James C Greer

List of Publications by Year
in descending order

125 papers	2,826 citations	159585 30 h-index	197818 49 g-index
130 all docs	130 docs citations	130 times ranked	3221 citing authors

#	Article	IF	Citations
1	Silicon Nanowire Band Gap Modification. Nano Letters, 2007, 7, 34-38.	9.1	215
2	Simulating the atomic layer deposition of alumina from first principles. Journal of Materials Chemistry, 2004, 14, 3246.	6.7	134
3	Correlated Electron Transport in Molecular Electronics. Physical Review Letters, 2004, 93, 036805.	7.8	123
4	Simulation of junctionless Si nanowire transistors with 3 nm gate length. Applied Physics Letters, 2010, 97, .	3.3	92
5	Interactions between Thiol Molecular Linkers and the Au13Nanoparticle. Journal of Physical Chemistry B, 2002, 106, 5931-5937.	2.6	80
6	Estimating full configuration interaction limits from a Monte Carlo selection of the expansion space. Journal of Chemical Physics, 1995, 103, 1821-1828.	3.0	79
7	Stress induced carbon fiber orientation for enhanced thermal conductivity of epoxy composites. Composites Part B: Engineering, 2021, 208, 108599.	12.0	76
8	C60 as a Faraday cage. Applied Physics Letters, 2004, 84, 431-433.	3.3	73
9	Orientation of individual<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>molecules adsorbed on Cu(111): Low-temperature scanning tunneling microscopy and density functional calculations. Physical Review B, 2008, 77, .	3.2	73
10	Nonâ€Covalent Functionalization of Graphene Using Selfâ€Assembly of Alkaneâ€Amines. Advanced Functional Materials, 2012, 22, 717-725.	14.9	73
11	Monte Carlo Configuration Interaction. Journal of Computational Physics, 1998, 146, 181-202.	3.8	72
12	Spin-Polarization Mechanisms of the Nitrogen-Vacancy Center in Diamond. Nano Letters, 2010, 10, 610-614.	9.1	68
13	Reaction/diffusion with Michaelisâ€“Menten kinetics in electroactive polymer films. Part 1. The steady-state amperometric response. Analyst, The, 1996, 121, 715-731.	3.5	59
14	Deformation Potentials and Electronâ^'Phonon Coupling in Silicon Nanowires. Nano Letters, 2010, 10, 869-873.	9.1	59
15	Device physics of back-contact perovskite solar cells. Energy and Environmental Science, 2020, 13, 1753-1765.	30.8	58
16	Phosphorous trapped within buckminsterfullerene. Journal of Chemical Physics, 2002, 116, 7849-7854.	3.0	54
17	The atomic nature of endohedrally encapsulated nitrogen N@C60 studied by density functional and Hartree-Fock methods. Chemical Physics Letters, 2000, 326, 567-572.	2.6	53
18	A Proposed Confinement Modulated Gap Nanowire Transistor Based on a Metal (Tin). Nano Letters, 2012, 12, 2222-2227.	9.1	45

