Luciano Colombo

List of Publications by Year
in descending order

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287 papers	27,173 citations	57758 44 h-index	5679 162 g-index
295 all docs	295 docs citations	295 times ranked	30857 citing authors

#	Article	IF	Citations
1	Large-Area Synthesis of High-Quality and Uniform Graphene Films on Copper Foils. Science, 2009, 324, 1312-1314.	12.6	10,000
2	A roadmap for graphene. Nature, 2012, 490, 192-200.	27.8	8,011
3	The Role of Surface Oxygen in the Growth of Large Single-Crystal Graphene on Copper. Science, 2013, 342, 720-723.	12.6	977
4	The effect of chemical residues on the physical and electrical properties of chemical vapor deposited graphene transferred to SiO2. Applied Physics Letters, 2011, 99, .	3.3	829
5	Elastic properties of hydrogenated graphene. Physical Review B, 2010, 82, .	3.2	476
6	Efficient Linear Scaling Algorithm for Tight-Binding Molecular Dynamics. Physical Review Letters, 1994, 73, 122-125.	7.8	412
7	Nonlinear Elasticity of Monolayer Graphene. Physical Review Letters, 2009, 102, 235502.	7.8	390
8	Gap opening in graphene by shear strain. Physical Review B, 2010, 81, .	3.2	310
9	Intrinsic point defects in crystalline silicon: Tight-binding molecular dynamics studiesof self-diffusion, interstitial-vacancy recombination, and formation volumes. Physical Review B, 1997, 55, 14279-14289.	3.2	256
10	Valence-band offsets at strained Si/Ge interfaces. Physical Review B, 1991, 44, 5572-5579.	3.2	177
11	Scaling of Al2O3 dielectric for graphene field-effect transistors. Applied Physics Letters, 2012, 100, .	3.3	105
12	Atomistic simulations of the sliding friction of graphene flakes. European Physical Journal B, 2009, 70, 449-459.	1.5	102
13	Atomic Scale Origin of Crack Resistance in Brittle Fracture. Physical Review Letters, 2005, 95, 115501.	7.8	83
14	Growth of Nanostructured Carbon Films by Cluster Assembly. Physical Review Letters, 1999, 83, 776-779.	7.8	82
15	First-principles study of the structural and elastic properties of zirconia. Physical Review B, 2009, 79, .	3.2	79
16	Effect of hydrogen coverage on the Young's modulus of graphene. Physical Review B, 2012, 85, .	3.2	76
17	Formation and annihilation of a bond defect in silicon: Anab initioquantum-mechanical characterization. Physical Review B, 1998, 57, 170-177.	3.2	73
18	Hydrogen Diffusion in Silicon from Tight-Binding Molecular Dynamics. Physical Review Letters, 1994, 73, 1636-1639.	7.8	72

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19	Calculating thermal conductivity in a transient conduction regime: theory and implementation. European Physical Journal B, 2014, 87, 1.	1.5	69
20	Surface phonons in Si(111) + H(1Ã—1). Physical Review B, 1988, 38, 3305-3310.	3.2	68
21	Boron ripening during solid-phase epitaxy of amorphous silicon. Physical Review B, 2004, 69, .	3.2	67
22	Thermal Rectification by Design in Telescopic Si Nanowires. Nano Letters, 2015, 15, 8255-8259.	9.1	66
23	Structural and binding properties of vacancy clusters in silicon. Europhysics Letters, 1998, 43, 695-700.	2.0	65
24	Simulation of the Amorphous-Silicon Properties and Their Dependence on Sample Preparation. Europhysics Letters, 1993, 22, 107-112.	2.0	64
25	Self-Assembling of Poly(3-hexylthiophene). Journal of Physical Chemistry C, 2011, 115, 576-581.	3.1	64
26	On the electrical activity of sp 2 -bonded grain boundaries in nanocrystalline diamond. Europhysics Letters, 1999, 46, 671-677.	2.0	62
27	Electrical and Thermal Transport in Coplanar Polycrystalline Grapheneâ€“hBN Heterostructures. Nano Letters, 2017, 17, 1660-1664.	9.1	62
28	Scaling properties of polycrystalline graphene: a review. 2D Materials, 2017, 4, 012002.	4.4	62
29	Intrinsic thermal conductivity in monolayer graphene is ultimately upper limited: A direct estimation by atomistic simulations. Physical Review B, 2015, 91, .	3.2	59
30	Understanding the Helical Wrapping of Poly(3-hexylthiophene) on Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 21109-21113.	3.1	55
31	Folded Graphene Membranes: Mapping Curvature at the Nanoscale. Nano Letters, 2012, 12, 5207-5212.	9.1	55
32	Elasticity of flexible and semiflexible polymers with extensible bonds in the Gibbs and Helmholtz ensembles. Journal of Chemical Physics, 2012, 136, 154906.	3.0	52
33	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. Physical Chemistry Chemical Physics, 2016, 18, 24318-24324.	2.8	52
34	Heat transport across a SiGe nanowire axial junction: Interface thermal resistance and thermal rectification. Physical Review B, 2014, 90, .	3.2	51
35	Lattice Thermal Conductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Si</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub><mml:mo>-</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ge</mml:mi></mml:mrow><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> Nanowires. Physical Review Letters, 2014, 112, 065901.	7.8	50
36	Absolute deformation potentials in semiconductors. Physical Review B, 1990, 41, 12358-12361.	3.2	49

