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	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
2	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
3	Stress induced carbon fiber orientation for enhanced thermal conductivity of epoxy composites. Composites Part B: Engineering, 2021, 208, 108599.	12.0	76
4	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
5	Epitaxial stabilisation of Ge1 â^' x Sn x alloys. Journal Physics D: Applied Physics, 2021, 54, 325302.	2.8	0
6	Effect of strain and many-body corrections on the band inversions and topology of bismuth. Physical Review B, 2021, 104, .	3.2	5
7	Electronic properties of bismuth nanostructures. Physical Review B, 2021, 104, .	3.2	6
8	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
9	Charge-carrier dynamics for silicon oxide tunneling junctions mediated by local pinholes. Cell Reports Physical Science, 2021, 2, 100667.	5.6	18
10	Device physics of back-contact perovskite solar cells. Energy and Environmental Science, 2020, 13, 1753-1765.	30.8	58
11	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
12	Influence of Surface Passivation on Indium Arsenide Nanowire Band Gap Energies. Journal of Electronic Materials, 2019, 48, 6654-6660.	2.2	2
13	Structural modification of thin Bi(1 1 1) films by passivation and native oxide model. Physical Review Materials, 2019, 3, .	2.4	5
14	Metal-semimetal Schottky diode relying on quantum confinement. Microelectronic Engineering, 2018, 195, 21-25.	2.4	17
15	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
16	Oxide removal and stabilization of bismuth thin films through chemically bound thiol layers. RSC Advances, 2018, 8, 33368-33373.	3.6	17
17	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
18	Properties of homo- and hetero-Schottky junctions from first principle calculations. Journal of Physics Condensed Matter, 2018, 30, 414003.	1.8	4

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19	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
20	First principles modeling of defects in the Al2O3/In0.53Ga0.47As system. Journal of Applied Physics, 2017, 121, .	2.5	5
21	Reinventing solid state electronics: Harnessing quantum confinement in bismuth thin films. Applied Physics Letters, 2017, 110, .	3.3	26
22	A Semimetal Nanowire Rectifier: Balancing Quantum Confinement and Surface Electronegativity. Nano Letters, 2016, 16, 7639-7644.	9.1	9
23	Electronic structure tuning via surface modification in semimetallic nanowires. Physical Review B, 2016, 94, .	3.2	6
24	A sub kBT/q semimetal nanowire field effect transistor. Applied Physics Letters, 2016, 109, 063108.	3.3	11
25	Multigate and Nanowire Transistors. , 2016, , 18-53.		1
26	Atomic-scale simulation of semimetal-to-semiconductor transition in bismuth nanowires for future generation of nanoelectronic devices. , 2016, , .		0
27	Energies of the X- and L-valleys in In0.53Ga0.47As from electronic structure calculations. Journal of Applied Physics, 2016, 119, .	2.5	5
28	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
29	Electron transport properties of sub-3-nm diameter copper nanowires. Physical Review B, 2015, 92, .	3.2	28
30	Strained semimetallic and semiconducting SnNW. , 2015, , .		0
31	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
32	Divacancies in carbon nanotubes and their influence on electron scattering. Journal of Physics Condensed Matter, 2014, 26, 045303.	1.8	9
33	Effect of structure on electronic properties of the iron-carbon nanotube interface. Chemical Physics Letters, 2014, 615, 11-15.	2.6	7
34	Strain induced effects on electronic structure of semi-metallic and semiconducting tin nanowires. Applied Physics Letters, 2014, 105, 123105.	3.3	11
35	Nanoscale Dynamics and Protein Adhesivity of Alkylamine Self-Assembled Monolayers on Graphene. Langmuir, 2013, 29, 7271-7282.	3.5	27
36	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

