensional nanostructures. <i>Carbon</i> , 2020, 157, 364-370.	5.4	14
4	Catalytic formation of narrow Nb nanowires inside carbon nanotubes. <i>Carbon</i> , 2020, 159, 195-200.	5.4	3
5	Changing the Phosphorus Allotrope from a Square Columnar Structure to a Planar Zigzag Nanoribbon by Increasing the Diameter of Carbon Nanotube Nanoreactors. <i>Nano Letters</i> , 2020, 20, 1280-1285.	4.5	29
6	Liquid Flow through Defective Layered Membranes: A Phenomenological Description. <i>Physical Review Applied</i> , 2020, 14, .	1.5	3
7	Efficient growth and characterization of one-dimensional transition metal tellurides inside carbon nanotubes. <i>Nanoscale</i> , 2020, 12, 17185-17190.	2.8	20
8	Periodically Gated Bilayer Graphene as an Electronic Metamaterial. <i>Physical Review Applied</i> , 2020, 13, .	1.5	4
9	Superior hardness and stiffness of diamond nanoparticles. <i>Carbon</i> , 2020, 162, 497-501.	5.4	7
10	Strain-controlled magnetic ordering in 2D carbon metamaterials. <i>Carbon</i> , 2020, 161, 219-223.	5.4	5
11	Low-symmetry two-dimensional $\text{BNP}_2$ and $\text{C}_2$ structures with high and anisotropic carrier mobilities. <i>Physical Review Materials</i> , 2020, 4, .	0.9	5
12	A water-resilient carbon nanotube based strain sensor for monitoring structural integrity. <i>Journal of Materials Chemistry A</i> , 2019, 7, 19996-20005.	5.2	36
13	Designing an All-Carbon Membrane for Water Desalination. <i>Physical Review Applied</i> , 2019, 12, .	1.5	16
14	Effect of Net Charge on the Relative Stability of 2D Boron Allotropes. <i>Nano Letters</i> , 2019, 19, 1359-1365.	4.5	23
15	Degenerately Doped Transition Metal Dichalcogenides as Ohmic Homojunction Contacts to Transition Metal Dichalcogenide Semiconductors. <i>ACS Nano</i> , 2019, 13, 5103-5111.	7.3	39
16	Towards room-temperature superconductivity in low-dimensional $\text{C}_{60}$ nanoarrays: An <i>ab initio</i> study. <i>Physical Review B</i> , 2018, 97, .	1.1	3
17	Formation Dynamics of Potassium-Based Graphite Intercalation Compounds: An <i>Ab Initio</i> Study. <i>Physical Review Applied</i> , 2018, 9, .	1.5	7
18	Shear instability in twisted bilayer graphene. <i>Physical Review B</i> , 2018, 98, .	1.1	31

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19	Two-Dimensional Mechanical Metamaterials with Unusual Poisson Ratio Behavior. <i>Physical Review Applied</i> , 2018, 10, .	1.5	17
20	Microscopic Mechanism of the Helix-to-Layer Transformation in Elemental Group VI Solids. <i>Nano Letters</i> , 2018, 18, 4908-4913.	4.5	19
21	Minimum model for the electronic structure of twisted bilayer graphene and related structures. <i>Physical Review B</i> , 2018, 98, .	1.1	34
22	Assembly of Ring-Shaped Phosphorus within Carbon Nanotube Nanoreactors. <i>Angewandte Chemie</i> , 2017, 129, 1876-1880.	1.6	21
23	Assembly of Ring-Shaped Phosphorus within Carbon Nanotube Nanoreactors. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 1850-1854.	7.2	64
24	Control of Surface and Edge Oxidation on Phosphorene. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 9126-9135.	4.0	135
25	Can CF <sub>3</sub> -Functionalized La@C <sub>60</sub> Be Isolated Experimentally and Become Superconducting?. <i>Nano Letters</i> , 2017, 17, 3402-3408.	4.5	22
26	Optimizing Charge Injection across Transition Metal Dichalcogenide Heterojunctions: Theory and Experiment. <i>ACS Nano</i> , 2017, 11, 3904-3910.	7.3	29
27	Long-wavelength deformations and vibrational modes in empty and liquid-filled microtubules and nanotubes: A theoretical study. <i>Physical Review B</i> , 2017, 95, .	1.1	8
28	Chemical and Electronic Repair Mechanism of Defects in MoS <sub>2</sub> Monolayers. <i>ACS Nano</i> , 2017, 11, 9989-9996.	7.3	80
29	Origin of Unusually High Rigidity in Selected Helical Coil Structures. <i>Physical Review Applied</i> , 2017, 8, .	1.5	1
30	Unusually Stable Helical Coil Allotrope of Phosphorus. <i>Nano Letters</i> , 2016, 16, 7865-7869.	4.5	29
31	Continuum approach for long-wavelength acoustic phonons in quasi-two-dimensional structures. <i>Physical Review B</i> , 2016, 94, .	1.1	45