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19	Binding energies and structures of NH3 clusters. Chemical Physics, 1989, 133, 191-197.	1.9	44
20	Tunnelling in alkanes anchored to gold electrodes via amine end groups. Nanotechnology, 2007, 18, 424010.	2.6	40
21	Predicting mask distortion, clogging and pattern transfer for stencil lithography. Microelectronic Engineering, 2007, 84, 42-53.	2.4	40
22	Impact of electronâ€“electron cusp on configuration interaction energies. Journal of Chemical Physics, 2001, 115, 1626-1634.	3.0	38
23	Tunnel Currents across Silane Diamines/Dithiols and Alkane Diamines/Dithiols: A Comparative Computational Study. Journal of Physical Chemistry C, 2009, 113, 744-750.	3.1	38
24	Proton transfer in ammonia cluster cations: molecular dynamics in a self consistent field. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 18, 413-426.	1.0	37
25	Monte Carlo configuration interaction predictions for the electronic spectra of Ne, CH2, C2, N2, and H2O compared to full configuration interaction calculations. Journal of Chemical Physics, 2008, 129, 064103.	3.0	37
26	Molecular Dynamics Study of Naturally Occurring Defects in Self-Assembled Monolayer Formation. ACS Nano, 2010, 4, 921-932.	14.6	37
27	Computational design ofSiâ•SiO2interfaces: Stress and strain on the atomic scale. Physical Review B, 2006, 73, .	3.2	36
28	Ballistic Conductance in Oxidized Si Nanowires. Nano Letters, 2009, 9, 1856-1860.	9.1	36
29	Independent particle descriptions of tunneling using the many-body quantum transport approach. Physical Review B, 2006, 73, .	3.2	32
30	A Monte Carlo configuration generation computer program for the calculation of electronic states of atoms, molecules, and quantum dots. Computer Physics Communications, 2000, 131, 142-163.	7.5	31
31	Corrugated membranes for improved pattern definition with micro/nanostencil lithography. Sensors and Actuators A: Physical, 2006, 130-131, 568-574.	4.1	31
32	Synergistic effect of carbon fiber and graphite on reducing thermal resistance of thermal interface materials. Composites Science and Technology, 2021, 212, 108883.	7.8	31
33	Crystallization induced realignment of carbon fibers in a phase change material to achieve exceptional thermal transportation properties. Journal of Materials Chemistry A, 2022, 10, 593-601.	10.3	29
34	Determination of complex absorbing potentials from the electron self-energy. Journal of Chemical Physics, 2006, 125, 244104.	3.0	28
35	Electron transport properties of sub-3-nm diameter copper nanowires. Physical Review B, 2015, 92, .	3.2	28
36	Nanoscale Dynamics and Protein Adhesivity of Alkylamine Self-Assembled Monolayers on Graphene. Langmuir, 2013, 29, 7271-7282.	3.5	27

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37	Reinventing solid state electronics: Harnessing quantum confinement in bismuth thin films. Applied Physics Letters, 2017, 110, .	3.3	26
38	Ab initio geometry and stability of a C120 torus. Chemical Physics Letters, 1994, 222, 621-625.	2.6	25
39	A force-field description of short-range repulsions for high density alkane molecular dynamics simulations. Journal of Computational Chemistry, 2004, 25, 1953-1966.	3.3	25
40	Consistent treatment of correlation effects in molecular dissociation studies using randomly chosen configurations. Journal of Chemical Physics, 1995, 103, 7996-8003.	3.0	24
41	Atomic scale model interfaces between high-khafnium silicates and silicon. Physical Review B, 2007, 75, .	3.2	24
42	Quantification of Ink Diffusion in Microcontact Printing with Self-Assembled Monolayers. Langmuir, 2009, 25, 242-247.	3.5	23
43	Symmetry, delocalization, and molecular conductance. Journal of Chemical Physics, 2005, 122, 044710.	3.0	22
44	Thermal decomposition mechanisms of hafnium and zirconium silicates at the atomic scale. Journal of Applied Physics, 2005, 97, 114911.	2.5	22
45	Quantum electronic transport in a configuration interaction basis. International Journal of Quantum Chemistry, 2004, 100, 1163-1169.	2.0	21
46	Subthreshold behavior of junctionless silicon nanowire transistors from atomic scale simulations. Solid-State Electronics, 2012, 71, 58-62.	1.4	21
47	Monte Carlo configuration interaction with perturbation corrections for dissociation energies of first row diatomic molecules: C2, N2, O2, CO, and NO. Journal of Chemical Physics, 2014, 140, 084114.	3.0	20
48	Structures and spectra of Na(NH3) n=1,2. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 30, 69-75.	1.0	18
49	Status and perspectives of nanoscale device modelling. Nanotechnology, 2001, 12, 136-142.	2.6	18
50	Charge-carrier dynamics for silicon oxide tunneling junctions mediated by local pinholes. Cell Reports Physical Science, 2021, 2, 100667.	5.6	18
51	Guanidinium Chloride Molecular Diffusion in Aqueous and Mixed Waterâ˜Ethanol Solutions. Journal of Physical Chemistry B, 2008, 112, 8906-8911.	2.6	17
52	Metal-semimetal Schottky diode relying on quantum confinement. Microelectronic Engineering, 2018, 195, 21-25.	2.4	17
53	Oxide removal and stabilization of bismuth thin films through chemically bound thiol layers. RSC Advances, 2018, 8, 33368-33373.	3.6	17
54	Mixed aggregation between lithium diisopropylamide and lithium chloride: NMR, solid-state structure and ab initio calculations. Inorganica Chimica Acta, 1997, 258, 1-9.	2.4	14

