David Tomanek

List of Publications by Year in Descending Order

229 papers	28,223 citations	70 h-index	166 g-index
247 ext. papers	30,320 ext. citations	5.9 avg, IF	7.1 L-index

#	Paper	IF	Citations
229	Efficient growth and characterization of one-dimensional transition metal tellurides inside carbon nanotubes. *Nanoscale*, **2020**, 12, 17185-17190	7.7	9
228	Superior hardness and stiffness of diamond nanoparticles. *Carbon*, **2020**, 162, 497-501	10.4	3
227	Strain-controlled magnetic ordering in 2D carbon metamaterials. *Carbon*, **2020**, 161, 219-223	10.4	4
226	Low-symmetry two-dimensional BNP2 and C2SiS structures with high and anisotropic carrier mobilities. *Physical Review Materials*, **2020**, 4,	3.2	3
225	In-plane breathing and shear modes in low-dimensional nanostructures. *Carbon*, **2020**, 157, 364-370	10.4	6
224	Catalytic formation of narrow Nb nanowires inside carbon nanotubes. *Carbon*, **2020**, 159, 195-200	10.4	2
223	Changing the Phosphorus Allotrope from a Square Columnar Structure to a Planar Zigzag Nanoribbon by Increasing the Diameter of Carbon Nanotube Nanoreactors. *Nano Letters*, **2020**, 20, 1280-1285	11.5	16
222	Designing an All-Carbon Membrane for Water Desalination. *Physical Review Applied*, **2019**, 12,	4.3	10
221	Effect of Net Charge on the Relative Stability of 2D Boron Allotropes. *Nano Letters*, **2019**, 19, 1359-1365	11.5	18
220	Degenerately Doped Transition Metal Dichalcogenides as Ohmic Homojunction Contacts to Transition Metal Dichalcogenide Semiconductors. *ACS Nano*, **2019**, 13, 5103-5111	16.7	25
219	A water-resilient carbon nanotube based strain sensor for monitoring structural integrity. *Journal of Materials Chemistry A*, **2019**, 7, 19996-20005	13	22
218	Towards room-temperature superconductivity in low-dimensional C60 nanoarrays: An ab initio study. *Physical Review B*, **2018**, 97,	3.3	3
217	Formation Dynamics of Potassium-Based Graphite Intercalation Compounds: An Ab Initio Study. *Physical Review Applied*, **2018**, 9,	4.3	2
216	Microscopic Mechanism of the Helix-to-Layer Transformation in Elemental Group VI Solids. *Nano Letters*, **2018**, 18, 4908-4913	11.5	15
215	Minimum model for the electronic structure of twisted bilayer graphene and related structures. *Physical Review B*, **2018**, 98,	3.3	22
214	Shear instability in twisted bilayer graphene. *Physical Review B*, **2018**, 98,	3.3	22
213	Two-Dimensional Mechanical Metamaterials with Unusual Poisson Ratio Behavior. *Physical Review Applied*, **2018**, 10,	4.3	14