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37	First Principle-Based Analysis of Single-Walled Carbon Nanotube and Silicon Nanowire Junctionless Transistors. IEEE Nanotechnology Magazine, 2013, 12, 1075-1081.	2.0	13
38	Quasiparticle energies and lifetimes in a metallic chain model of a tunnel junction. Journal of Chemical Physics, 2013, 138, 144105.	3.0	11
39	Formation of contacts between doped carbon nanotubes and aluminum electrodes. Journal of Applied Physics, 2013, 114, 153709.	2.5	1
40	Semi-Metal Nanowire Transistors from First Principle Calculations. ECS Transactions, 2013, 53, 259-267.	0.5	1
41	Many-electron scattering applied to atomic point contacts. Journal of Physics Condensed Matter, 2012, 24, 125602.	1.8	2
42	Tin nanowire field effect transistor. , 2012, , .		1
43	A Proposed Confinement Modulated Gap Nanowire Transistor Based on a Metal (Tin). Nano Letters, 2012, 12, 2222-2227.	9.1	45
44	Subthreshold behavior of junctionless silicon nanowire transistors from atomic scale simulations. Solid-State Electronics, 2012, 71, 58-62.	1.4	21
45	Nonâ€Covalent Functionalization of Graphene Using Selfâ€Assembly of Alkaneâ€Amines. Advanced Functional Materials, 2012, 22, 717-725.	14.9	73
46	Comment on â€œCritical analysis of a variational method used to describe molecular electron transportâ€• Physical Review B, 2011, 84, .	3.2	2
47	Variational method with scattering boundary conditions imposed by the Wigner distribution. Physical Review B, 2011, 83, .	3.2	4
48	Atomic scale simulation of a junctionless silicon nanowire transistor. , 2011, , .		2
49	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
50	Spin-Polarization Mechanisms of the Nitrogen-Vacancy Center in Diamond. Nano Letters, 2010, 10, 610-614.	9.1	68
51	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
52	Electronegativity and Electron Currents in Molecular Tunnel Junctions. Journal of Physical Chemistry C, 2010, 114, 20564-20568.	3.1	6
53	Simulation of junctionless Si nanowire transistors with 3 nm gate length. Applied Physics Letters, 2010, 97, .	3.3	92
54	Molecular Dynamics Study of Naturally Occurring Defects in Self-Assembled Monolayer Formation. ACS Nano, 2010, 4, 921-932.	14.6	37

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55	Deformation Potentials and Electronâ^'Phonon Coupling in Silicon Nanowires. Nano Letters, 2010, 10, 869-873.	9.1	59
56	Transient activation model for antimony in relaxed and strained silicon. Solid-State Electronics, 2009, 53, 1173-1176.	1.4	2
57	Quantification of Ink Diffusion in Microcontact Printing with Self-Assembled Monolayers. Langmuir, 2009, 25, 242-247.	3.5	23
58	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
59	Ballistic Conductance in Oxidized Si Nanowires. Nano Letters, 2009, 9, 1856-1860.	9.1	36
60	Mechanical stabilisation and design optimisation of masks for stencil lithography: Numerical approach and experimental validation. Microelectronic Engineering, 2008, 85, 2243-2249.	2.4	2
61	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
62	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
63	Guanidinium Chloride Molecular Diffusion in Aqueous and Mixed Waterâ^'Ethanol Solutions. Journal of Physical Chemistry B, 2008, 112, 8906-8911.	2.6	17
64	Electronic current density expanded in natural orbitals. Molecular Physics, 2008, 106, 1363-1367.	1.7	5
65	Atomic scale model interfaces between high-khafnium silicates and silicon. Physical Review B, 2007, 75, .	3.2	24
66	Stress in silicon interlayers at the SiOxâ^•Ge interface. Applied Physics Letters, 2007, 90, 143511.	3.3	2
67	Reduced Density Matrices in Quantum Electronic Transport. AIP Conference Proceedings, 2007, , .	0.4	0
68	Tunnelling in alkanes anchored to gold electrodes via amine end groups. Nanotechnology, 2007, 18, 424010.	2.6	40
69	Computational Design and Optimisation of Mechanically Reinforced Masks for Stencil Lithography. , 2007, , .		0
70	Silicon Nanowire Band Gap Modification. Nano Letters, 2007, 7, 34-38.	9.1	215
71	Predicting mask distortion, clogging and pattern transfer for stencil lithography. Microelectronic Engineering, 2007, 84, 42-53.	2.4	40
72	Computational design ofSiâ^•SiO2interfaces: Stress and strain on the atomic scale. Physical Review B, 2006, 73, .	3.2	36