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55	Electrostatic ordering of the lanthanum endoatom inLa@C82adsorbed on metal surfaces. Physical Review B, 2005, 71, .	3.2	13
56	First Principle-Based Analysis of Single-Walled Carbon Nanotube and Silicon Nanowire Junctionless Transistors. IEEE Nanotechnology Magazine, 2013, 12, 1075-1081.	2.0	13
57	Quasiparticle energies and lifetimes in a metallic chain model of a tunnel junction. Journal of Chemical Physics, 2013, 138, 144105.	3.0	11
58	Strain induced effects on electronic structure of semi-metallic and semiconducting tin nanowires. Applied Physics Letters, 2014, 105, 123105.	3.3	11
59	A sub kBT/q semimetal nanowire field effect transistor. Applied Physics Letters, 2016, 109, 063108.	3.3	11
60	Error analysis for pseudo-logarithmic amplification. Measurement Science and Technology, 1992, 3, 939-942.	2.6	10
61	Amidolithium-mediated enolization: does proton transfer occur via a dimer intermediate with bridging carbonyls?. New Journal of Chemistry, 2001, 25, 262-267.	2.8	10
62	Many-electron systems with constrained current. Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 291, 46-50.	2.1	10
63	Bonding of Atomic Phosphorus to Polycyclic Hydrocarbons and Curved Graphitic Surfaces. Journal of the American Chemical Society, 2003, 125, 2301-2306.	13.7	10
64	Transport properties and electrical device characteristics with the TiMeS computational platform: Application in silicon nanowires. Journal of Applied Physics, 2013, 113, 203708.	2.5	9
65	Divacancies in carbon nanotubes and their influence on electron scattering. Journal of Physics Condensed Matter, 2014, 26, 045303.	1.8	9
66	A Semimetal Nanowire Rectifier: Balancing Quantum Confinement and Surface Electronegativity. Nano Letters, 2016, 16, 7639-7644.	9.1	9
67	A basis set study for the calculation of electronic excitations using Monte Carlo configuration interaction. Journal of Chemical Physics, 2001, 114, 15.	3.0	8
68	Effect of strain, thickness, and local surface environment on electron transport properties of oxygen-terminated copper thin films. Physical Review B, 2016, 94, .	3.2	8
69	Quantum mechanics at the core of multi-scale simulations. Journal of Computer-Aided Materials Design, 2006, 13, 89-109.	0.7	7
70	Effect of structure on electronic properties of the iron-carbon nanotube interface. Chemical Physics Letters, 2014, 615, 11-15.	2.6	7
71	Electronegativity and Electron Currents in Molecular Tunnel Junctions. Journal of Physical Chemistry C, 2010, 114, 20564-20568.	3.1	6
72	Electronic structure tuning via surface modification in semimetallic nanowires. Physical Review B, 2016, 94, .	3.2	6