212	Assembly of Ring-Shaped Phosphorus within Carbon Nanotube Nanoreactors. *Angewandte Chemie*, **2017**, 129, 1876-1880	3.6	19
211	Assembly of Ring-Shaped Phosphorus within Carbon Nanotube Nanoreactors. *Angewandte Chemie - International Edition*, **2017**, 56, 1850-1854	16.4	47
210	Control of Surface and Edge Oxidation on Phosphorene. *ACS Applied Materials & Interfaces*, **2017**, 9, 9126-9135	9.5	102
209	Can CF-Functionalized La@C Be Isolated Experimentally and Become Superconducting?. *Nano Letters*, **2017**, 17, 3402-3408	11.5	16
208	Optimizing Charge Injection across Transition Metal Dichalcogenide Heterojunctions: Theory and Experiment. *ACS Nano*, **2017**, 11, 3904-3910	16.7	23
207	Long-wavelength deformations and vibrational modes in empty and liquid-filled microtubules and nanotubes: A theoretical study. *Physical Review B*, **2017**, 95,	3.3	4
206	Chemical and Electronic Repair Mechanism of Defects in MoS Monolayers. *ACS Nano*, **2017**, 11, 9989-9996	16.7	62
205	Two-Dimensional Phosphorus Carbide: Competition between sp(2) and sp(3) Bonding. *Nano Letters*, **2016**, 16, 3247-52	11.5	98
204	A metallic mosaic phase and the origin of Mott-insulating state in 1T-TaS2. *Nature Communications*, **2016**, 7, 10956	17.4	131
203	Low-Resistance 2D/2D Ohmic Contacts: A Universal Approach to High-Performance WSe2, MoS2, and MoSe2 Transistors. *Nano Letters*, **2016**, 16, 1896-902	11.5	266
202	Unusually Stable Helical Coil Allotrope of Phosphorus. *Nano Letters*, **2016**, 16, 7865-7869	11.5	24
201	Continuum approach for long-wavelength acoustic phonons in quasi-two-dimensional structures. *Physical Review B*, **2016**, 94,	3.3	35
200	Strain-controlled fundamental gap and structure of bulk black phosphorus. *Physical Review B*, **2016**, 94,	3.3	31
199	Designing Isoelectronic Counterparts to Layered Group V Semiconductors. *ACS Nano*, **2015**, 9, 8284-90	16.7	115
198	Relative stability and local curvature analysis in carbon nanotori. *Physical Review B*, **2015**, 91,	3.3	9
197	Strain-induced metal-semiconductor transition in monolayers and bilayers of gray arsenic: A computational study. *Physical Review B*, **2015**, 91,	3.3	159
196	Interfacing graphene and related 2D materials with the 3D world. *Journal of Physics Condensed Matter*, **2015**, 27, 133203	1.8	22
195	Electronic structure and transport in graphene/haeckelite hybrids: an ab initio study. *2D Materials*, **2015**, 2, 035001	5.9	15

194	Structural Transition in Layered As(1-x)P(x) Compounds: A Computational Study. *Nano Letters*, **2015** , 15, 6042-6	11.5	63
193	Enhancing mechanical toughness of aluminum surfaces by nano-boron implantation: An ab initio study. *Chemical Physics Letters*, **2015**, 620, 25-28	2.5	1
192	Interpreting core-level spectra of oxidizing phosphorene: Theory and experiment. *Physical Review B* , **2015**, 92,	3.3	31
191	Simulated scanning tunneling microscopy images of few-layer phosphorus capped by graphene and hexagonal boron nitride monolayers. *Physical Review B*, **2015**, 91,	3.3	27
190	Effect of structural defects on the thermal conductivity of graphene: From point to line defects to haeckelites. *Physical Review B*, **2014**, 89,	3.3	51
189	Spontaneous graphitization of ultrathin cubic structures: a computational study. *Nano Letters*, **2014** , 14, 7126-30	11.5	26
188	Graphitic Phase of NaCl. Bulk Properties and Nanoscale Stability. *Journal of Physical Chemistry Letters*, **2014**, 5, 4014-9	6.4	11
187	Semiconducting layered blue phosphorus: a computational study. *Physical Review Letters*, **2014**, 112, 176802	7.4	836
186	Phase coexistence and metal-insulator transition in few-layer phosphorene: a computational study. *Physical Review Letters*, **2014**, 113, 046804	7.4	451
185	Magic numbers in small iron clusters: A first-principles study. *Chemical Physics Letters*, **2014**, 613, 59-63	2.5	23
184	Phosphorene: an unexplored 2D semiconductor with a high hole mobility. *ACS Nano*, **2014**, 8, 4033-41	16.7	4487
183	High mobility WSe2 p- and n-type field-effect transistors contacted by highly doped graphene for low-resistance contacts. *Nano Letters*, **2014**, 14, 3594-601	11.5	341
182	2014 symposium on phosphorene: An emerging 2D semiconductor. *Materials Express*, **2014**, 4, 545-547	1.3	5
181	Topologically protected conduction state at carbon foam surfaces: an ab initio study. *Physical Review Letters*, **2014**, 112, 026803	7.4	30
180	Local curvature and stability of two-dimensional systems. *Physical Review B*, **2014**, 90,	3.3	19
179	High Stability of Faceted Nanotubes and Fullerenes of Multiphase Layered Phosphorus: A Computational Study. *Physical Review Letters*, **2014**, 113, 226801	7.4	73
178	Tiling phosphorene. *ACS Nano*, **2014**, 8, 12763-8	16.7	109
177	Evidence of diamond nanowires formed inside carbon nanotubes from diamantane dicarboxylic acid. *Angewandte Chemie - International Edition*, **2013**, 52, 3717-21	16.4	57