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37	Nonlinear elasticity in nanostructured materials. Reports on Progress in Physics, 2011, 74, 116501.	20.1	48
38	Thermal boundary resistance at Si/Ge interfaces determined by approach-to-equilibrium molecular dynamics simulations. Physical Review B, 2015, 91, .	3.2	48
39	Structure and properties of amorphous gallium arsenide by tight-binding molecular dynamics. Physical Review B, 1994, 50, 4371-4377.	3.2	47
40	Model for thermal conductivity in nanoporous silicon from atomistic simulations. Physical Review B, 2015, 91, .	3.2	46
41	Surface phonon calculation for Si(111): H(1Ã—1). Physica Scripta, 1988, 37, 768-772.	2.5	45
42	Role of Extended Vacancy-Vacancy Interaction on the Ripening of Voids in Silicon. Physical Review Letters, 1999, 82, 1720-1723.	7.8	45
43	Evolution of energetics and bonding of compact self-interstitial clusters in Si. Europhysics Letters, 2000, 50, 608-614.	2.0	45
44	Self-interstitial trapping by carbon complexes in crystalline silicon. Physical Review B, 2002, 66, .	3.2	45
45	Role of lattice discreteness on brittle fracture: Atomistic simulations versus analytical models. Physical Review B, 2006, 73, .	3.2	45
46	Non-ohmic behavior and resistive switching of Au cluster-assembled films beyond the percolation threshold. Nanoscale Advances, 2019, 1, 3119-3130.	4.6	45
47	Elastic fields and moduli in defected graphene. Journal of Physics Condensed Matter, 2012, 24, 104020.	1.8	44
48	Atomic-scale characterization of boron diffusion in silicon. Physical Review B, 2001, 64, .	3.2	43
49	Calculating lattice thermal conductivity: a synopsis. Physica Scripta, 2018, 93, 043002.	2.5	40
50	Observation of second sound in a rapidly varying temperature field in Ge. Science Advances, 2021, 7, .	10.3	40
51	Theory and Monte Carlo simulations for the stretching of flexible and semiflexible single polymer chains under external fields. Journal of Chemical Physics, 2012, 137, 244907.	3.0	39
52	Correlation between atomic structure and localized gap states in silicon grain boundaries. Physical Review B, 1998, 57, 6247-6250.	3.2	38
53	Effect of hydrogenation on graphene thermal transport. Carbon, 2014, 80, 167-173.	10.3	38
54	Leaving the fullerene road: presence and stability of sp chains in sp2carbon clusters and cluster-assembled solids. New Journal of Physics, 2005, 7, 81-81.	2.9	37

