David Tomanek

List of Publications by Citations

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	Crystalline Ropes of Metallic Carbon Nanotubes. *Science*, **1996**, 273, 483-7	33.3	4692
228	Phosphorene: an unexplored 2D semiconductor with a high hole mobility. *ACS Nano*, **2014**, 8, 4033-41	16.7	4487
227	Unusually high thermal conductivity of carbon nanotubes. *Physical Review Letters*, **2000**, 84, 4613-6	7.4	2415
226	Semiconducting layered blue phosphorus: a computational study. *Physical Review Letters*, **2014**, 112, 176802	7.4	836
225	Phase coexistence and metal-insulator transition in few-layer phosphorene: a computational study. *Physical Review Letters*, **2014**, 113, 046804	7.4	451
224	Electron-phonon coupling and superconductivity in alkali-intercalated C60 solid. *Physical Review Letters*, **1992**, 68, 526-529	7.4	451
223	Self-Assembly of Tubular Fullerenes. *The Journal of Physical Chemistry*, **1995**, 99, 10694-10697		422
222	Designing electrical contacts to MoS2 monolayers: a computational study. *Physical Review Letters*, **2012**, 108, 156802	7.4	413
221	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
220	Simple theory for the electronic and atomic structure of small clusters. *Physical Review B*, **1983**, 28, 665-673	3.7	333
219	A novel hybrid carbon material. *Nature Nanotechnology*, **2007**, 2, 156-61	28.7	326
218	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
217	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
216	Catalytic Growth of Single-Wall Carbon Nanotubes: An Ab Initio Study. *Physical Review Letters*, **1997**, 78, 2393-2396	7.4	304
215	Collective plasmon excitations in C60 clusters. *Physical Review Letters*, **1991**, 67, 2690-2693	7.4	300
214	Improved carrier mobility in few-layer MoS2 field-effect transistors with ionic-liquid gating. *ACS Nano*, **2013**, 7, 4449-58	16.7	267
213	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

212	Structural rigidity and low frequency vibrational modes of long carbon tubules. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1993**, 27, 93-96		266
211	Structure and bonding of small semiconductor clusters. *Physical Review B*, **1987**, 36, 1208-1217	3.3	264
210	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
209	Spin currents in rough graphene nanoribbons: universal fluctuations and spin injection. *Physical Review Letters*, **2008**, 100, 177207	7.4	240
208	Calculation of magic numbers and the stability of small Si clusters. *Physical Review Letters*, **1986**, 56, 1055-1058	7.4	234
207	First-principles calculation of highly asymmetric structure in scanning-tunneling-microscopy images of graphite. *Physical Review B*, **1988**, 37, 8327-8336	3.3	222
206	First-principles theory of atomic-scale friction. *Physical Review Letters*, **1990**, 64, 3054-3057	7.4	211
205	Electronic and structural properties of multiwall carbon nanotubes. *Physical Review B*, **1998**, 58, R16001-R16004	3.3	209
204	Growth regimes of carbon clusters. *Physical Review Letters*, **1991**, 67, 2331-2334	7.4	207
203	Calculation of elastic strain and electronic effects on surface segregation. *Physical Review B*, **1985**, 32, 5051-5056	3.3	177
202	Conducting linear chains of sulphur inside carbon nanotubes. *Nature Communications*, **2013**, 4, 2162	17.4	176
201	Magnetism in all-carbon nanostructures with negative Gaussian curvature. *Physical Review Letters*, **2003**, 91, 237204	7.4	176
200	Thermal contraction of carbon fullerenes and nanotubes. *Physical Review Letters*, **2004**, 92, 015901	7.4	173
199	Calculation of electronic and structural properties of BC3. *Physical Review B*, **1988**, 37, 3134-3136	3.3	172
198	Calculation of an Atomically Modulated Friction Force in Atomic-Force Microscopy. *Europhysics Letters*, **1991**, 15, 887-892	1.6	169
197	Contact dependence of carrier injection in carbon nanotubes: an ab initio study. *Physical Review Letters*, **2006**, 96, 076802	7.4	168
196	Melting the fullerenes: A molecular dynamics study. *Physical Review Letters*, **1994**, 72, 2418-2421	7.4	165
195	Strain-induced metal-semiconductor transition in monolayers and bilayers of gray arsenic: A computational study. *Physical Review B*, **2015**, 91,	3.3	159

