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	Thermal conduction and rectification phenomena in nanoporous silicon membranes. Physical Chemistry Chemical Physics, 2022, 24, 13625-13632.	2.8	3
2	Room temperature second sound in cumulene. Physical Chemistry Chemical Physics, 2021, 23, 15275-15281.	2.8	3
3	Intrinsic thermoelectric figure of merit of bulk compositional SiGe alloys: A first-principles study. Physical Review Materials, 2021, 5, .	2.4	9
4	Observation of second sound in a rapidly varying temperature field in Ge. Science Advances, 2021, 7, .	10.3	40
5	Engineering the Thermal Conductivity of Doped SiGe by Mass Variance: A First-Principles Proof of Concept. Frontiers in Mechanical Engineering, 2021, 7, .	1.8	2
6	Thermal transport in amorphous graphene with varying structural quality. 2D Materials, 2021, 8, 015028.	4.4	6
7	Modeling charge transport in gold nanogranular films. Physical Review Materials, 2021, 5, .	2.4	2
8	Impact of oxidation morphology on reduced graphene oxides upon thermal annealing. JPhys Materials, 2020, 3, 015011.	4.2	14
9	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
10	Modeling resistive switching in nanogranular metal films. Physical Review Research, 2020, 2, .	3.6	7
11	Lattice Thermal Boundary Resistance. , 2020, , 845-863.		0
12	Non-ohmic behavior and resistive switching of Au cluster-assembled films beyond the percolation threshold. Nanoscale Advances, 2019, 1, 3119-3130.	4.6	45
13	Obituary for Professor Sandro Massidda. Journal of Physics Condensed Matter, 2019, 31, 270202.	1.8	1
14	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
15	Strain engineering of ZnO thermal conductivity. Physical Review Materials, 2019, 3, .	2.4	13
16	Calculating lattice thermal conductivity: a synopsis. Physica Scripta, 2018, 93, 043002.	2.5	40
17	Understanding the Polymerization Process of Eumelanin by Computer Simulations. Journal of Physical Chemistry C, 2018, 122, 28368-28374.	3.1	11
18	Physical and Chemical Control of Interface Stability in Porous Siâ€“Eumelanin Hybrids. Journal of Physical Chemistry C, 2018, 122, 28405-28415.	3.1	14

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19	Phonon Scattering in Silicon by Multiple Morphological Defects: A Multiscale Analysis. Journal of Electronic Materials, 2018, 47, 5148-5157.	2.2	9
20	Lattice Thermal Boundary Resistance. , 2018, , 1-19.		1
21	The thermal boundary resistance at semiconductor interfaces: a critical appraisal of the Onsager vs. Kapitza formalisms. Physical Chemistry Chemical Physics, 2018, 20, 22623-22628.	2.8	2
22	Assessing the anomalous superdiffusive heat transport in a single one-dimensional PEDOT chain. Physical Review Materials, 2018, 2, .	2.4	17
23	Evidence of thermal transport anisotropy in stable glasses of vapor deposited organic molecules. Physical Review Materials, 2018, 2, .	2.4	17
24	Nature of microscopic heat carriers in nanoporous silicon. Physical Review Materials, 2018, 2, .	2.4	4
25	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
26	Thermal boundary resistance from transient nanocalorimetry: A multiscale modeling approach. Physical Review B, 2017, 95, .	3.2	20
27	Electrical and Thermal Transport in Coplanar Polycrystalline Grapheneâ€“hBN Heterostructures. Nano Letters, 2017, 17, 1660-1664.	9.1	62
28	Assessing the Performance of Eumelanin/Si Interface for Photovoltaic Applications. Journal of Physical Chemistry C, 2017, 121, 11576-11584.	3.1	15
29	Scaling properties of polycrystalline graphene: a review. 2D Materials, 2017, 4, 012002.	4.4	62
30	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
31	Thermal Transport in Nanocrystalline Graphene: The Role of Grain Boundaries. Carbon Nanostructures, 2017, , 1-17.	0.1	1
32	Linking morphology to thermal conductivity in PEDOT: an atomistic investigation. Journal Physics D: Applied Physics, 2017, 50, 494002.	2.8	17
33	Surface elastic properties in silicon nanoparticles. Europhysics Letters, 2017, 119, 66005.	2.0	4
34	Deciphering Molecular Mechanisms of Interface Buildup and Stability in Porous Si/Eumelanin Hybrids. International Journal of Molecular Sciences, 2017, 18, 1567.	4.1	15
35	Thermal and transport properties of pristine single-layer hexagonal boron nitride: A first principles investigation. Physical Review Materials, 2017, 1, .	2.4	11
36	Thermal transport in porous Si nanowires from approach-to-equilibrium molecular dynamics calculations. Applied Physics Letters, 2016, 109, .	3.3	24