32	Strain-controlled fundamental gap and structure of bulk black phosphorus. <i>Physical Review B</i> , 2016, 94, .	1.1	40
33	Two-Dimensional Phosphorus Carbide: Competition between sp <sup>2</sup> and sp <sup>3</sup> Bonding. <i>Nano Letters</i> , 2016, 16, 3247-3252.	4.5	137
34	A metallic mosaic phase and the origin of Mott-insulating state in 1T-TaS <sub>2</sub> . <i>Nature Communications</i> , 2016, 7, 10956.	5.8	196
35	Low-Resistance 2D/2D Ohmic Contacts: A Universal Approach to High-Performance WSe <sub>2</sub> , MoS <sub>2</sub> , and MoSe <sub>2</sub> Transistors. <i>Nano Letters</i> , 2016, 16, 1896-1902.	4.5	334
36	Interpreting core-level spectra of oxidizing phosphorene: Theory and experiment. <i>Physical Review B</i> , 2015, 92, .	1.1	35

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37	Administration's grand victory over academia. <i>Materials Express</i> , 2015, 5, 79-81.	0.2	0
38	Simulated scanning tunneling microscopy images of few-layer phosphorus capped by graphene and hexagonal boron nitride monolayers. <i>Physical Review B</i> , 2015, 91, .	1.1	27
39	Designing Isoelectronic Counterparts to Layered Group V Semiconductors. <i>ACS Nano</i> , 2015, 9, 8284-8290.	7.3	128
40	Relative stability and local curvature analysis in carbon nanotori. <i>Physical Review B</i> , 2015, 91, .	1.1	9
41	Strain-induced metal-semiconductor transition in monolayers and bilayers of gray arsenic: A computational study. <i>Physical Review B</i> , 2015, 91, .	1.1	178
42	Interfacing graphene and related 2D materials with the 3D world. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 133203.	0.7	24
43	Electronic structure and transport in graphene/haeckelite hybrids: an <i>ab initio</i> study. <i>2D Materials</i> , 2015, 2, 035001.	2.0	18
44	Structural Transition in Layered As <sub>1-x</sub> P <sub>x</sub> Compounds: A Computational Study. <i>Nano Letters</i> , 2015, 15, 6042-6046.	4.5	74
45	Enhancing mechanical toughness of aluminum surfaces by nano-boron implantation: An <i>ab initio</i> study. <i>Chemical Physics Letters</i> , 2015, 620, 25-28.	1.2	3
46	2014 symposium on phosphorene: An emerging 2D semiconductor. <i>Materials Express</i> , 2014, 4, 545-547.	0.2	5
47	Topologically Protected Conduction State at Carbon Foam Surfaces: An <i>Ab initio</i> Study. <i>Physical Review Letters</i> , 2014, 112, 026803.	2.9	32
48	Local curvature and stability of two-dimensional systems. <i>Physical Review B</i> , 2014, 90, .	1.1	24
49	High Stability of Faceted Nanotubes and Fullerenes of Multiphase Layered Phosphorus: A Computational Study. <i>Physical Review Letters</i> , 2014, 113, 226801.	2.9	91
50	Tiling Phosphorene. <i>ACS Nano</i> , 2014, 8, 12763-12768.	7.3	122
51	Effect of structural defects on the thermal conductivity of graphene: From point to line defects to haeckelites. <i>Physical Review B</i> , 2014, 89, .	1.1	64
52	Spontaneous Graphitization of Ultrathin Cubic Structures: A Computational Study. <i>Nano Letters</i> , 2014, 14, 7126-7130.	4.5	31
53	Graphitic Phase of NaCl. Bulk Properties and Nanoscale Stability. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4014-4019.	2.1	16
54	Semiconducting Layered Blue Phosphorus: A Computational Study. <i>Physical Review Letters</i> , 2014, 112, 176802.	2.9	996

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55	Phase Coexistence and Metal-Insulator Transition in Few-Layer Phosphorene: A Computational Study. <i>Physical Review Letters</i> , 2014, 113, 046804.	2.9	556
56	Magic numbers in small iron clusters: A first-principles study. <i>Chemical Physics Letters</i> , 2014, 613, 59-63.	1.2	36
57	Phosphorene: An Unexplored 2D Semiconductor with a High Hole Mobility. <i>ACS Nano</i> , 2014, 8, 4033-4041.	7.3	5,474
58	High Mobility $WSe_2$ p- and n-Type Field-Effect Transistors Contacted by Highly Doped Graphene for Low-Resistance Contacts. <i>Nano Letters</i> , 2014, 14, 3594-3601.	4.5	399
