John W Mintmire

List of Publications by Citations

56 papers	6,188 citations	28 h-index	58 g-index
58 ext. papers	6,465 ext. citations	4.5 avg, IF	5.46 L-index

#	Paper	IF	Citations
56	Are fullerene tubules metallic?. *Physical Review Letters*, **1992**, 68, 631-634	7.4	1869
55	Energetics of nanoscale graphitic tubules. *Physical Review B*, **1992**, 45, 12592-12595	3.3	826
54	Helical and rotational symmetries of nanoscale graphitic tubules. *Physical Review B*, **1993**, 47, 5485-5488	3.3	540
53	Electronic and structural properties of carbon nanotubes. *Carbon*, **1995**, 33, 893-902	10.4	302
52	Electrostatic potentials for metal-oxide surfaces and interfaces. *Physical Review B*, **1994**, 50, 11996-12003	3.3	301
51	Fitting the Coulomb potential variationally in linear-combination-of-atomic-orbitals density-functional calculations. *Physical Review A*, **1982**, 25, 88-95	2.6	237
50	Hidden one-electron interactions in carbon nanotubes revealed in graphene nanostrips. *Nano Letters*, **2007**, 7, 825-30	11.5	166
49	Local-density-functional methods in two-dimensionally periodic systems. Hydrogen and beryllium monolayers. *Physical Review B*, **1982**, 26, 1743-1753	3.3	166
48	Density of states reflects diameter in nanotubes. *Nature*, **1998**, 394, 29-30	50.4	150
47	Graphene nanostrip digital memory device. *Nano Letters*, **2007**, 7, 3608-11	11.5	135
46	Altering low-bias transport in zigzag-edge graphene nanostrips with edge chemistry. *Applied Physics Letters*, **2007**, 91, 112108	3.4	135
45	Properties of fullerene nanotubules. *Journal of Physics and Chemistry of Solids*, **1993**, 54, 1835-1840	3.9	129
44	Fundamental properties of single-wall carbon nanotubes. *Journal of Physical Chemistry B*, **2005**, 109, 52-65	3.4	128
43	Conformational effects in organopolysilanes: A first-principles approach. *Physical Review B*, **1989**, 39, 13350-13357	3.3	95
42	X□Approach for the Determination of Electronic and Geometric Structure of Polyacetylene and Other Chain Polymers. *Physical Review Letters*, **1983**, 50, 101-105	7.4	84
41	Local-density-functional approach to all-trans-polyacetylene. *Physical Review B*, **1983**, 28, 3283-3290	3.3	84
40	Local-density-functional results for the dimerization of trans-polyacetylene: Relationship to the band-gap problem. *Physical Review B*, **1987**, 35, 4180-4183	3.3	75

39	Edges bring new dimension to graphene nanoribbons. *Nano Letters*, **2010**, 10, 3638-42	11.5	64
38	Transport in multiterminal graphene nanodevices. *Nanotechnology*, **2007**, 18, 424033	3.4	60
37	Local-density-functional calculation of photoelectron spectra of fullerenes. *Physical Review B*, **1991**, 43, 14281-14284	3.3	56
36	Molecular-dynamics simulations of void collapse in shocked model-molecular solids. *Physical Review B*, **1994**, 49, 14859-14864	3.3	51
35	Local-density-functional total energy gradients in the linear combination of Gaussian-type orbitals method. *Physical Review A*, **1990**, 42, 6354-6359	2.6	49
34	Stability and electronic structure of phosphorus nanotubes. *Europhysics Letters*, **2004**, 65, 82-88	1.6	48
33	Electronic structure simulations of carbon nanotubes. *Synthetic Metals*, **1996**, 77, 231-234	3.6	38
32	First-Principles Study of the Optical Properties of ZnO Single-Wall Nanotubes *Journal of Physical Chemistry C*, **2007**, 111, 17821-17826	3.8	34
31	Heteroatom effects in heterocyclic ring chain polymers. *Synthetic Metals*, **1986**, 16, 235-243	3.6	32
30	Charge transfer and bonding in metallic oxides. *Journal of Adhesion Science and Technology*, **1994**, 8, 853-864	2	31
29	First-principles calculation of the conformation and electronic structure of polyparaphenylene. *Journal of Chemical Physics*, **1998**, 109, 9623-9631	3.9	28
28	Molecular dynamics simulations of the oxidation of aluminum nanoparticles. *Journal of Physical Chemistry B*, **2005**, 109, 209-14	3.4	28
27	Stability of narrow zigzag carbon nanotubes. *International Journal of Quantum Chemistry*, **2003**, 91, 51-56	2.1	26
26	Group-IV covalent clusters: Si45 and C44 versus Si44 and C45. *Physical Review B*, **1991**, 44, 3479-3482	3.3	25
25	Theoretical treatment of the dielectric response of all-trans-polyacetylene. *Physical Review B*, **1983**, 27, 1447-1449	3.3	23
24	Chemical forces associated with deuterium confinement in palladium. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1989**, 138, 51-54	2.3	16
23	Conformation and electronic structure of heterocyclic ring chain polymers. *Synthetic Metals*, **1988**, 25, 109-119	3.6	15
22	Structural and elastic properties of transition-metal superlattices. *Physical Review B*, **1992**, 45, 13624-13630	3.3	14