176	Conducting linear chains of sulphur inside carbon nanotubes. *Nature Communications*, **2013**, 4, 2162	17.4	176
175	Improved carrier mobility in few-layer MoS2 field-effect transistors with ionic-liquid gating. *ACS Nano*, **2013**, 7, 4449-58	16.7	267
174	Formation and properties of selenium double-helices inside double-wall carbon nanotubes: experiment and theory. *ACS Nano*, **2013**, 7, 5607-13	16.7	43
173	Theoretical investigation of the electronic structure and quantum transport in the graphene-C(111) diamond surface system. *Journal of Physics Condensed Matter*, **2013**, 25, 435302	1.8	10
172	Limits of mechanical energy storage and structural changes in twisted carbon nanotube ropes. *Physical Review B*, **2013**, 88,	3.3	12
171	Optimizing electronic structure and quantum transport at the graphene-Si(111) interface: an ab initio density-functional study. *Physical Review Letters*, **2013**, 110, 176805	7.4	22
170	Evidence of Diamond Nanowires Formed inside Carbon Nanotubes from Diamantane Dicarboxylic Acid. *Angewandte Chemie*, **2013**, 125, 3805-3809	3.6	13
169	Formation and stability of cellular carbon foam structures: an ab initio study. *Physical Review Letters*, **2012**, 109, 135501	7.4	27
168	Designing electrical contacts to MoS2 monolayers: a computational study. *Physical Review Letters*, **2012**, 108, 156802	7.4	413
167	Synthesis and transformation of linear adamantane assemblies inside carbon nanotubes. *ACS Nano*, **2012**, 6, 8674-83	16.7	61
166	Computational study of the thermal conductivity in defective carbon nanostructures. *Physical Review B*, **2012**, 86,	3.3	33
165	Helicity in ropes of chiral nanotubes: calculations and observation. *Physical Review Letters*, **2012**, 108, 235501	7.4	4
164	Nanomechanical energy storage in twisted nanotube ropes. *Physical Review Letters*, **2012**, 109, 255501	7.4	16
163	Selective probe of the morphology and local vibrations at carbon nanoasperities. *Journal of Chemical Physics*, **2012**, 136, 064505	3.9	4
162	Fame on Sale: Pitfalls of the Ranking Game. *Materials Express*, **2011**, 1, 355-356	1.3	2
161	Nanoconfinement effects on the reversibility of hydrogen storage in ammonia borane: a first-principles study. *Journal of Chemical Physics*, **2011**, 134, 214501	3.9	14
160	Search for the largest two-dimensional aggregates of boron: An ab initio study. *Physical Review B*, **2011**, 83,	3.3	29
159	Photoexfoliation of graphene from graphite: an ab initio study. *Physical Review Letters*, **2010**, 104, 208302	7.4	64