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73	A Physical Compact Model for Electron Transport Across Single Molecules. IEEE Nanotechnology Magazine, 2006, 5, 745-749.	2.0	2
74	Statistical estimates of electron correlations. Journal of Chemical Physics, 2006, 125, 054104.	3.0	3
75	Determination of complex absorbing potentials from the electron self-energy. Journal of Chemical Physics, 2006, 125, 244104.	3.0	28
76	Corrugated membranes for improved pattern definition with micro/nanostencil lithography. Sensors and Actuators A: Physical, 2006, 130-131, 568-574.	4.1	31
77	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
78	Quantum mechanics at the core of multi-scale simulations. Journal of Computer-Aided Materials Design, 2006, 13, 89-109.	0.7	7
79	Independent particle descriptions of tunneling using the many-body quantum transport approach. Physical Review B, 2006, 73, .	3.2	32
80	Symmetry, delocalization, and molecular conductance. Journal of Chemical Physics, 2005, 122, 044710.	3.0	22
81	Thermal decomposition mechanisms of hafnium and zirconium silicates at the atomic scale. Journal of Applied Physics, 2005, 97, 114911.	2.5	22
82	Electrostatic ordering of the lanthanum endoatom inLa@C82adsorbed on metal surfaces. Physical Review B, 2005, 71, .	3.2	13
83	E-MRS 2004 Spring Meeting Symposium H: Atomic Scale Materials Design: Modelling and Characterization. Computational Materials Science, 2005, 33, 1-2.	3.0	1
84	Correlated Electron Transport in Molecular Electronics. Physical Review Letters, 2004, 93, 036805.	7.8	123
85	Quantum electronic transport in a configuration interaction basis. International Journal of Quantum Chemistry, 2004, 100, 1163-1169.	2.0	21
86	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
87	Side gating in silicon germanium hetero-dimensional field effect transistors. Microelectronic Engineering, 2004, 71, 197-208.	2.4	2
88	Heterodimensional FET With Split Drain. IEEE Electron Device Letters, 2004, 25, 737-739.	3.9	2
89	Simulating the atomic layer deposition of alumina from first principles. Journal of Materials Chemistry, 2004, 14, 3246.	6.7	134
90	C60 as a Faraday cage. Applied Physics Letters, 2004, 84, 431-433.	3.3	73

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91	Bonding of Atomic Phosphorus to Polycyclic Hydrocarbons and Curved Graphitic Surfaces. Journal of the American Chemical Society, 2003, 125, 2301-2306.	13.7	10
92	E-MRS 2002 Spring Meeting Symposium A: Atomic Scale Materials Design. Computational Materials Science, 2003, 27, xi-xii.	3.0	0
93	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
94	Tools for analysing configuration interaction wavefunctions. Computational Materials Science, 2003, 28, 240-249.	3.0	1
95	Phosphorous trapped within buckminsterfullerene. Journal of Chemical Physics, 2002, 116, 7849-7854.	3.0	54
96	Extraction of analytical potential function parameters from abÂinitio potential energy surfaces and analytical forces. Computer Physics Communications, 2002, 147, 803-825.	7.5	3
97	Interactions between Thiol Molecular Linkers and the Au13Nanoparticle. Journal of Physical Chemistry B, 2002, 106, 5931-5937.	2.6	80
98	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
99	Many-electron systems with constrained current. Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 291, 46-50.	2.1	10
100	Status and perspectives of nanoscale device modelling. Nanotechnology, 2001, 12, 136-142.	2.6	18
101	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
102	Impact of electronâ€“electron cusp on configuration interaction energies. Journal of Chemical Physics, 2001, 115, 1626-1634.	3.0	38
103	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
104	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
105	Cluster ion implantation: a molecular dynamics study. Materials Science in Semiconductor Processing, 2000, 3, 91-95.	4.0	2
106	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
107	Electronic correlation energy in linear and cyclic carbon tetramers. Chemical Physics Letters, 1999, 306, 197-201.	2.6	2
108	Monte Carlo Configuration Interaction. Journal of Computational Physics, 1998, 146, 181-202.	3.8	72

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109	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
110	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
111	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
112	Alternative equations of motion for dynamical simulated annealing of the density functional. Physical Review B, 1996, 53, 10651-10655.	3.2	0
113	Consistent treatment of correlation effects in molecular dissociation studies using randomly chosen configurations. Journal of Chemical Physics, 1995, 103, 7996-8003.	3.0	24
114	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
115	Structures and spectra of Na(NH3) n=1,2. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 30, 69-75.	1.0	18
116	Constrained mechanics for the dynamical simulated annealing of Coulomb systems. Theoretica Chimica Acta, 1994, 88, 363-373.	0.8	1
117	An Approximate Time Evolution Operator to Generate the Verlet Algorithm. Journal of Computational Physics, 1994, 115, 245-247.	3.8	2
118	Ab initio geometry and stability of a C120 torus. Chemical Physics Letters, 1994, 222, 621-625.	2.6	25
119	Error analysis for pseudo-logarithmic amplification. Measurement Science and Technology, 1992, 3, 939-942.	2.6	10
120	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
121	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
122	TREPICO observation of the threshold region of N2O clusters. Chemical Physics Letters, 1990, 168, 330-336.	2.6	2
123	Binding energies and structures of NH3 clusters. Chemical Physics, 1989, 133, 191-197.	1.9	44
124	Nanowire Electronic Structure. , 0, , 107-166.		0
125	Charge Transport in Quasi-1d Nanostructures. , 0, , 167-220.		0