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55	Thermal conductivity of MoS ₂ polycrystalline nanomembranes. 2D Materials, 2016, 3, 035016.	4.4	37
56	Two-state theory of single-molecule stretching experiments. Physical Review E, 2013, 87, .	2.1	36
57	Atomistic modeling of brittleness in covalent materials. Physical Review B, 2007, 76, .	3.2	35
58	Efficient particle labeling in atomistic simulations. Journal of Chemical Physics, 2007, 126, 121102.	3.0	35
59	Record Low Thermal Conductivity of Polycrystalline MoS₂ Films: Tuning the Thermal Conductivity by Grain Orientation. ACS Applied Materials & Interfaces, 2017, 9, 37905-37911.	8.0	35
60	Structure and chemical order of bulkSi1âˆ’xCxamorphous alloys. Physical Review B, 1998, 58, 10357-10362.	3.2	34
61	Pressure-induced structural transformations in a medium-sized silicon nanocrystal by tight-binding molecular dynamics. Journal of Chemical Physics, 2002, 117, 11329-11335.	3.0	34
62	Patterning of goldâ€“polydimethylsiloxane (Auâ€“PDMS) nanocomposites by supersonic cluster beam implantation. Journal Physics D: Applied Physics, 2014, 47, 015301.	2.8	34
63	Interaction between a monovacancy and a vacancy cluster in silicon. Physical Review B, 1998, 57, 8767-8769.	3.2	33
64	Solidâ€“liquid interface velocity and diffusivity in laser-melt amorphous silicon. Applied Physics Letters, 2000, 77, 2337-2339.	3.3	33
65	Thermal transport in nanocrystalline graphene investigated by approach-to-equilibrium molecular dynamics simulations. Carbon, 2016, 96, 429-438.	10.3	33
66	Nanocrystalline silicon films as multifunctional material for optoelectronic and photovoltaic applications. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2006, 134, 118-124.	3.5	32
67	Atomistic Investigation of Poly(3-hexylthiophene) Adhesion on Nanostructured Titania. Journal of Physical Chemistry C, 2010, 114, 3401-3406.	3.1	32
68	Structural Properties of Liquid and Amorphous GaAs by Tight-Binding Molecular Dynamics. Europhysics Letters, 1993, 24, 659-664.	2.0	30
69	Tight-Binding Theory of Native Point Defects in Silicon. Annual Review of Materials Research, 2002, 32, 271-295.	9.3	30
70	First-principles study of the effect of pressure on the five zirconia polymorphs. I. Structural, vibrational, and thermoelastic properties. Physical Review B, 2010, 82, .	3.2	30
71	Quantum Confinement by an Order-Disorder Boundary in Nanocrystalline Silicon. Physical Review Letters, 2010, 104, 176803.	7.8	30
72	Polymer Crystallinity and Transport Properties at the Poly(3-hexylthiophene)/Zinc Oxide Interface. Journal of Physical Chemistry C, 2011, 115, 9651-9655.	3.1	30

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73	Thermal rectification in silicon by a graded distribution of defects. Journal of Applied Physics, 2016, 119, .	2.5	30
74	Routes to carbon schwarzites from fullerene fragments. Europhysics Letters, 1997, 39, 269-274.	2.0	29
75	A source code for tight-binding molecular dynamics simulations. Computational Materials Science, 1998, 12, 278-287.	3.0	29
76	A lattice kinetic Monte Carlo code for the description of vacancy diffusion and self-organization in Si. Nuclear Instruments & Methods in Physics Research B, 1999, 148, 262-267.	1.4	29
77	Diffusion of small self-interstitial clusters in silicon: Temperature-accelerated tight-binding molecular dynamics simulations. Physical Review B, 2005, 71, .	3.2	29
78	Laser-induced melting of silicon: A tight-binding molecular dynamics simulation. Physical Review B, 2000, 61, 8233-8237.	3.2	28
79	Effects of the Orientational Distribution of Cracks in Solids. Physical Review Letters, 2007, 98, 055503.	7.8	28
80	Interplay between bending and stretching in carbon nanoribbons. Physical Review B, 2010, 81, .	3.2	28
81	Lattice-strain field induced by{311}self-interstitial defects in silicon. Physical Review B, 2000, 62, 1815-1820.	3.2	27
82	Growth of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>sp</mml:mi><mml:mtext>â^'</mml:mtext><mml:msup><mml:mi>sp</mml:mi><mml:mn>2</mml:m in a carbon plasma. Physical Review B, 2007, 76, .	3.2	27
83	Interface structure and defects of silicon nanocrystals embedded into a-SiO2. Applied Physics Letters, 2008, 93, 153109.	3.3	27
84	A theoretical study of the smallest tetrahedral carbon schwarzites. Europhysics Letters, 1998, 44, 525-530.	2.0	26
85	Atomistic study of the interaction between a microcrack and a hard inclusion inÎ²â^'SiC. Physical Review B, 2004, 70, .	3.2	26
86	Exploiting hydrogenation for thermal rectification in graphene nanoribbons. Physical Review B, 2015, 92, .	3.2	26
87	Heat transport through a solidâ€“solid junction: the interface as an autonomous thermodynamic system. Physical Chemistry Chemical Physics, 2016, 18, 13741-13745.	2.8	25
88	Hollow Diamonds from Fullerenes. Materials Science Forum, 1996, 232, 247-274.	0.3	24
89	Atomistic study of the dissolution of small boron interstitial clusters in c-Si. Applied Physics Letters, 2005, 87, 191912.	3.3	24
90	Nonlinear elasticity of composite materials. European Physical Journal B, 2009, 68, 89-101.	1.5	24