194	Fractional quantum conductance in carbon nanotubes. *Physical Review Letters*, **2000**, 84, 1974-7	7.4	150
193	Bucky Shuttle Memory Device: Synthetic Approach and Molecular Dynamics Simulations. *Physical Review Letters*, **1999**, 82, 1470-1473	7.4	145
192	Jahn-Teller effect for the negatively charged C60 molecule: Analogy with the silicon vacancy. *Physical Review B*, **1991**, 44, 12106-12108	3.3	140
191	A metallic mosaic phase and the origin of Mott-insulating state in 1T-TaS2. *Nature Communications*, **2016**, 7, 10956	17.4	131
190	Diamond fragments as building blocks of functional nanostructures. *Physical Review B*, **2004**, 70,	3.3	131
189	Superconductivity in alkali intercalated C60. *Journal of Physics and Chemistry of Solids*, **1992**, 53, 1473-1485	3.9	130
188	Spectroscopic characterization of Stone-Wales defects in nanotubes. *Physical Review B*, **2004**, 69,	3.3	126
187	Effect of intertube coupling on the electronic structure of carbon nanotube ropes. *Physical Review B*, **1998**, 58, R13314-R13317	3.3	124
186	Role of electronic excitations in ion collisions with carbon nanostructures. *Physical Review Letters*, **2007**, 99, 016104	7.4	122
185	Calculation of chemisorption and absorption induced surface segregation. *Surface Science*, **1982**, 114, 11-22	1.8	121
184	Direct observation of optically induced transient structures in graphite using ultrafast electron crystallography. *Physical Review Letters*, **2008**, 101, 077401	7.4	116
183	Designing Isoelectronic Counterparts to Layered Group V Semiconductors. *ACS Nano*, **2015**, 9, 8284-90	16.7	115
182	Tiling phosphorene. *ACS Nano*, **2014**, 8, 12763-8	16.7	109
181	Thermal line broadening in small metal clusters. *Physical Review B*, **1989**, 40, 2749-2751	3.3	109
180	Defective fullerenes and nanotubes as molecular magnets: An ab initio study. *Physical Review B*, **2003**, 68,	3.3	107
179	Control of Surface and Edge Oxidation on Phosphorene. *ACS Applied Materials & Interfaces*, **2017**, 9, 9126-9135	9.5	102
178	Morphology and Stability of Growing Multiwall Carbon Nanotubes. *Physical Review Letters*, **1997**, 79, 2065-2068	7.4	99
177	Two-Dimensional Phosphorus Carbide: Competition between sp(2) and sp(3) Bonding. *Nano Letters*, **2016**, 16, 3247-52	11.5	98

176	Microscopic formation mechanism of nanotube peapods. *Physical Review Letters*, **2002**, 88, 185502	7.4	97
175	Stability of multishell fullerenes. *Physical Review B*, **1993**, 48, 15461-15464	3.3	95
174	Electronic interwall interactions and charge redistribution in multiwall nanotubes. *Physical Review B* , **2001**, 65,	3.3	89
173	Stiffness of a solid composed of C60 clusters. *Physical Review B*, **1991**, 44, 6562-6565	3.3	88
172	Quasiparticle calculation of valence band offset of AlAs-GaAs(001). *Solid State Communications*, **1988**, 66, 585-588	1.6	88
171	Self-assembly of long chain alkanes and their derivatives on graphite. *Journal of Chemical Physics*, **2008**, 128, 124709	3.9	86
170	Cavities and Channels in Electrides. *Journal of the American Chemical Society*, **1996**, 118, 7329-7336	16.4	86
169	Laser-Driven Atomic Pump. *Physical Review Letters*, **1999**, 82, 5373-5376	7.4	82
168	Electronic and structural properties of carbon nanohorns. *Physical Review B*, **2000**, 62, R2291-R2294	3.3	79
167	Ab initio calculation of chemisorption systems: H on Pd(001) and Pd(110). *Physical Review B*, **1991**, 43, 4699-4713	3.3	79
166	Scrolls and nested tubes in multiwall carbon nanotubes. *Carbon*, **2002**, 40, 1123-1130	10.4	76
165	Stability and fragmentation of complex structures in ferrofluids. *Physical Review Letters*, **1995**, 74, 3049-3052	7.4	76
164	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
163	Zipper mechanism of nanotube fusion: theory and experiment. *Physical Review Letters*, **2004**, 92, 075504	7.4	75
162	High Stability of Faceted Nanotubes and Fullerenes of Multiphase Layered Phosphorus: A Computational Study. *Physical Review Letters*, **2014**, 113, 226801	7.4	73
161	Itinerant ferromagnetism in heterostructured C/BN nanotubes. *Physical Review B*, **2003**, 67,	3.3	72
160	Carbon foam: Spanning the phase space between graphite and diamond. *Physical Review B*, **2001**, 64,	3.3	70
159	Precursors to C60 fullerene formation. *Physical Review B*, **1992**, 46, 7326-7328	3.3	70