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37	Predicting the thermal conductivity in a graphene nanoflake from its response to a thermal impulse. Physical Review B, 2016, 94, .	3.2	2
38	Effect of asymmetric concentration profile on thermal conductivity in Ge/SiGe superlattices. Applied Physics Letters, 2016, 108, 203102.	3.3	11
39	Thermal boundary resistance in semiconductors by non-equilibrium thermodynamics. Advances in Physics: X, 2016, 1, 246-261.	4.1	9
40	Thermal conductivity of MoS ₂ polycrystalline nanomembranes. 2D Materials, 2016, 3, 035016.	4.4	37
41	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. Physical Chemistry Chemical Physics, 2016, 18, 24318-24324.	2.8	52
42	Density functional theory calculations of the stress of oxidised (1 1 0) silicon surfaces. Metrologia, 2016, 53, 1339-1345.	1.2	11
43	Thermal rectification in silicon by a graded distribution of defects. Journal of Applied Physics, 2016, 119, .	2.5	30
44	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
45	Structural, Vibrational, and Thermal Properties of Nanocrystalline Graphene in Atomistic Simulations. Journal of Physical Chemistry C, 2016, 120, 3026-3035.	3.1	15
46	Thermal transport in nanocrystalline graphene investigated by approach-to-equilibrium molecular dynamics simulations. Carbon, 2016, 96, 429-438.	10.3	33
47	Exploiting hydrogenation for thermal rectification in graphene nanoribbons. Physical Review B, 2015, 92, .	3.2	26
48	Intrinsic thermal conductivity in monolayer graphene is ultimately upper limited: A direct estimation by atomistic simulations. Physical Review B, 2015, 91, .	3.2	59
49	Thermal boundary resistance at Si/Ge interfaces determined by approach-to-equilibrium molecular dynamics simulations. Physical Review B, 2015, 91, .	3.2	48
50	SixGe1-x alloy as efficient phonon barrier in Ge/Si superlattices for thermoelectric applications. European Physical Journal B, 2015, 88, 1.	1.5	9
51	Model for thermal conductivity in nanoporous silicon from atomistic simulations. Physical Review B, 2015, 91, .	3.2	46
52	Lattice strain at c-Si surfaces: a density functional theory calculation. Metrologia, 2015, 52, 214-221.	1.2	13
53	Stretchable nanocomposite electrodes with tunable mechanical properties by supersonic cluster beam implantation in elastomers. Applied Physics Letters, 2015, 106, 121902.	3.3	20
54	Thermal Rectification by Design in Telescopic Si Nanowires. Nano Letters, 2015, 15, 8255-8259.	9.1	66

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55	Patterning of goldâ€“polydimethylsiloxane (Auâ€“PDMS) nanocomposites by supersonic cluster beam implantation. Journal Physics D: Applied Physics, 2014, 47, 015301.	2.8	34
56	Heat transport across a SiGe nanowire axial junction: Interface thermal resistance and thermal rectification. Physical Review B, 2014, 90, .	3.2	51
57	Atomistic study of the structural and electronic properties of a-Si:H/c-Si interfaces. Journal of Physics Condensed Matter, 2014, 26, 095001.	1.8	8
58	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 Physical Review Letters, 2014, 112, 065901.	7.8	50
59	Effect of hydrogenation on graphene thermal transport. Carbon, 2014, 80, 167-173.	10.3	38
60	Effect of structural features on the thermal conductivity of SiGe-based materials. European Physical Journal B, 2014, 87, 1.	1.5	14
61	Calculating thermal conductivity in a transient conduction regime: theory and implementation. European Physical Journal B, 2014, 87, 1.	1.5	69
62	Folds and Buckles at the Nanoscale: Experimental and Theoretical Investigation of the Bending Properties of Graphene Membranes. Topics in Current Chemistry, 2013, 348, 205-236.	4.0	1
63	The Role of Surface Oxygen in the Growth of Large Single-Crystal Graphene on Copper. Science, 2013, 342, 720-723.	12.6	977
64	Two-state theory of single-molecule stretching experiments. Physical Review E, 2013, 87, .	2.1	36
65	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
66	Neutral-cluster implantation in polymers by computer experiments. Journal of Applied Physics, 2013, 113, .	2.5	13
67	Monte Carlo simulations of single polymer force-extension relations. Journal of Physics: Conference Series, 2012, 383, 012016.	0.4	7
68	Scaling of Al2O3 dielectric for graphene field-effect transistors. Applied Physics Letters, 2012, 100, .	3.3	105
69	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
70	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
71	A roadmap for graphene. Nature, 2012, 490, 192-200.	27.8	8,011
72	Optoelectronic properties of (ZnO)60 isomers. Physical Chemistry Chemical Physics, 2012, 14, 14293.	2.8	14