158	Effect of bundling on the stability, equilibrium geometry, and electronic structure of Mo6S9□Ix nanowires. *Physical Review B*, **2010**, 82,	3.3	8
157	Reinforcing multiwall carbon nanotubes by electron beam irradiation. *Journal of Applied Physics*, **2010**, 108, 084314	2.5	13
156	Structural and magnetic properties of Tcn@C60 endohedral metalofullerenes: First-principles predictions. *Physical Review B*, **2010**, 81,	3.3	18
155	Interplay between structural and electronic properties of bundled Mo6S(9-x)I(x) nanowires. *Journal of Physics Condensed Matter*, **2010**, 22, 505301	1.8	5
154	Designing rigid carbon foams. *Journal of Physics Condensed Matter*, **2010**, 22, 334220	1.8	23
153	Equilibrium structure of ferrofluid aggregates. *Journal of Physics Condensed Matter*, **2010**, 22, 455105	1.8	10
152	Hydrogen-induced disintegration of fullerenes and nanotubes: An ab initio study. *Physical Review B*, **2009**, 80,	3.3	17
151	Trapping cold atoms using surface-grown carbon nanotubes. *Physical Review A*, **2009**, 79,	2.6	20
150	Revealing subsurface vibrational modes by atom-resolved damping force spectroscopy. *Physical Review Letters*, **2009**, 102, 195503	7.4	11
149	Molecular self-assembly of functionalized fullerenes on a metal surface. *Physical Review Letters*, **2009**, 102, 056102	7.4	25
148	Modeling extended contacts for nanotube and graphene devices. *Physical Review B*, **2008**, 77,	3.3	61
147	Modeling the destruction of realistic nanotube emitters: Relative role of charging and temperature. *Physical Review B*, **2008**, 77,	3.3	2
146	Hydrogenation of single-wall carbon nanotubes using polyamine reagents: combined experimental and theoretical study. *Journal of the American Chemical Society*, **2008**, 130, 2296-303	16.4	48
145	Direct observation of optically induced transient structures in graphite using ultrafast electron crystallography. *Physical Review Letters*, **2008**, 101, 077401	7.4	116
144	Self-assembly of long chain alkanes and their derivatives on graphite. *Journal of Chemical Physics*, **2008**, 128, 124709	3.9	86
143	Origin of torsion-induced conductance oscillations in carbon nanotubes. *Physical Review B*, **2008**, 78,	3.3	30
142	Compositional ordering and quantum transport in Mo6S9□Ix nanowires: Ab initio calculations. *Physical Review B*, **2008**, 77,	3.3	15
141	Spin currents in rough graphene nanoribbons: universal fluctuations and spin injection. *Physical Review Letters*, **2008**, 100, 177207	7.4	240

140	Transforming carbon nanotubes by silylation: an ab initio study. *Physical Review Letters*, **2008**, 100, 236102	7.4	11
139	Mechanism of fullerene hydrogenation by polyamines: Ab initio density functional calculations. *Physical Review B*, **2008**, 78,	3.3	28
138	A novel hybrid carbon material. *Nature Nanotechnology*, **2007**, 2, 156-61	28.7	326
137	Targeted medication delivery using magnetic nanostructures. *Journal of Physics Condensed Matter*, **2007**, 19, 086210	1.8	3
136	Unique structural and transport properties of molybdenum chalcohalide nanowires. *Physical Review Letters*, **2007**, 99, 085503	7.4	25
135	Effect of electron and hole doping on the structure of C, Si, and S nanowires. *Physical Review B*, **2007**, 75,	3.3	14
134	Role of electronic excitations in ion collisions with carbon nanostructures. *Physical Review Letters*, **2007**, 99, 016104	7.4	122
133	Introduction to the Important and Exciting Aspects of Carbon-Nanotube Science and Technology. *Topics in Applied Physics*, **2007**, 1-12	0.5	16
132	Interplay between structure and magnetism in Mo12S9I9 nanowires. *Physical Review Letters*, **2006**, 96, 125502	7.4	35
131	Toward uniform nanotubular compounds: synthetic approach and ab initio calculations. *Journal of Chemical Physics*, **2006**, 124, 121102	3.9	6
130	Contact dependence of carrier injection in carbon nanotubes: an ab initio study. *Physical Review Letters*, **2006**, 96, 076802	7.4	168
129	Real-time ab initio simulations of excited carrier dynamics in carbon nanotubes. *Physical Review Letters*, **2006**, 97, 126104	7.4	43
128	Effect of SOCl2 treatment on electrical and mechanical properties of single-wall carbon nanotube networks. *Journal of the American Chemical Society*, **2005**, 127, 5125-31	16.4	312
127	Carbon-based nanotechnology on a supercomputer. *Journal of Physics Condensed Matter*, **2005**, 17, R413-R459	1.8	16
126	Kwon, Berber, and Tománek Reply:. *Physical Review Letters*, **2005**, 94,	7.4	8
125	Energetics and packing of fullerenes in nanotube peapods. *Physical Review B*, **2005**, 71,	3.3	46
124	Stability differences and conversion mechanism between nanotubes and scrolls. *Physical Review B*, **2004**, 69,	3.3	21
123	Quantum size effects in the polarizability of carbon fullerenes. *Physical Review Letters*, **2004**, 92, 215501	7.4	57