59	Evidence of Diamond Nanowires Formed inside Carbon Nanotubes from Diamantane Dicarboxylic Acid. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 3717-3721.	7.2	71
60	Conducting linear chains of sulphur inside carbon nanotubes. <i>Nature Communications</i> , 2013, 4, 2162.	5.8	228
61	Improved Carrier Mobility in Few-Layer $MoS_2$ Field-Effect Transistors with Ionic-Liquid Gating. <i>ACS Nano</i> , 2013, 7, 4449-4458.	7.3	301
62	Formation and Properties of Selenium Double-Helices inside Double-Wall Carbon Nanotubes: Experiment and Theory. <i>ACS Nano</i> , 2013, 7, 5607-5613.	7.3	57
63	Theoretical investigation of the electronic structure and quantum transport in the graphene-C(111) diamond surface system. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 435302.	0.7	13
64	Limits of mechanical energy storage and structural changes in twisted carbon nanotube ropes. <i>Physical Review B</i> , 2013, 88, .	1.1	16
65	Optimizing Electronic Structure and Quantum Transport at the Graphene-Si(111) Interface: An <i>Ab Initio</i> Density-Functional Study. <i>Physical Review Letters</i> , 2013, 110, 176805.	2.9	23
66	Nanomechanical Energy Storage in Twisted Nanotube Ropes. <i>Physical Review Letters</i> , 2012, 109, 255501.	2.9	18
67	Selective probe of the morphology and local vibrations at carbon nanoasperities. <i>Journal of Chemical Physics</i> , 2012, 136, 064505.	1.2	8
68	Formation and Stability of Cellular Carbon Foam Structures: An <i>Ab Initio</i> Study. <i>Physical Review Letters</i> , 2012, 109, 135501.	2.9	27
69	Designing Electrical Contacts to $MoS_2$ Monolayers: A Computational Study. <i>Physical Review Letters</i> , 2012, 108, 156802.	2.9	475
70	Synthesis and Transformation of Linear Adamantane Assemblies inside Carbon Nanotubes. <i>ACS Nano</i> , 2012, 6, 8674-8683.	7.3	70
71	Computational study of the thermal conductivity in defective carbon nanostructures. <i>Physical Review B</i> , 2012, 86, .	1.1	38
72	Helicity in Ropes of Chiral Nanotubes: Calculations and Observation. <i>Physical Review Letters</i> , 2012, 108, 235501.	2.9	6

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73	Calling to Be Your Best: Your Calling to Science. <i>Materials Express</i> , 2011, 1, 86-87.	0.2	0
74	Fame on Sale: Pitfalls of the Ranking Game. <i>Materials Express</i> , 2011, 1, 355-356.	0.2	2
75	Nanoconfinement effects on the reversibility of hydrogen storage in ammonia borane: A first-principles study. <i>Journal of Chemical Physics</i> , 2011, 134, 214501.	1.2	15
76	Search for the largest two-dimensional aggregates of boron: An ab initio study. <i>Physical Review B</i> , 2011, 83, .	1.1	31
77	Photoexfoliation of Graphene from Graphite: An <i>ab initio</i> Study. <i>Physical Review Letters</i> , 2010, 104, 208302.	2.9	75
78	Effect of bundling on the stability, equilibrium geometry, and electronic structure of $\text{Mo}_6\text{S}_8$ . <i>Physical Review B</i> , 2010, 82, .	1.1	8
79	Reinforcing multiwall carbon nanotubes by electron beam irradiation. <i>Journal of Applied Physics</i> , 2010, 108, 084314.	1.1	16
80	Structural and magnetic properties of $\text{Tc}_n\text{M}_m$ metallofullerenes: First-principles predictions. <i>Physical Review B</i> , 2010, 81, .	1.1	19
81	Interplay between structural and electronic properties of bundled $\text{Mo}_6\text{S}_9\hat{\alpha}\text{I}$ nanowires. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 505301.	0.7	5
82	Designing rigid carbon foams. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 334220.	0.7	29
83	Equilibrium structure of ferrofluid aggregates. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 455105.	0.7	12
84	Hydrogen-induced disintegration of fullerenes and nanotubes: An <i>ab initio</i> study. <i>Physical Review B</i> , 2009, 80, .	1.1	18
85	Trapping cold atoms using surface-grown carbon nanotubes. <i>Physical Review A</i> , 2009, 79, .	1.0	22
86	Revealing Subsurface Vibrational Modes by Atom-Resolved Damping Force Spectroscopy. <i>Physical Review Letters</i> , 2009, 102, 195503.	2.9	14