158	How free are encapsulated atoms in C60?. *Chemical Physics Letters*, **1994**, 221, 453-458	2.5	68
157	Photogalvanic effects in heteropolar nanotubes. *Physical Review Letters*, **2000**, 85, 1512-5	7.4	67
156	Photoexfoliation of graphene from graphite: an ab initio study. *Physical Review Letters*, **2010**, 104, 208302	7.4	64
155	Structural Transition in Layered As(1-x)P(x) Compounds: A Computational Study. *Nano Letters*, **2015**, 15, 6042-6	11.5	63
154	Electronic Structure of (n,0) Zigzag Carbon Nanotubes:´Cluster and Crystal Approach. *Journal of Physical Chemistry A*, **1998**, 102, 975-981	2.8	63
153	Theory for the atomic force microscopy of deformable surfaces. *Physical Review Letters*, **1989**, 63, 876-879	7.4	63
152	Chemical and Electronic Repair Mechanism of Defects in MoS Monolayers. *ACS Nano*, **2017**, 11, 9989-9996	16.7	62
151	Electronic model for energies, relaxations and reconstruction trends at metal surfaces. *Surface Science*, **1985**, 163, 503-515	1.8	62
150	Synthesis and transformation of linear adamantane assemblies inside carbon nanotubes. *ACS Nano*, **2012**, 6, 8674-83	16.7	61
149	Modeling extended contacts for nanotube and graphene devices. *Physical Review B*, **2008**, 77,	3.3	61
148	Fullereneynes: a new family of porous fullerenes. *Chemical Physics Letters*, **1993**, 204, 8-14	2.5	61
147	Noble gas temperature control of metal clusters: A molecular dynamics study. *Journal of Chemical Physics*, **1997**, 107, 3071-3079	3.9	60
146	Stability of M@C60 endohedral complexes. *Chemical Physics Letters*, **1993**, 208, 79-85	2.5	58
145	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. *Physical Review B*, **1989**, 40, 3162-3168	3.3	58
144	Evidence of diamond nanowires formed inside carbon nanotubes from diamantane dicarboxylic acid. *Angewandte Chemie - International Edition*, **2013**, 52, 3717-21	16.4	57
143	Quantum size effects in the polarizability of carbon fullerenes. *Physical Review Letters*, **2004**, 92, 215501	7.4	57
142	Effect of adsorbates on surface phonon modes: H on Pd(001) and Pd(110). *Physical Review B*, **1991**, 44, 13053-13062	3.3	56
141	Cold fusion: How close can deuterium atoms come inside palladium?. *Physical Review Letters*, **1989**, 63, 59-61	7.4	56

140	Ab initio calculation of coverage-dependent adsorption properties of H on Pd(001). *Physical Review Letters*, **1986**, 57, 2594-2597	7.4	56
139	Electronic structure of single-wall, multiwall, and filled carbon nanotubes. *Physical Review B*, **1997**, 55, 13980-13988	3.3	55
138	Microscopic mechanism of fullerene fusion. *Physical Review B*, **2004**, 70,	3.3	55
137	Structural properties of Fe crystals. *Physical Review B*, **1993**, 47, 95-99	3.3	54
136	Semiempirical theory for surface core-level shifts. *Solid State Communications*, **1982**, 41, 273-279	1.6	52
135	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
134	Energetics and electronic structure of a polyacetylene chain contained in a carbon nanotube. *Physical Review B*, **2003**, 67,	3.3	50
133	Mesoscopic origami with graphite: scrolls, nanotubes, peapods. *Physica B: Condensed Matter*, **2002**, 323, 86-89	2.8	49
132	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
131	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
130	Assembly of Ring-Shaped Phosphorus within Carbon Nanotube Nanoreactors. *Angewandte Chemie - International Edition*, **2017**, 56, 1850-1854	16.4	47
129	Coherent control of photocurrents in graphene and carbon nanotubes. *Physical Review B*, **2000**, 61, 7669-7677	3.3	47
128	Energetics and packing of fullerenes in nanotube peapods. *Physical Review B*, **2005**, 71,	3.3	46
127	Quasiparticle band gaps for ultrathin GaAs/AlAs(001) superlattices. *Physical Review Letters*, **1989**, 63, 1495-1498	7.4	44
126	Formation and properties of selenium double-helices inside double-wall carbon nanotubes: experiment and theory. *ACS Nano*, **2013**, 7, 5607-13	16.7	43
125	Real-time ab initio simulations of excited carrier dynamics in carbon nanotubes. *Physical Review Letters*, **2006**, 97, 126104	7.4	43
124	Computer simulation of hydrogen embrittlement in metals. *Nature*, **1993**, 362, 435-437	50.4	42
123	Orientational melting in carbon nanotube ropes. *Physical Review Letters*, **2000**, 84, 1483-6	7.4	41