122	Zipper mechanism of nanotube fusion: theory and experiment. *Physical Review Letters*, **2004**, 92, 075504	7.4	75
121	Photodesorption of oxygen from carbon nanotubes. *Physical Review B*, **2004**, 70,	3.3	18
120	Microscopic mechanism of fullerene fusion. *Physical Review B*, **2004**, 70,	3.3	55
119	Diamond fragments as building blocks of functional nanostructures. *Physical Review B*, **2004**, 70,	3.3	131
118	Can photo excitations heal defects in carbon nanotubes?. *Chemical Physics Letters*, **2004**, 392, 209-213	2.5	21
117	Thermal contraction of carbon fullerenes and nanotubes. *Physical Review Letters*, **2004**, 92, 015901	7.4	173
116	Spectroscopic characterization of Stone-Wales defects in nanotubes. *Physical Review B*, **2004**, 69,	3.3	126
115	Rigid crystalline phases of polymerized fullerenes. *Physical Review B*, **2004**, 70,	3.3	27
114	Energetics and Bandstructure for a Polyacetylene Chain Enclosed inside a Carbon Nanotube. *Synthetic Metals*, **2003**, 135-136, 729-730	3.6	2
113	Bonding and energy dissipation in a nanohook assembly. *Physical Review Letters*, **2003**, 91, 165503	7.4	23
112	Magnetism in all-carbon nanostructures with negative Gaussian curvature. *Physical Review Letters*, **2003**, 91, 237204	7.4	176
111	Energetics and electronic structure of a polyacetylene chain contained in a carbon nanotube. *Physical Review B*, **2003**, 67,	3.3	50
110	Defective fullerenes and nanotubes as molecular magnets: An ab initio study. *Physical Review B*, **2003**, 68,	3.3	107
109	Itinerant ferromagnetism in heterostructured C/BN nanotubes. *Physical Review B*, **2003**, 67,	3.3	72
108	Onset of nanotube decay under extreme thermal and electronic excitations. *Physica B: Condensed Matter*, **2002**, 323, 78-85	2.8	32
107	Mesoscopic origami with graphite: scrolls, nanotubes, peapods. *Physica B: Condensed Matter*, **2002**, 323, 86-89	2.8	49
106	Ballistic conductance in quantum devices: from organic polymers to nanotubes. *Current Applied Physics*, **2002**, 2, 47-49	2.6	8
105	Scrolls and nested tubes in multiwall carbon nanotubes. *Carbon*, **2002**, 40, 1123-1130	10.4	76

104	Hierarchical assembly of nanostructured carbon foam. *Molecular Crystals and Liquid Crystals*, **2002**, 386, 189-195	0.5	8
103	Microscopic formation mechanism of nanotube peapods. *Physical Review Letters*, **2002**, 88, 185502	7.4	97
102	Giant magneto-conductance in twisted carbon nanotubes. *Europhysics Letters*, **2002**, 59, 75-80	1.6	11
101	Paradoxical magnetic cooling in a structural transition model. *European Physical Journal B*, **2001**, 19, 117-119	1.1	1
100	Carbon foam: Spanning the phase space between graphite and diamond. *Physical Review B*, **2001**, 64,	3.3	70
99	Electronic interwall interactions and charge redistribution in multiwall nanotubes. *Physical Review B* , **2001**, 65,	3.3	89
98	Imaging the interlayer interactions of multiwall carbon nanotubes using scanning tunneling microscopy and spectroscopy. *Applied Physics Letters*, **2001**, 79, 4210-4212	3.4	16
97	Electronic structure and properties of rhombohedrally polymerized C60. *Journal of Chemical Physics* , **2001**, 115, 5637-5641	3.9	16
96	Effect of van der Waals interactions on the Raman modes in single walled carbon nanotubes. *Physical Review Letters*, **2001**, 86, 3895-8	7.4	313
95	Synthesis of high-density carbon nanotube films by microwave plasma chemical vapor deposition. *Diamond and Related Materials*, **2001**, 10, 1947-1951	3.5	21
94	Thermal and Electrical Conductance of Carbon Nanostructures **2001**, 263-272		
93	Stability, electronic structure and reactivity of the polymerized fullerite forms. *Journal of Physics and Chemistry of Solids*, **2000**, 61, 1901-1911	3.9	14
92	Electronic and structural properties of carbon nanohorns. *Physical Review B*, **2000**, 62, R2291-R2294	3.3	79
91	Coherent control of photocurrents in graphene and carbon nanotubes. *Physical Review B*, **2000**, 61, 7669-7677	3.5	47
90	Fractional quantum conductance in carbon nanotubes. *Physical Review Letters*, **2000**, 84, 1974-7	7.4	150
89	Unusually high thermal conductivity of carbon nanotubes. *Physical Review Letters*, **2000**, 84, 4613-6	7.4	2415
88	Photogalvanic effects in heteropolar nanotubes. *Physical Review Letters*, **2000**, 85, 1512-5	7.4	67
87	Orientational melting in carbon nanotube ropes. *Physical Review Letters*, **2000**, 84, 1483-6	7.4	41