87	Molecular Self-Assembly of Functionalized Fullerenes on a Metal Surface. <i>Physical Review Letters</i> , 2009, 102, 056102.	2.9	26
88	Modeling extended contacts for nanotube and graphene devices. <i>Physical Review B</i> , 2008, 77, .	1.1	71
89	Modeling the destruction of realistic nanotube emitters: Relative role of charging and temperature. <i>Physical Review B</i> , 2008, 77, .	1.1	2
90	Hydrogenation of Single-Wall Carbon Nanotubes Using Polyamine Reagents: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 2296-2303.	6.6	55

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91	Direct Observation of Optically Induced Transient Structures in Graphite Using Ultrafast Electron Crystallography. <i>Physical Review Letters</i> , 2008, 101, 077401.	2.9	128
92	Self-assembly of long chain alkanes and their derivatives on graphite. <i>Journal of Chemical Physics</i> , 2008, 128, 124709.	1.2	99
93	Origin of torsion-induced conductance oscillations in carbon nanotubes. <i>Physical Review B</i> , 2008, 78, .	1.1	33
94	Compositional ordering and quantum transport in $\text{Mo}_6\text{S}_9\text{S}'$ nanowires: <i>Ab initio</i> calculations. <i>Physical Review B</i> , 2008, 77, .	1.1	16
95	Spin Currents in Rough Graphene Nanoribbons: Universal Fluctuations and Spin Injection. <i>Physical Review Letters</i> , 2008, 100, 177207.	2.9	288
96	Transforming Carbon Nanotubes by Silylation: An <i>Ab Initio</i> Study. <i>Physical Review Letters</i> , 2008, 100, 236102.	2.9	11
97	Mechanism of fullerene hydrogenation by polyamines: <i>Ab initio</i> density functional calculations. <i>Physical Review B</i> , 2008, 78, .	1.1	45
98	Targeted medication delivery using magnetic nanostructures. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 086210.	0.7	4
99	Unique Structural and Transport Properties of Molybdenum Chalcogenide Nanowires. <i>Physical Review Letters</i> , 2007, 99, 085503.	2.9	30
100	Effect of electron and hole doping on the structure of C, Si, and S nanowires. <i>Physical Review B</i> , 2007, 75, .	1.1	15
101	Role of Electronic Excitations in Ion Collisions with Carbon Nanostructures. <i>Physical Review Letters</i> , 2007, 99, 016104.	2.9	142
102	A novel hybrid carbon material. <i>Nature Nanotechnology</i> , 2007, 2, 156-161.	15.6	369
103	Introduction to the Important and Exciting Aspects of Carbon-Nanotube Science and Technology. <i>Topics in Applied Physics</i> , 2007, , 1-12.	0.4	18
104	Real-Time <i>Ab Initio</i> Simulations of Excited Carrier Dynamics in Carbon Nanotubes. <i>Physical Review Letters</i> , 2006, 97, 126104.	2.9	47
105	Interplay between Structure and Magnetism in $\text{Mo}_6\text{S}_9\text{S}'$ Nanowires. <i>Physical Review Letters</i> , 2006, 96, 125502.	2.9	37
106	Toward uniform nanotubular compounds: Synthetic approach and <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2006, 124, 121102.	1.2	6
107	Contact Dependence of Carrier Injection in Carbon Nanotubes: An <i>Ab Initio</i> Study. <i>Physical Review Letters</i> , 2006, 96, 076802.	2.9	194
108	Computational Nanotechnology: From Clusters to Devices. <i>AIP Conference Proceedings</i> , 2005, , .	0.3	0

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109	Energetics and packing of fullerenes in nanotube peapods. <i>Physical Review B</i> , 2005, 71, .	1.1	48
110	Effect of SOCl <sub>2</sub> Treatment on Electrical and Mechanical Properties of Single-Wall Carbon Nanotube Networks. <i>Journal of the American Chemical Society</i> , 2005, 127, 5125-5131.	6.6	330
111	Carbon-based nanotechnology on a supercomputer. <i>Journal of Physics Condensed Matter</i> , 2005, 17, R413-R459.	0.7	18
112	Kwon, Berber, and Tománek Reply:. <i>Physical Review Letters</i> , 2005, 94, .	2.9	8
113	Stability differences and conversion mechanism between nanotubes and scrolls. <i>Physical Review B</i> , 2004, 69, .	1.1	22
114	Quantum Size Effects in the Polarizability of Carbon Fullerenes. <i>Physical Review Letters</i> , 2004, 92, 215501.	2.9	62
115	Zipper Mechanism of Nanotube Fusion: Theory and Experiment. <i>Physical Review Letters</i> , 2004, 92, 075504.	2.9	78