21	Electrostatic-based model for alumina surfaces. *Thin Solid Films*, **1994**, 253, 179-184	2.2	13
20	Photoelectron spectra from local-density-functional calculations: Application to chain polymers. *Physical Review B*, **1987**, 36, 3312-3318	3.3	13
19	A comparison of the LCAO-Xα method with the hartree□fock and multiple-scattering-Xα methods on carbon monoxide. *Chemical Physics*, **1980**, 50, 91-103	2.3	13
18	Comment on "Ground state of trans-polyacetylene and the Peierls mechanism". *Physical Review Letters*, **1989**, 63, 2532	7.4	11
17	Robust Ballistic Transport in Narrow Armchair-Edge Graphene Nanoribbons with Chemical Edge Disorder. *Journal of Physical Chemistry Letters*, **2010**, 1, 1082-1085	6.4	9
16	Reactive Bond-Order Simulations Using Both Spatial and Temporal Approaches to Parallelism. *Structural Chemistry*, **2004**, 15, 479-486	1.8	9
15	Model studies of composition-modulated Cu?Ni superlattices. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1990**, 126, 29-31	5.3	8
14	Theoretical elastic properties of single-walled carbon nanotubes. *International Journal of Quantum Chemistry*, **2005**, 105, 767-771	2.1	7
13	Multiscale Modeling of Metal□Metal Contact Dynamics Under High Electromagnetic Stress: Timescales and Mechanisms for Joule Melting of Al□Cu Asperities. *IEEE Transactions on Magnetics*, **2009**, 45, 331-335	2	6
12	Endohedral carbon chains in chiral single-wall carbon nanotubes. *International Journal of Quantum Chemistry*, **2006**, 106, 2324-2330	2.1	6
11	Simulations of metal nanowires. *International Journal of Quantum Chemistry*, **2005**, 105, 772-780	2.1	6
10	Lattice vacancy effects on electron transport in multiterminal graphene nanodevices. *International Journal of Quantum Chemistry*, **2007**, 107, 3071-3076	2.1	5
9	First-principles properties of organic polymer photovoltaic materials. *International Journal of Quantum Chemistry*, **2007**, 107, 3120-3125	2.1	4
8	Surface passivation effects in silicon nanowires. *Molecular Physics*, **2015**, 113, 274-281	1.7	3
7	Electronic transport of silicon nanowires with surface defects. *International Journal of Quantum Chemistry*, **2009**, 109, 3705-3710	2.1	3
6	Endohedral selenium chains in carbon, boron nitride, and BC2N nanotubes. *International Journal of Quantum Chemistry*, **2000**, 80, 480-485	2.1	3
5	Effect of phase-breaking events on electron transport in mesoscopic and nanodevices. *International Journal of Quantum Chemistry*, **2008**, 108, 2896-2905	2.1	2
4	Limits of chemical effects on cold fusion. *Journal of Fusion Energy*, **1990**, 9, 363-366	1.6	2

3	Linear combination of Gaussian-type orbitals-local-density-functional cluster studies of D-D interactions in titanium and palladium. *Physical Review B*, **1990**, 41, 9683-9687	3.3	2
2	First-principles simulations of chiral double-wall carbon nanotubes. *International Journal of Quantum Chemistry*, **2008**, 108, 2943-2949	2.1	1
1	First-Principles Study of Helical Silver Single-Wall Nanotubes and Nanowires. *Materials Research Society Symposia Proceedings*, **2005**, 900, 1		1