86	Thermodynamics of finite magnetic two-isomer systems. *Journal of Chemical Physics*, **1999**, 111, 10689-10693	3.9	6
85	Bucky Shuttle Memory Device: Synthetic Approach and Molecular Dynamics Simulations. *Physical Review Letters*, **1999**, 82, 1470-1473	7.4	145
84	Laser-Driven Atomic Pump. *Physical Review Letters*, **1999**, 82, 5373-5376	7.4	82
83	X-ray spectroscopic and quantum chemical study of carbon tubes produced in arc-discharge. *Chemical Physics Letters*, **1998**, 289, 341-349	2.5	16
82	Electronic Structure of (n,0) Zigzag Carbon Nanotubes: ´Cluster and Crystal Approach. *Journal of Physical Chemistry A*, **1998**, 102, 975-981	2.8	63
81	Electronic and structural properties of multiwall carbon nanotubes. *Physical Review B*, **1998**, 58, R16001-R16004	3.3	209
80	Do Carbon Nanotubes Spin When Bundled?. *Journal of Materials Research*, **1998**, 13, 2363-2367	2.5	12
79	Effect of intertube coupling on the electronic structure of carbon nanotube ropes. *Physical Review B*, **1998**, 58, R13314-R13317	3.3	124
78	Morphology and Stability of Growing Multiwall Carbon Nanotubes. *Physical Review Letters*, **1997**, 79, 2065-2068	7.4	99
77	Hydrogen-Induced Polymorphism of the Pd(110) Surface. *Physical Review Letters*, **1997**, 79, 1329-1332	7.4	22
76	Noble gas temperature control of metal clusters: A molecular dynamics study. *Journal of Chemical Physics*, **1997**, 107, 3071-3079	3.9	60
75	Electronic structure of single-wall, multiwall, and filled carbon nanotubes. *Physical Review B*, **1997**, 55, 13980-13988	3.3	55
74	Tight-binding molecular dynamics simulations of semiconductor alloys: clusters, surfaces, and defects. *Journal of Physics Condensed Matter*, **1997**, 9, 4345-4364	1.8	5
73	Self-assembly of magnetic nanostructures. *Zeitschrift Fur Physik D-Atoms Molecules and Clusters*, **1997**, 40, 539-541		16
72	Catalytic Growth of Single-Wall Carbon Nanotubes: An Ab Initio Study. *Physical Review Letters*, **1997** , 78, 2393-2396	7.4	304
71	Does hydrogen pre-melt palladium clusters?. *Chemical Physics Letters*, **1997**, 264, 39-43	2.5	16
70	Disintegration of finite carbon chains in electric fields. *Chemical Physics Letters*, **1997**, 264, 345-350	2.5	18
69	Field-induced unraveling of carbon nanotubes. *Chemical Physics Letters*, **1997**, 265, 667-672	2.5	29