116	Photodesorption of oxygen from carbon nanotubes. <i>Physical Review B</i> , 2004, 70, .	1.1	19
117	Microscopic mechanism of fullerene fusion. <i>Physical Review B</i> , 2004, 70, .	1.1	62
118	Diamond fragments as building blocks of functional nanostructures. <i>Physical Review B</i> , 2004, 70, .	1.1	137
119	Can photo excitations heal defects in carbon nanotubes?. <i>Chemical Physics Letters</i> , 2004, 392, 209-213.	1.2	23
120	Thermal Contraction of Carbon Fullerenes and Nanotubes. <i>Physical Review Letters</i> , 2004, 92, 015901.	2.9	195
121	Spectroscopic characterization of Stone-Wales defects in nanotubes. <i>Physical Review B</i> , 2004, 69, .	1.1	134
122	Rigid crystalline phases of polymerized fullerenes. <i>Physical Review B</i> , 2004, 70, .	1.1	36
123	Energetics and Bandstructure for a Polyacetylene Chain Enclosed inside a Carbon Nanotube. <i>Synthetic Metals</i> , 2003, 135-136, 729-730.	2.1	2
124	Bonding and Energy Dissipation in a Nanohook Assembly. <i>Physical Review Letters</i> , 2003, 91, 165503.	2.9	26
125	Magnetism in All-Carbon Nanostructures with Negative Gaussian Curvature. <i>Physical Review Letters</i> , 2003, 91, 237204.	2.9	200
126	Energetics and electronic structure of a polyacetylene chain contained in a carbon nanotube. <i>Physical Review B</i> , 2003, 67, .	1.1	52



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127	Defective fullerenes and nanotubes as molecular magnets: Anab initio study. Physical Review B, 2003, 68, .	1.1	114
128	Itinerant ferromagnetism in heterostructured C/BN nanotubes. Physical Review B, 2003, 67, .	1.1	75
129	MAGNETO-CONDUCTANCE IN TWISTED CARBON NANOTUBES. , 2003, , .		0
130	Hierarchical assembly of nanostructured carbon foam. Molecular Crystals and Liquid Crystals, 2002, 386, 189-195.	0.4	9
131	Microscopic Formation Mechanism of Nanotube Peapods. Physical Review Letters, 2002, 88, 185502.	2.9	101
132	Giant magneto-conductance in twisted carbon nanotubes. Europhysics Letters, 2002, 59, 75-80.	0.7	11
133	Onset of nanotube decay under extreme thermal and electronic excitations. Physica B: Condensed Matter, 2002, 323, 78-85.	1.3	37
134	Mesoscopic origami with graphite: scrolls, nanotubes, peapods. Physica B: Condensed Matter, 2002, 323, 86-89.	1.3	52
135	Ballistic conductance in quantum devices: from organic polymers to nanotubes. Current Applied Physics, 2002, 2, 47-49.	1.1	8
136	Scrolls and nested tubes in multiwall carbon nanotubes. Carbon, 2002, 40, 1123-1130.	5.4	84
137	Effect of van der Waals Interactions on the Raman Modes in Single Walled Carbon Nanotubes. Physical Review Letters, 2001, 86, 3895-3898.	2.9	340
138	Synthesis of high-density carbon nanotube films by microwave plasma chemical vapor deposition. Diamond and Related Materials, 2001, 10, 1947-1951.	1.8	22
139	Optical current injection in carbon and boron nitride nanotubes. AIP Conference Proceedings, 2001, , .	0.3	0
140	Photo-galvano-mechanical phenomena in nanotubes. AIP Conference Proceedings, 2001, , .	0.3	0
141	Paradoxical magnetic cooling in a structural transition model. European Physical Journal B, 2001, 19, 117-119.	0.6	1
142	Carbon foam: Spanning the phase space between graphite and diamond. Physical Review B, 2001, 64, .	1.1	74
143	Electronic interwall interactions and charge redistribution in multiwall nanotubes. Physical Review B, 2001, 65, .	1.1	103
144	Imaging the interlayer interactions of multiwall carbon nanotubes using scanning tunneling microscopy and spectroscopy. Applied Physics Letters, 2001, 79, 4210-4212.	1.5	19

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145	Electronic structure and properties of rhombohedrally polymerized C60. Journal of Chemical Physics, 2001, 115, 5637-5641.	1.2	22
146	Thermal and Electrical Conductance of Carbon Nanostructures. , 2001, , 263-272.		0
147	Electrical and thermal transport in carbon nanotubes. AIP Conference Proceedings, 2000, , .	0.3	1