122	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
121	Limits of Resolution in Atomic Force Microscopy Images of Graphite. *Europhysics Letters*, **1991**, 15, 49-54	1.6	37
120	Theory of elastic tip□urface 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
119	Collective electronic excitations in small metal clusters. *Physical Review B*, **1991**, 43, 6804-6807	3.3	37
118	Ionicity of the MC60 bond in M@C60 endohedral complexes. *Chemical Physics Letters*, **1995**, 243, 42-44	2.5	36
117	Interplay between structure and magnetism in Mo12S9I9 nanowires. *Physical Review Letters*, **2006**, 96, 125502	7.4	35
116	Continuum approach for long-wavelength acoustic phonons in quasi-two-dimensional structures. *Physical Review B*, **2016**, 94,	3.3	35
115	Computational study of the thermal conductivity in defective carbon nanostructures. *Physical Review B*, **2012**, 86,	3.3	33
114	Onset of nanotube decay under extreme thermal and electronic excitations. *Physica B: Condensed Matter*, **2002**, 323, 78-85	2.8	32
113	Hyperpolarizability of the C60 fullerene cluster. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1993**, 25, 181-184		32
112	Thermodynamic interpretation of core-level binding energies in adsorbates. *Surface Science*, **1983**, 126, 112-119	1.8	32
111	Interpreting core-level spectra of oxidizing phosphorene: Theory and experiment. *Physical Review B* , **2015**, 92,	3.3	31
110	□tates contribution to the conductivity of BC3. *Solid State Communications*, **1988**, 67, 515-518	1.6	31
109	Multi-adatom interactions on metal surfaces. *Surface Science*, **1986**, 173, 538-554	1.8	31
108	Strain-controlled fundamental gap and structure of bulk black phosphorus. *Physical Review B*, **2016**, 94,	3.3	31
107	Topologically protected conduction state at carbon foam surfaces: an ab initio study. *Physical Review Letters*, **2014**, 112, 026803	7.4	30
106	Origin of torsion-induced conductance oscillations in carbon nanotubes. *Physical Review B*, **2008**, 78,	3.3	30
105	Search for the largest two-dimensional aggregates of boron: An ab initio study. *Physical Review B*, **2011**, 83,	3.3	29