68	Crystalline Ropes of Metallic Carbon Nanotubes. *Science*, **1996**, 273, 483-7	33.3	4692
67	Cavities and Channels in Electrides. *Journal of the American Chemical Society*, **1996**, 118, 7329-7336	16.4	86
66	MAGNETISM OF SMALL TRANSITION-METAL CLUSTERS AND EFFECTS OF ISOMERIZATION. *Surface Review and Letters*, **1996**, 03, 463-466	1.1	4
65	Self-Assembly of Tubular Fullerenes. *The Journal of Physical Chemistry*, **1995**, 99, 10694-10697		422
64	Stability and fragmentation of complex structures in ferrofluids. *Physical Review Letters*, **1995**, 74, 3049-3052	7.4	76
63	Stability and elastic properties of hydrogen-loaded Ti1-xAlx alloys: An ab initio study. *Physical Review B*, **1995**, 51, 9569-9580	3.3	11
62	Ionicity of the MC60 bond in M@C60 endohedral complexes. *Chemical Physics Letters*, **1995**, 243, 42-44	2.5	36
61	How free are encapsulated atoms in C60?. *Chemical Physics Letters*, **1994**, 221, 453-458	2.5	68
60	Melting the fullerenes: A molecular dynamics study. *Physical Review Letters*, **1994**, 72, 2418-2421	7.4	165
59	Vibrational spectra of multishell fullerenes. *Physical Review B*, **1994**, 50, 12207-12210	3.3	9
58	Modifying the buckyball. *Computational Materials Science*, **1994**, 2, 468-474	3.2	
57	Stability of multishell fullerenes. *Physical Review B*, **1993**, 48, 15461-15464	3.3	95
56	Structural properties of Fe crystals. *Physical Review B*, **1993**, 47, 95-99	3.3	54
55	Stability of C60 fullerite intercalation compounds. *Physical Review B*, **1993**, 47, 6711-6720	3.3	26
54	Collective electronic excitations and their damping in small alkali clusters. *Chemical Physics Letters*, **1993**, 205, 521-528	2.5	22
53	Stability of M@C60 endohedral complexes. *Chemical Physics Letters*, **1993**, 208, 79-85	2.5	58
52	Lanthanide- and actinide-based fullerite compounds: potential AxC60 superconductors?. *Chemical Physics Letters*, **1993**, 203, 438-443	2.5	13
51	Fullereneynes: a new family of porous fullerenes. *Chemical Physics Letters*, **1993**, 204, 8-14	2.5	61

50	Total energy calculations for extremely large clusters: The recursive approach. *Solid State Communications*, **1993**, 86, 607-612	1.6	25
49	Stability of fullerene-based systems. *Journal of Physics and Chemistry of Solids*, **1993**, 54, 1679-1684	3.9	19
48	Computer simulation of hydrogen embrittlement in metals. *Nature*, **1993**, 362, 435-437	50.4	42
47	Structural rigidity and low frequency vibrational modes of long carbon tubules. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1993**, 27, 93-96		266
46	Hyperpolarizability of the C60 fullerene cluster. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1993**, 25, 181-184		32
45	Theory for the atomic force microscopy of layered elastic surfaces. *Journal of Physics Condensed Matter*, **1992**, 4, 4233-4249	1.8	14
44	Reply to "Comment on 'Jahn-Teller effect for the negatively charged C60 molecule: Analogy with the silicon vacancy' ". *Physical Review B*, **1992**, 46, 14264-14265	3.3	
43	Schl er et al. reply. *Physical Review Letters*, **1992**, 69, 213	7.4	16
42	Electron-phonon coupling and superconductivity in alkali-intercalated C60 solid. *Physical Review Letters*, **1992**, 68, 526-529	7.4	451
41	Precursors to C60 fullerene formation. *Physical Review B*, **1992**, 46, 7326-7328	3.3	70
40	Superconductivity in alkali intercalated C60. *Journal of Physics and Chemistry of Solids*, **1992**, 53, 1473-1485	3.9	130
39	Mechanical stability of Pd-H systems: A molecular-dynamics study. *Physical Review B*, **1992**, 46, 8099-8108	3.3	29
38	Growth regimes of carbon clusters. *Physical Review Letters*, **1991**, 67, 2331-2334	7.4	207
37	Collective plasmon excitations in C60 clusters. *Physical Review Letters*, **1991**, 67, 2690-2693	7.4	300
36	Calculation of an Atomically Modulated Friction Force in Atomic-Force Microscopy. *Europhysics Letters*, **1991**, 15, 887-892	1.6	169
35	Limits of Resolution in Atomic Force Microscopy Images of Graphite. *Europhysics Letters*, **1991**, 15, 49-54	1.6	37
34	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		37
33	Ab initio calculation of chemisorption systems: H on Pd(001) and Pd(110). *Physical Review B*, **1991**, 43, 4699-4713	3.3	79