148	Stability, electronic structure and reactivity of the polymerized fullerite forms. Journal of Physics and Chemistry of Solids, 2000, 61, 1901-1911.	1.9	17
149	Electronic and structural properties of carbon nanohorns. Physical Review B, 2000, 62, R2291-R2294.	1.1	90
150	Coherent control of photocurrents in graphene and carbon nanotubes. Physical Review B, 2000, 61, 7669-7677.	1.1	54
151	Fractional Quantum Conductance in Carbon Nanotubes. Physical Review Letters, 2000, 84, 1974-1977.	2.9	166
152	Unusually High Thermal Conductivity of Carbon Nanotubes. Physical Review Letters, 2000, 84, 4613-4616.	2.9	2,775
153	Photogalvanic Effects in Heteropolar Nanotubes. Physical Review Letters, 2000, 85, 1512-1515.	2.9	85
154	Orientalional Melting in Carbon Nanotube Ropes. Physical Review Letters, 2000, 84, 1483-1486.	2.9	45
155	Thermodynamics of finite magnetic two-isomer systems. Journal of Chemical Physics, 1999, 111, 10689-10693.	1.2	7
156	“Bucky Shuttle”-Memory Device: Synthetic Approach and Molecular Dynamics Simulations. Physical Review Letters, 1999, 82, 1470-1473.	2.9	155
157	Laser-Driven Atomic Pump. Physical Review Letters, 1999, 82, 5373-5376.	2.9	93
158	X-ray spectroscopic and quantum “chemical study of carbon tubes produced in arc-discharge. Chemical Physics Letters, 1998, 289, 341-349.	1.2	18
159	Electronic Structure of (n,0) Zigzag Carbon Nanotubes: A Cluster and Crystal Approach. Journal of Physical Chemistry A, 1998, 102, 975-981.	1.1	66
160	Electronic and structural properties of multiwall carbon nanotubes. Physical Review B, 1998, 58, R16001-R16004.	1.1	241
161	Do Carbon Nanotubes Spin When Bundled?. Journal of Materials Research, 1998, 13, 2363-2367.	1.2	13
162	Effect of intertube coupling on the electronic structure of carbon nanotube ropes. Physical Review B, 1998, 58, R13314-R13317.	1.1	130

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163	Self-assembly and electronic structure of bundled single- and multi-wall nanotubes. , 1998, , .		0
164	Morphology and Stability of Growing Multiwall Carbon Nanotubes. Physical Review Letters, 1997, 79, 2065-2068.	2.9	106
165	Hydrogen-Induced Polymorphism of the Pd(110) Surface. Physical Review Letters, 1997, 79, 1329-1332.	2.9	25
166	Noble gas temperature control of metal clusters: A molecular dynamics study. Journal of Chemical Physics, 1997, 107, 3071-3079.	1.2	71
167	Electronic structure of single-wall, multiwall, and filled carbon nanotubes. Physical Review B, 1997, 55, 13980-13988.	1.1	59
168	Tight-binding molecular dynamics simulations of semiconductor alloys: clusters, surfaces, and defects. Journal of Physics Condensed Matter, 1997, 9, 4345-4364.	0.7	6
169	Self-assembly of magnetic nanostructures. Zeitschrift für Physik D-Atoms Molecules and Clusters, 1997, 40, 539-541.	1.0	16
170	Catalytic Growth of Single-Wall Carbon Nanotubes: An Ab Initio Study. Physical Review Letters, 1997, 78, 2393-2396.	2.9	320
171	Does hydrogen pre-melt palladium clusters?. Chemical Physics Letters, 1997, 264, 39-43.	1.2	17
172	Disintegration of finite carbon chains in electric fields. Chemical Physics Letters, 1997, 264, 345-350.	1.2	20
173	Field-induced unraveling of carbon nanotubes. Chemical Physics Letters, 1997, 265, 667-672.	1.2	34
174	Crystalline Ropes of Metallic Carbon Nanotubes. Science, 1996, 273, 483-487.	6.0	5,226
175	Cavities and Channels in Electrified. Journal of the American Chemical Society, 1996, 118, 7329-7336.	6.6	91
176	<title>From astrophysics to mesoscopic physics: a sightseeing tour in the world of clusters and fullerenes</title>. , 1996, , .		0
177	MAGNETISM OF SMALL TRANSITION-METAL CLUSTERS AND EFFECTS OF ISOMERIZATION. Surface Review and Letters, 1996, 03, 463-466.	0.5	4
178	Ionicity of the M@C60 bond in M@C60 endohedral complexes. Chemical Physics Letters, 1995, 243, 42-44.	1.2	42
179	Self-Assembly of Tubular Fullerenes. The Journal of Physical Chemistry, 1995, 99, 10694-10697.	2.9	499
180	Stability and Fragmentation of Complex Structures in Ferrofluids. Physical Review Letters, 1995, 74, 3049-3052.	2.9	77