104	Field-induced unraveling of carbon nanotubes. *Chemical Physics Letters*, **1997**, 265, 667-672	2.5	29
103	Mechanical stability of Pd-H systems: A molecular-dynamics study. *Physical Review B*, **1992**, 46, 8099-8108	3.3	29
102	Mechanism of fullerene hydrogenation by polyamines: Ab initio density functional calculations. *Physical Review B*, **2008**, 78,	3.3	28
101	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
100	Formation and stability of cellular carbon foam structures: an ab initio study. *Physical Review Letters*, **2012**, 109, 135501	7.4	27
99	Rigid crystalline phases of polymerized fullerenes. *Physical Review B*, **2004**, 70,	3.3	27
98	Spontaneous graphitization of ultrathin cubic structures: a computational study. *Nano Letters*, **2014** , 14, 7126-30	11.5	26
97	Stability of C60 fullerite intercalation compounds. *Physical Review B*, **1993**, 47, 6711-6720	3.3	26
96	Degenerately Doped Transition Metal Dichalcogenides as Ohmic Homojunction Contacts to Transition Metal Dichalcogenide Semiconductors. *ACS Nano*, **2019**, 13, 5103-5111	16.7	25
95	Molecular self-assembly of functionalized fullerenes on a metal surface. *Physical Review Letters*, **2009**, 102, 056102	7.4	25
94	Unique structural and transport properties of molybdenum chalcohalide nanowires. *Physical Review Letters*, **2007**, 99, 085503	7.4	25
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91	Optimizing Charge Injection across Transition Metal Dichalcogenide Heterojunctions: Theory and Experiment. *ACS Nano*, **2017**, 11, 3904-3910	16.7	23
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88	Bonding and energy dissipation in a nanohook assembly. *Physical Review Letters*, **2003**, 91, 165503	7.4	23
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86	Minimum model for the electronic structure of twisted bilayer graphene and related structures. *Physical Review B*, **2018**, 98,	3.3	22
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84	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
83	Hydrogen-Induced Polymorphism of the Pd(110) Surface. *Physical Review Letters*, **1997**, 79, 1329-1332	7.4	22
82	Collective electronic excitations and their damping in small alkali clusters. *Chemical Physics Letters*, **1993**, 205, 521-528	2.5	22
81	Shear instability in twisted bilayer graphene. *Physical Review B*, **2018**, 98,	3.3	22
80	Stability differences and conversion mechanism between nanotubes and scrolls. *Physical Review B*, **2004**, 69,	3.3	21
79	Can photo excitations heal defects in carbon nanotubes?. *Chemical Physics Letters*, **2004**, 392, 209-213	2.5	21
78	Synthesis of high-density carbon nanotube films by microwave plasma chemical vapor deposition. *Diamond and Related Materials*, **2001**, 10, 1947-1951	3.5	21
77	Trapping cold atoms using surface-grown carbon nanotubes. *Physical Review A*, **2009**, 79,	2.6	20
76	Assembly of Ring-Shaped Phosphorus within Carbon Nanotube Nanoreactors. *Angewandte Chemie*, **2017**, 129, 1876-1880	3.6	19
75	Local curvature and stability of two-dimensional systems. *Physical Review B*, **2014**, 90,	3.3	19
74	Stability of fullerene-based systems. *Journal of Physics and Chemistry of Solids*, **1993**, 54, 1679-1684	3.9	19
73	Effect of Net Charge on the Relative Stability of 2D Boron Allotropes. *Nano Letters*, **2019**, 19, 1359-1365	11.5	18
72	Structural and magnetic properties of Tcn@C60 endohedral metalofullerenes: First-principles predictions. *Physical Review B*, **2010**, 81,	3.3	18
71	Disintegration of finite carbon chains in electric fields. *Chemical Physics Letters*, **1997**, 264, 345-350	2.5	18
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67	Can CF-Functionalized La@C Be Isolated Experimentally and Become Superconducting?. *Nano Letters*, **2017**, 17, 3402-3408	11.5	16
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64	Does hydrogen pre-melt palladium clusters?. *Chemical Physics Letters*, **1997**, 264, 39-43	2.5	16
63	X-ray spectroscopic and quantum chemical study of carbon tubes produced in arc-discharge. *Chemical Physics Letters*, **1998**, 289, 341-349	2.5	16
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53	Compositional ordering and quantum transport in Mo6S9Ix nanowires: Ab initio calculations. *Physical Review B*, **2008**, 77,	3.3	15
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49	Stability, electronic structure and reactivity of the polymerized fullerite forms. *Journal of Physics and Chemistry of Solids*, **2000**, 61, 1901-1911	3.9	14
48	Theory for the atomic force microscopy of layered elastic surfaces. *Journal of Physics Condensed Matter*, **1992**, 4, 4233-4249	1.8	14
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46	Evidence of Diamond Nanowires Formed inside Carbon Nanotubes from Diamantane Dicarboxylic Acid. *Angewandte Chemie*, **2013**, 125, 3805-3809	3.6	13
45	Reinforcing multiwall carbon nanotubes by electron beam irradiation. *Journal of Applied Physics*, **2010**, 108, 084314	2.5	13
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43	Limits of mechanical energy storage and structural changes in twisted carbon nanotube ropes. *Physical Review B*, **2013**, 88,	3.3	12
42	Do Carbon Nanotubes Spin When Bundled?. *Journal of Materials Research*, **1998**, 13, 2363-2367	2.5	12
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