32	Effect of adsorbates on surface phonon modes: H on Pd(001) and Pd(110). *Physical Review B*, **1991**, 44, 13053-13062	3.3	56
31	Collective electronic excitations in small metal clusters. *Physical Review B*, **1991**, 43, 6804-6807	3.3	37
30	Palladium-graphite interaction potentials based on first-principles calculations. *Physical Review B*, **1991**, 43, 12623-12625	3.3	15
29	Stiffness of a solid composed of C60 clusters. *Physical Review B*, **1991**, 44, 6562-6565	3.3	88
28	Jahn-Teller effect for the negatively charged C60 molecule: Analogy with the silicon vacancy. *Physical Review B*, **1991**, 44, 12106-12108	3.3	140
27	First-principles theory of atomic-scale friction. *Physical Review Letters*, **1990**, 64, 3054-3057	7.4	211
26	Quasiparticle band offset at the (001) interface and band gaps in ultrathin superlattices of GaAs-AlAs heterojunctions. *Physical Review B*, **1990**, 41, 10058-10067	3.3	39
25	Theory for the atomic force microscopy of deformable surfaces. *Physical Review Letters*, **1989**, 63, 876-879	7.4	63
24	Thermal effects in the equilibrium structure and size distribution of small Si clusters. *Physical Review B*, **1989**, 39, 5361-5365	3.3	17
23	Theory for the Atomic Force Microscopy of Deformable Surfaces. *Physical Review Letters*, **1989**, 63, 1896-1896	7.4	7
22	Thermal line broadening in small metal clusters. *Physical Review B*, **1989**, 40, 2749-2751	3.3	109
21	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. *Physical Review B*, **1989**, 40, 3162-3168	3.3	58
20	Quasiparticle band gaps for ultrathin GaAs/AlAs(001) superlattices. *Physical Review Letters*, **1989**, 63, 1495-1498	7.4	44
19	Cold fusion: How close can deuterium atoms come inside palladium?. *Physical Review Letters*, **1989**, 63, 59-61	7.4	56
18	Quasiparticle calculation of valence band offset of AlAs-GaAs(001). *Solid State Communications*, **1988**, 66, 585-588	1.6	88
17	□states contribution to the conductivity of BC3. *Solid State Communications*, **1988**, 67, 515-518	1.6	31
16	Calculation of electronic and structural properties of BC3. *Physical Review B*, **1988**, 37, 3134-3136	3.3	172
15	First-principles calculation of highly asymmetric structure in scanning-tunneling-microscopy images of graphite. *Physical Review B*, **1988**, 37, 8327-8336	3.3	222

14	Structure and bonding of small semiconductor clusters. *Physical Review B*, **1987**, 36, 1208-1217	3.3	264
13	Theory and observation of highly asymmetric atomic structure in scanning-tunneling-microscopy images of graphite. *Physical Review B*, **1987**, 35, 7790-7793	3.3	254
12	Calculation of magic numbers and the stability of small Si clusters. *Physical Review Letters*, **1986**, 56, 1055-1058	7.4	234
11	Ab initio calculation of coverage-dependent adsorption properties of H on Pd(001). *Physical Review Letters*, **1986**, 57, 2594-2597	7.4	56
10	Multi-adatom interactions on metal surfaces. *Surface Science*, **1986**, 173, 538-554	1.8	31
9	Total-energy calculations for N2 dissociation on Fe(111): Characterization of precursor and dissociative states. *Physical Review B*, **1985**, 31, 2488-2490	3.3	49
8	Electronic model for energies, relaxations and reconstruction trends at metal surfaces. *Surface Science*, **1985**, 163, 503-515	1.8	62
7	Calculation of elastic strain and electronic effects on surface segregation. *Physical Review B*, **1985**, 32, 5051-5056	3.3	177
6	Thermodynamic interpretation of core-level binding energies in adsorbates. *Surface Science*, **1983**, 126, 112-119	1.8	32
5	Simple theory for the electronic and atomic structure of small clusters. *Physical Review B*, **1983**, 28, 665-673	3.3	333
4	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	1.8	76
3	Calculation of chemisorption and absorption induced surface segregation. *Surface Science*, **1982**, 114, 11-22	1.8	121
2	Semiempirical theory for surface core-level shifts. *Solid State Communications*, **1982**, 41, 273-279	1.6	52
1	Surface core-level binding energy shifts in alloys. *Solid State Communications*, **1981**, 39, 987-989	1.6	16