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91	Thermal transport in porous Si nanowires from approach-to-equilibrium molecular dynamics calculations. Applied Physics Letters, 2016, 109, .	3.3	24
92	Defect-Induced Amorphization in Silicon. Europhysics Letters, 1995, 29, 623-628.	2.0	22
93	Energetics of native point defects in cubic silicon carbide. European Physical Journal B, 2004, 38, 437-444.	1.5	22
94	Lattice dynamics and Raman response of (113) GaAs/AlAs superlattices. Physical Review B, 1994, 49, 10362-10372.	3.2	21
95	Calculation of elastic constants in defected and amorphous silicon by quantum simulations. Physical Review B, 1996, 54, 11857-11860.	3.2	21
96	Structural properties of silica surface: a classical molecular dynamics study. Journal of Non-Crystalline Solids, 1997, 220, 164-168.	3.1	21
97	Native defects and their interactions in silicon. Physica B: Condensed Matter, 1999, 273-274, 458-462.	2.7	21
98	Low-energy recoils in crystalline silicon: Quantum simulations. Physical Review B, 2001, 63, .	3.2	21
99	Silicon self-diffusion constants by tight-binding molecular dynamics. Physical Review B, 2001, 64, .	3.2	21
100	First-principles study of the effect of pressure on the five zirconia polymorphs. II. Static dielectric properties and Raman spectra. Physical Review B, 2010, 82, .	3.2	21
101	Phonon calculations in superperiodic structures: The surface Green-function matching approach. Physical Review B, 1988, 38, 3172-3179.	3.2	20
102	Pre-fragmentation dynamics of C60. A molecular dynamics investigation. Chemical Physics Letters, 1994, 225, 191-195.	2.6	20
103	Atomistic fracture: QFM vs. MD. Engineering Fracture Mechanics, 2008, 75, 1794-1803.	4.3	20
104	Effective permittivity of materials containing graded ellipsoidal inclusions. European Physical Journal B, 2008, 66, 29-35.	1.5	20
105	Poly(3-hexylthiophene) Adhesion on Zinc Oxide Nanoneedles. Journal of Physical Chemistry C, 2011, 115, 16833-16837.	3.1	20
106	Stretchable nanocomposite electrodes with tunable mechanical properties by supersonic cluster beam implantation in elastomers. Applied Physics Letters, 2015, 106, 121902.	3.3	20
107	Thermal boundary resistance from transient nanocalorimetry: A multiscale modeling approach. Physical Review B, 2017, 95, .	3.2	20
108	Vibrational properties and infrared spectra ofAlxGa1â^'xAs systems. I. Average-t-matrix approximation versus supercell calculation for homogeneous alloys. Physical Review B, 1991, 43, 14447-14456.	3.2	19