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73	Effect of strain and diameter on electronic and charge transport properties of indium arsenide nanowires. Solid-State Electronics, 2018, 149, 6-14.	1.4	6
74	Electronic properties of bismuth nanostructures. Physical Review B, 2021, 104, .	3.2	6
75	Comment on: Structures, stabilities, and intermolecular vibrational frequencies of small ammonia complexes by molecular mechanics for clusters analysis. Journal of Chemical Physics, 1991, 95, 3861-3862.	3.0	5
76	Band structure engineering of a molecular wire system composed of dimercaptoacetoamidobenzene, its derivatives, and gold clusters. Computational Materials Science, 2003, 27, 166-174.	3.0	5
77	Electronic current density expanded in natural orbitals. Molecular Physics, 2008, 106, 1363-1367.	1.7	5
78	Energies of the X- and L-valleys in In0.53Ga0.47As from electronic structure calculations. Journal of Applied Physics, 2016, 119, .	2.5	5
79	Electronic and structural properties of rhombohedral [1â€‰1â€‰1] and [1â€‰1â€‰0] oriented ultra-thin bismuth nanowires. Journal of Physics Condensed Matter, 2017, 29, 065301.	1.8	5
80	First principles modeling of defects in the Al2O3/In0.53Ga0.47As system. Journal of Applied Physics, 2017, 121, .	2.5	5
81	Effect of strain and many-body corrections on the band inversions and topology of bismuth. Physical Review B, 2021, 104, .	3.2	5
82	Structural modification of thin Bi(1 1 1) films by passivation and native oxide model. Physical Review Materials, 2019, 3, .	2.4	5
83	Impact of Metal Hybridization on Contact Resistance and Leakage Current of Carbon Nanotube Transistors. IEEE Electron Device Letters, 2022, 43, 1367-1370.	3.9	5
84	Alloy corrections to the virtual crystal approximation and explicit band structure calculations for silicon-germanium. Materials Science in Semiconductor Processing, 2000, 3, 109-114.	4.0	4
85	Computational Design of Silicon Suboxides: Chemical and Mechanical Forces on the Atomic Scale. Journal of Computer-Aided Materials Design, 2006, 13, 185-200.	0.7	4
86	Variational method with scattering boundary conditions imposed by the Wigner distribution. Physical Review B, 2011, 83, .	3.2	4
87	Properties of homo- and hetero-Schottky junctions from first principle calculations. Journal of Physics Condensed Matter, 2018, 30, 414003.	1.8	4
88	Impact of stoichiometry and strain on Ge1â^'x Sn x alloys from first principles calculations. Journal Physics D: Applied Physics, 2021, 54, 245103.	2.8	4
89	Extraction of analytical potential function parameters from abÂinitio potential energy surfaces and analytical forces. Computer Physics Communications, 2002, 147, 803-825.	7.5	3
90	Statistical estimates of electron correlations. Journal of Chemical Physics, 2006, 125, 054104.	3.0	3