#	ARTICLE	IF	CITATIONS
181	Stability and elastic properties of hydrogen-loaded $Ti_{1-x}Al_x$ alloys: An ab initio study. <i>Physical Review B</i> , 1995, 51, 9569-9580.	1.1	14
182	How free are encapsulated atoms in C60?. <i>Chemical Physics Letters</i> , 1994, 221, 453-458.	1.2	74
183	Melting the fullerenes: A molecular dynamics study. <i>Physical Review Letters</i> , 1994, 72, 2418-2421.	2.9	185
184	Vibrational spectra of multishell fullerenes. <i>Physical Review B</i> , 1994, 50, 12207-12210.	1.1	9
185	Modifying the buckyball. <i>Computational Materials Science</i> , 1994, 2, 468-474.	1.4	0
186	Collective electronic excitations and their damping in small alkali clusters. <i>Chemical Physics Letters</i> , 1993, 205, 521-528.	1.2	23
187	Stability of M@C60 endohedral complexes. <i>Chemical Physics Letters</i> , 1993, 208, 79-85.	1.2	62
188	Lanthanide- and actinide-based fullerite compounds: potential $A_xC_{60}$ superconductors?. <i>Chemical Physics Letters</i> , 1993, 203, 438-443.	1.2	14
189	Fullereneynes: a new family of porous fullerenes. <i>Chemical Physics Letters</i> , 1993, 204, 8-14.	1.2	67
190	Total energy calculations for extremely large clusters: The recursive approach. <i>Solid State Communications</i> , 1993, 86, 607-612.	0.9	28
191	Stability of fullerene-based systems. <i>Journal of Physics and Chemistry of Solids</i> , 1993, 54, 1679-1684.	1.9	19
192	Computer simulation of hydrogen embrittlement in metals. <i>Nature</i> , 1993, 362, 435-437.	13.7	55
193	Structural rigidity and low frequency vibrational modes of long carbon tubules. <i>Zeitschrift für Physik D-Atoms Molecules and Clusters</i> , 1993, 27, 93-96.	1.0	309
194	Hyperpolarizability of the C60 fullerene cluster. <i>Zeitschrift für Physik D-Atoms Molecules and Clusters</i> , 1993, 25, 181-184.	1.0	35
195	Stability of multishell fullerenes. <i>Physical Review B</i> , 1993, 48, 15461-15464.	1.1	105
196	Structural properties of Fe crystals. <i>Physical Review B</i> , 1993, 47, 95-99.	1.1	56
197	Stability of C60 fullerite intercalation compounds. <i>Physical Review B</i> , 1993, 47, 6711-6720.	1.1	28
198	Theory for the atomic force microscopy of layered elastic surfaces. <i>Journal of Physics Condensed Matter</i> , 1992, 4, 4233-4249.	0.7	15

#	ARTICLE	IF	CITATIONS
199	Reply to "Comment on Jahn-Teller effect for the negatively charged C <sub>60</sub> molecule: Analogy with the silicon vacancy". Physical Review B, 1992, 46, 14264-14265.	1.1	0
200	Schlüter et al. reply. Physical Review Letters, 1992, 69, 213-213.	2.9	19
201	Electron-phonon coupling and superconductivity in alkali-intercalated C <sub>60</sub> solid. Physical Review Letters, 1992, 68, 526-529.	2.9	473
202	Precursors to C <sub>60</sub> fullerene formation. Physical Review B, 1992, 46, 7326-7328.	1.1	75
203	Superconductivity in alkali intercalated C <sub>60</sub> . Journal of Physics and Chemistry of Solids, 1992, 53, 1473-1485.	1.9	142
204	Mechanical stability of Pd-H systems: A molecular-dynamics study. Physical Review B, 1992, 46, 8099-8108.	1.1	31
205	Jahn-Teller effect for the negatively charged C <sub>60</sub> molecule: Analogy with the silicon vacancy. Physical Review B, 1991, 44, 12106-12108.	1.1	146
206	Growth regimes of carbon clusters. Physical Review Letters, 1991, 67, 2331-2334.	2.9	220
207	Collective plasmon excitations in C <sub>60</sub> clusters. Physical Review Letters, 1991, 67, 2690-2693.	2.9	310
208	Calculation of an Atomically Modulated Friction Force in Atomic-Force Microscopy. Europhysics Letters, 1991, 15, 887-892.	0.7	205
209	Limits of Resolution in Atomic Force Microscopy Images of Graphite. Europhysics Letters, 1991, 15, 49-54.	0.7	43
210	Theory of elastic tip-surface interactions in atomic force microscopy. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1991, 9, 479.	1.6	44
211	Ab initio calculation of chemisorption systems: H on Pd(001) and Pd(110). Physical Review B, 1991, 43, 4699-4713.	1.1	83
212	Effect of adsorbates on surface phonon modes: H on Pd(001) and Pd(110). Physical Review B, 1991, 44, 13053-13062.	1.1	59