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109	Structural and electronic properties of strained Si/GaAs heterostructures. Physical Review B, 1993, 48, 12047-12052.	3.2	19
110	TIGHT-BINDING MOLECULAR DYNAMICS. , 1996, , 147-183.		19
111	Neutral boron-interstitial clusters in crystalline silicon. Physical Review B, 2004, 69, .	3.2	19
112	Nonuniform Growth of Embedded Silicon Nanocrystals in an Amorphous Matrix. Physical Review Letters, 2007, 99, 205501.	7.8	19
113	Tight-binding molecular dynamics in liquid III-V compounds. I. Potential generation. Journal of Physics Condensed Matter, 1994, 6, 5243-5254.	1.8	18
114	Electronic states in one-dimensional polymeric superlattices: A tight-binding approach. Physical Review B, 1995, 51, 1624-1630.	3.2	18
115	Solidâ€toâ€liquid phase change and fragmentation in C60. Journal of Chemical Physics, 1995, 102, 2151-2155.	3.0	18
116	Hydrogen bonding and migration in amorphous silicon. Europhysics Letters, 1996, 36, 295-300.	2.0	18
117	Molecular dynamics simulation of defect production in irradiated Î²-SiC. Journal of Nuclear Materials, 2000, 283-287, 794-798.	2.7	18
118	Defect energetics of Î²-SiC using a new tight-binding molecular dynamics model. Journal of Nuclear Materials, 2004, 329-333, 1219-1222.	2.7	18
119	Atomic scale simulations of vapor cooled carbon clusters. Applied Physics A: Materials Science and Processing, 2007, 86, 275-281.	2.3	18
120	Crystallization kinetics of mixed amorphous-crystalline nanosystems. Physical Review B, 2008, 78, .	3.2	18
121	Simulating Energy Relaxation in Pumpâ€“Probe Vibrational Spectroscopy of Hydrogen-Bonded Liquids. Journal of Chemical Theory and Computation, 2017, 13, 1284-1292.	5.3	18
122	Phonon properties and Raman response of (113) GaAs/AlAs corrugated superlattices. Physical Review B, 1995, 51, 1647-1652.	3.2	17
123	Triple junctions and elastic stability of polycrystalline silicon. Physical Review B, 2000, 63, .	3.2	17
124	Atomic-scale model ofcâ^'Si/a-Si:H interfaces. Physical Review B, 2004, 69, .	3.2	17
125	Fracture toughness of nanostructured silicon carbide. Applied Physics Letters, 2005, 87, 141912.	3.3	17
126	Electronic localization and optical absorption in embedded silicon nanograins. Applied Physics Letters, 2009, 94, 053115.	3.3	17

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127	Linking morphology to thermal conductivity in PEDOT: an atomistic investigation. Journal Physics D: Applied Physics, 2017, 50, 494002.	2.8	17
128	Assessing the anomalous superdiffusive heat transport in a single one-dimensional PEDOT chain. Physical Review Materials, 2018, 2, .	2.4	17
129	Evidence of thermal transport anisotropy in stable glasses of vapor deposited organic molecules. Physical Review Materials, 2018, 2, .	2.4	17
130	Prediction of newsp2andsp2/sp3hollow carbon crystals. Journal of Chemical Physics, 1997, 106, 2311-2316.	3.0	16
131	Hydrogen diffusion in crystalline SiO2. Chemical Physics Letters, 1997, 264, 435-440.	2.6	16
132	Parallel tight-binding molecular dynamics simulations on symmetric multi-processing platforms. Computer Physics Communications, 2000, 128, 108-117.	7.5	16
133	Interaction of doping impurities with the 30Â° partial dislocations in SiC: Anab initioinvestigation. Physical Review B, 2005, 72, .	3.2	16
134	Elucidating the atomistic mechanisms driving self-diffusion of amorphous Si during annealing. Physical Review B, 2011, 83, .	3.2	16
135	A planar approach to the lattice dynamics of polar semiconductor superlattices. Surface Science, 1989, 221, 486-512.	1.9	15
136	On the Use of the Reverse Monte Carlo Technique to Generate Amorphous Carbon Structures. International Journal of Modern Physics C, 1998, 09, 917-926.	1.7	15
137	Channeling characterization of defects in silicon: an atomistic approach. Nuclear Instruments & Methods in Physics Research B, 2005, 230, 185-192.	1.4	15
138	Depth resolved study of impurity sites in low energy ion implanted As in Si. Journal of Applied Physics, 2007, 102, 043524.	2.5	15
139	Nonlinear elastic Landau coefficients in heterogeneous materials. Europhysics Letters, 2008, 83, 66003.	2.0	15
140	Structural, Vibrational, and Thermal Properties of Nanocrystalline Graphene in Atomistic Simulations. Journal of Physical Chemistry C, 2016, 120, 3026-3035.	3.1	15
141	Assessing the Performance of Eumelanin/Si Interface for Photovoltaic Applications. Journal of Physical Chemistry C, 2017, 121, 11576-11584.	3.1	15
142	Deciphering Molecular Mechanisms of Interface Buildup and Stability in Porous Si/Eumelanin Hybrids. International Journal of Molecular Sciences, 2017, 18, 1567.	4.1	15
143	Geometric construction of large dynamical matrices: Applications to reconstructed surfaces, superlattices and mixed crystals. Superlattices and Microstructures, 1990, 7, 139-146.	3.1	14
144	Vibrational properties and infrared spectra ofAlxGa1â^'xAs systems. II. Order and disorder features in superlattice configuration. Physical Review B, 1991, 43, 14457-14464.	3.2	14