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91	Comment on â€œElectron transport through correlated molecules computed using the time-independent Wigner function: Two critical testsâ€• Physical Review B, 2010, 82, .	3.2	3
92	Structural and energetic origin of defects at the interface between germanium and a high-k dielectric from first principles. Applied Physics Letters, 2011, 98, 082904.	3.3	3
93	TREPICO observation of the threshold region of N2O clusters. Chemical Physics Letters, 1990, 168, 330-336.	2.6	2
94	An Approximate Time Evolution Operator to Generate the Verlet Algorithm. Journal of Computational Physics, 1994, 115, 245-247.	3.8	2
95	Parallelization model for successive approximations to the Rayleigh-Ritz linear variational problem. IEEE Transactions on Parallel and Distributed Systems, 1998, 9, 938-946.	5.6	2
96	Electronic correlation energy in linear and cyclic carbon tetramers. Chemical Physics Letters, 1999, 306, 197-201.	2.6	2
97	Cluster ion implantation: a molecular dynamics study. Materials Science in Semiconductor Processing, 2000, 3, 91-95.	4.0	2
98	Side gating in silicon germanium hetero-dimensional field effect transistors. Microelectronic Engineering, 2004, 71, 197-208.	2.4	2
99	Heterodimensional FET With Split Drain. IEEE Electron Device Letters, 2004, 25, 737-739.	3.9	2
100	A Physical Compact Model for Electron Transport Across Single Molecules. IEEE Nanotechnology Magazine, 2006, 5, 745-749.	2.0	2
101	Stress in silicon interlayers at the SiOxâ•Ge interface. Applied Physics Letters, 2007, 90, 143511.	3.3	2
102	Mechanical stabilisation and design optimisation of masks for stencil lithography: Numerical approach and experimental validation. Microelectronic Engineering, 2008, 85, 2243-2249.	2.4	2
103	Transient activation model for antimony in relaxed and strained silicon. Solid-State Electronics, 2009, 53, 1173-1176.	1.4	2
104	Comment on â€œCritical analysis of a variational method used to describe molecular electron transportâ€• Physical Review B, 2011, 84, .	3.2	2
105	Atomic scale simulation of a junctionless silicon nanowire transistor. , 2011, , .		2
106	Many-electron scattering applied to atomic point contacts. Journal of Physics Condensed Matter, 2012, 24, 125602.	1.8	2
107	Influence of surface stoichiometry and quantum confinement on the electronic structure of small diameter InxGa1-xAs nanowires. Materials Chemistry and Physics, 2018, 206, 35-39.	4.0	2
108	Influence of Surface Passivation on Indium Arsenide Nanowire Band Gap Energies. Journal of Electronic Materials, 2019, 48, 6654-6660.	2.2	2

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109	Electrode-molecule energy level offsets in a gold-benzene diamine-gold single molecule tunnel junction. Journal of Chemical Physics, 2020, 153, 174104.	3.0	2
110	Constrained mechanics for the dynamical simulated annealing of Coulomb systems. Theoretica Chimica Acta, 1994, 88, 363-373.	0.8	1
111	Tools for analysing configuration interaction wavefunctions. Computational Materials Science, 2003, 28, 240-249.	3.0	1
112	E-MRS 2004 Spring Meeting Symposium H: Atomic Scale Materials Design: Modelling and Characterization. Computational Materials Science, 2005, 33, 1-2.	3.0	1
113	Tin nanowire field effect transistor. , 2012, , .		1
114	Formation of contacts between doped carbon nanotubes and aluminum electrodes. Journal of Applied Physics, 2013, 114, 153709.	2.5	1
115	Semi-Metal Nanowire Transistors from First Principle Calculations. ECS Transactions, 2013, 53, 259-267.	0.5	1
116	Multigate and Nanowire Transistors. , 2016, , 18-53.		1
117	Alternative equations of motion for dynamical simulated annealing of the density functional. Physical Review B, 1996, 53, 10651-10655.	3.2	0
118	E-MRS 2002 Spring Meeting Symposium A: Atomic Scale Materials Design. Computational Materials Science, 2003, 27, xi-xii.	3.0	0
119	Reduced Density Matrices in Quantum Electronic Transport. AIP Conference Proceedings, 2007, , .	0.4	0
120	Computational Design and Optimisation of Mechanically Reinforced Masks for Stencil Lithography. , 2007, , .		0
121	Strained semimetallic and semiconducting SnNW. , 2015, , .		0
122	Nanowire Electronic Structure. , 0, , 107-166.		0
123	Charge Transport in Quasi-1d Nanostructures. , 0, , 167-220.		0
124	Atomic-scale simulation of semimetal-to-semiconductor transition in bismuth nanowires for future generation of nanoelectronic devices. , 2016, , .		0
125	Epitaxial stabilisation of Ge1 â^' x Sn x alloys. Journal Physics D: Applied Physics, 2021, 54, 325302.	2.8	0