213	Collective electronic excitations in small metal clusters. Physical Review B, 1991, 43, 6804-6807.	1.1	40
214	Palladium-graphite interaction potentials based on first-principles calculations. Physical Review B, 1991, 43, 12623-12625.	1.1	18
215	Stiffness of a solid composed of C <sub>60</sub> clusters. Physical Review B, 1991, 44, 6562-6565.	1.1	97
216	First-principles theory of atomic-scale friction. Physical Review Letters, 1990, 64, 3054-3057.	2.9	255

#	ARTICLE	IF	CITATIONS
217	Quasiparticle band offset at the (001) interface and band gaps in ultrathin superlattices of GaAs-AlAs heterojunctions. Physical Review B, 1990, 41, 10058-10067.	1.1	42
218	Theory for the Atomic Force Microscopy of Deformable Surfaces. Physical Review Letters, 1989, 63, 876-879.	2.9	76
219	Thermal effects in the equilibrium structure and size distribution of small Si clusters. Physical Review B, 1989, 39, 5361-5365.	1.1	17
220	Theory for the Atomic Force Microscopy of Deformable Surfaces. Physical Review Letters, 1989, 63, 1896-1896.	2.9	7
221	Thermal line broadening in small metal clusters. Physical Review B, 1989, 40, 2749-2751.	1.1	113
222	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. Physical Review B, 1989, 40, 3162-3168.	1.1	69
223	Quasiparticle band gaps for ultrathin GaAs/AlAs(001) superlattices. Physical Review Letters, 1989, 63, 1495-1498.	2.9	44
224	Cold fusion: How close can deuterium atoms come inside palladium?. Physical Review Letters, 1989, 63, 59-61.	2.9	63
225	Quasiparticle calculation of valence band offset of AlAs-GaAs(001). Solid State Communications, 1988, 66, 585-588.	0.9	91
226	$\pi$ -states contribution to the conductivity of BC3. Solid State Communications, 1988, 67, 515-518.	0.9	34
227	Calculation of electronic and structural properties of BC3. Physical Review B, 1988, 37, 3134-3136.	1.1	182
228	First-principles calculation of highly asymmetric structure in scanning-tunneling-microscopy images of graphite. Physical Review B, 1988, 37, 8327-8336.	1.1	243
229	Structure and bonding of small semiconductor clusters. Physical Review B, 1987, 36, 1208-1217.	1.1	280
230	Theory and observation of highly asymmetric atomic structure in scanning-tunneling-microscopy images of graphite. Physical Review B, 1987, 35, 7790-7793.	1.1	276
231	Multi-adatom interactions on metal surfaces. Surface Science, 1986, 173, 538-554.	0.8	31
232	Calculation of Magic Numbers and the Stability of Small Si Clusters. Physical Review Letters, 1986, 56, 1055-1058.	2.9	251
233	Ab Initio Calculation of Coverage-Dependent Adsorption Properties of H on Pd(001). Physical Review Letters, 1986, 57, 2594-2597.	2.9	57
234	Total-energy calculations for N <sub>2</sub> dissociation on Fe(111): Characterization of precursor and dissociative states. Physical Review B, 1985, 31, 2488-2490.	1.1	53

#	ARTICLE	IF	CITATIONS
235	Electronic model for energies, relaxations and reconstruction trends at metal surfaces. Surface Science, 1985, 163, 503-515.	0.8	67
236	Calculation of elastic strain and electronic effects on surface segregation. Physical Review B, 1985, 32, 5051-5056.	1.1	186
237	Thermodynamic interpretation of core-level binding energies in adsorbates. Surface Science, 1983, 126, 112-119.	0.8	34
238	Simple theory for the electronic and atomic structure of small clusters. Physical Review B, 1983, 28, 665-673.	1.1	345
239	Adsorption and decomposition of ammonia on a W(110) surface: Photoemission fingerprinting and interpretation of the core level binding energies using the equivalent core approximation. Surface Science, 1982, 119, 133-149.	0.8	79
240	Calculation of chemisorption and absorption induced surface segregation. Surface Science, 1982, 114, 11-22.	0.8	133
241	Semiempirical theory for surface core-level shifts. Solid State Communications, 1982, 41, 273-279.	0.9	52
242	Surface core-level binding energy shifts in alloys. Solid State Communications, 1981, 39, 987-989.	0.9	17
243	Large scale simulations for carbon nanotubes. , 0, , .		0