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145	Effects of the orientational distribution of cracks in isotropic solids. Engineering Fracture Mechanics, 2007, 74, 1983-2003.	4.3	14
146	Lattice model describing scale effects in nonlinear elasticity of nanoinhomogeneities. Physical Review B, 2010, 81, .	3.2	14
147	Self-Assembling of Zinc Phthalocyanines on ZnO (101Ì…0) Surface through Multiple Time Scales. ACS Nano, 2011, 5, 9639-9647.	14.6	14
148	Optoelectronic properties of (ZnO)60 isomers. Physical Chemistry Chemical Physics, 2012, 14, 14293.	2.8	14
149	Effect of structural features on the thermal conductivity of SiGe-based materials. European Physical Journal B, 2014, 87, 1.	1.5	14
150	Physical and Chemical Control of Interface Stability in Porous Siâ€“Eumelanin Hybrids. Journal of Physical Chemistry C, 2018, 122, 28405-28415.	3.1	14
151	Impact of oxidation morphology on reduced graphene oxides upon thermal annealing. JPhys Materials, 2020, 3, 015011.	4.2	14
152	Tight-binding molecular dynamics in liquid III-V compounds. II. Simulations for GaAs and GaSb. Journal of Physics Condensed Matter, 1994, 6, 5255-5271.	1.8	13
153	Microstructure evolution from the atomic scale up. Computational Materials Science, 2002, 24, 21-27.	3.0	13
154	Failure strength of brittle materials containing nanovoids. Physical Review B, 2007, 75, .	3.2	13
155	Mechanisms of self-diffusion in stoichiometric and substoichiometric amorphous silicon dioxide. Physical Review B, 2010, 81, .	3.2	13
156	Electronic Properties of Hybrid Zinc Oxideâ€“Oligothiophene Nanostructures. Journal of Physical Chemistry C, 2012, 116, 8174-8180.	3.1	13
157	Response to â€œComment on â€˜Elasticity of flexible and semiflexible polymers with extensible bonds in the Gibbs and Helmholtz ensemblesâ€â€™ [J. Chem. Phys. 138, 157101 (2013)]. Journal of Chemical Physics, 2013, 138, 157102.	3.0	13
158	Neutral-cluster implantation in polymers by computer experiments. Journal of Applied Physics, 2013, 113, .	2.5	13
159	Lattice strain at c-Si surfaces: a density functional theory calculation. Metrologia, 2015, 52, 214-221.	1.2	13
160	Strain engineering of ZnO thermal conductivity. Physical Review Materials, 2019, 3, .	2.4	13
161	Impact of synthetic conditions on the anisotropic thermal conductivity of poly(3,4-ethylenedioxythiophene) (PEDOT): A molecular dynamics investigation. Physical Review Materials, 2020, 4, .	2.4	13
162	Dispersive-linear-chain approach to the interpretation of surface phonons: Application to GaSe(001) andTaSe2(001). Physical Review B, 1988, 37, 3025-3036.	3.2	12

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163	Ab initiostructures ofAsmVcomplexes and the simulation of Rutherford backscattering channeling spectra in heavily As-doped crystalline silicon. Physical Review B, 2005, 72, .	3.2	12
164	Role of defects in the electronic properties of amorphous/crystalline Si interface. Physical Review B, 2001, 64, .	3.2	11
165	Simulation of atomic force microscopy of fractal nanostructured carbon films. Europhysics Letters, 2001, 54, 72-76.	2.0	11
166	Local lattice distortion inSi1â^'xâ^'yGexCyepitaxial layers from x-ray absorption fine structure. Physical Review B, 2001, 63, .	3.2	11
167	Interpretation of ion-channeling spectra in ion-implanted Si with models of structurally relaxed point defects and clusters. Physical Review B, 2004, 69, .	3.2	11
168	Hydrogen Uptake in Cluster-Assembled Carbon Thin Films:Â Experiment and Computer Simulation. Journal of Physical Chemistry B, 2004, 108, 5157-5160.	2.6	11
169	Effect of asymmetric concentration profile on thermal conductivity in Ge/SiGe superlattices. Applied Physics Letters, 2016, 108, 203102.	3.3	11
170	Density functional theory calculations of the stress of oxidised (1 1 0) silicon surfaces. Metrologia, 2016, 53, 1339-1345.	1.2	11
171	Understanding the Polymerization Process of Eumelanin by Computer Simulations. Journal of Physical Chemistry C, 2018, 122, 28368-28374.	3.1	11
172	Thermal and transport properties of pristine single-layer hexagonal boron nitride: A first principles investigation. Physical Review Materials, 2017, 1, .	2.4	11
173	Migration of atomic hydrogen in crystalline and amorphous SiO2: a molecular dynamics study. Journal of Non-Crystalline Solids, 1997, 216, 30-35.	3.1	10
174	Energetics and diffusivity of atomic boron in silicon by density-functional-based tight-binding simulations. Computational Materials Science, 2001, 22, 44-48.	3.0	10
175	Structural, electronic, and energetic properties of small self-interstitial clusters in GaAs by tight-binding molecular dynamics. Physical Review B, 2005, 71, .	3.2	10
176	Atomistic Investigation of the Solidâ€“Liquid Interface between the Crystalline Zinc Oxide Surface and the Liquid Tetrahydrofuran Solvent. Journal of Physical Chemistry C, 2012, 116, 12644-12648.	3.1	10
177	Energy Relaxation and Thermal Diffusion in Infrared Pumpâ€“Probe Spectroscopy of Hydrogen-Bonded Liquids. Journal of Physical Chemistry Letters, 2019, 10, 3447-3452.	4.6	10
178	Amorphization of fullerite crystals. Chemical Physics Letters, 1995, 238, 281-285.	2.6	9
179	Computational Materials Science application programming interface (CMSapi): a tool for developing applications for atomistic simulations. Computer Physics Communications, 2005, 169, 462-466.	7.5	9
180	Interfacial elastic properties betweena-Siandc-Si. Physical Review B, 2008, 78, .	3.2	9

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181	SixGe1-x alloy as efficient phonon barrier in Ge/Si superlattices for thermoelectric applications. European Physical Journal B, 2015, 88, 1.	1.5	9
182	Thermal boundary resistance in semiconductors by non-equilibrium thermodynamics. Advances in Physics: X, 2016, 1, 246-261.	4.1	9
183	Phonon Scattering in Silicon by Multiple Morphological Defects: A Multiscale Analysis. Journal of Electronic Materials, 2018, 47, 5148-5157.	2.2	9
184	Intrinsic thermoelectric figure of merit of bulk compositional SiGe alloys: A first-principles study. Physical Review Materials, 2021, 5, .	2.4	9
185	Disorder configurations from vibrational structure in Al_xGa_{1â^'x},As systems. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1992, 65, 325-337.	0.6	8
186	A first-principles derived parametrization for the adiabatic bond charge model. Solid State Communications, 1995, 96, 49-52.	1.9	8
187	On the effect of quench rate on the structure of amorphous carbon. Computational Materials Science, 1998, 10, 67-74.	3.0	8
188	Atomistic simulation of ion channeling in heavily doped Si:As. Nuclear Instruments & Methods in Physics Research B, 2005, 230, 112-117.	1.4	8
189	Local elastic fields around cracks and their stress density of states. Physical Review B, 2007, 76, .	3.2	8
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