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73	Elastic fields and moduli in defected graphene. Journal of Physics Condensed Matter, 2012, 24, 104020.	1.8	44
74	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
75	Folded Graphene Membranes: Mapping Curvature at the Nanoscale. Nano Letters, 2012, 12, 5207-5212.	9.1	55
76	Effect of hydrogen coverage on the Young's modulus of graphene. Physical Review B, 2012, 85, .	3.2	76
77	Electronic Properties of Hybrid Zinc Oxideâ€“Oligothiophene Nanostructures. Journal of Physical Chemistry C, 2012, 116, 8174-8180.	3.1	13
78	Poly(3-hexylthiophene) Adhesion on Zinc Oxide Nanoneedles. Journal of Physical Chemistry C, 2011, 115, 16833-16837.	3.1	20
79	Adhesion and Diffusion of Zinc-Phthalocyanines on the ZnO (101Ì…0) Surface. Journal of Physical Chemistry C, 2011, 115, 18208-18212.	3.1	8
80	Self-Assembling of Poly(3-hexylthiophene). Journal of Physical Chemistry C, 2011, 115, 576-581.	3.1	64
81	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
82	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
83	Self-Assembling of Zinc Phthalocyanines on ZnO (101Ì…0) Surface through Multiple Time Scales. ACS Nano, 2011, 5, 9639-9647.	14.6	14
84	Order-disorder phase change in embedded Si nanoparticles. Physical Review B, 2011, 83, .	3.2	8
85	Nonlinear elasticity in nanostructured materials. Reports on Progress in Physics, 2011, 74, 116501.	20.1	48
86	Elucidating the atomistic mechanisms driving self-diffusion of amorphous Si during annealing. Physical Review B, 2011, 83, .	3.2	16
87	Elastic properties of multi-cracked composite materials. European Physical Journal B, 2010, 76, 261-269.	1.5	3
88	Lattice model describing scale effects in nonlinear elasticity of nanoinhomogeneities. Physical Review B, 2010, 81, .	3.2	14
89	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
90	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

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91	Understanding the Helical Wrapping of Poly(3-hexylthiophene) on Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 21109-21113.	3.1	55
92	Gap opening in graphene by shear strain. Physical Review B, 2010, 81, .	3.2	310
93	Atomistic Investigation of Poly(3-hexylthiophene) Adhesion on Nanostructured Titania. Journal of Physical Chemistry C, 2010, 114, 3401-3406.	3.1	32
94	Elastic properties of hydrogenated graphene. Physical Review B, 2010, 82, .	3.2	476
95	Quantum Confinement by an Order-Disorder Boundary in Nanocrystalline Silicon. Physical Review Letters, 2010, 104, 176803.	7.8	30
96	Mechanisms of self-diffusion in stoichiometric and substoichiometric amorphous silicon dioxide. Physical Review B, 2010, 81, .	3.2	13
97	Interplay between bending and stretching in carbon nanoribbons. Physical Review B, 2010, 81, .	3.2	28
98	Calculation of the local optoelectronic properties of nanostructured silicon. Physical Review B, 2009, 79, .	3.2	4
99	Electronic localization and optical absorption in embedded silicon nanograins. Applied Physics Letters, 2009, 94, 053115.	3.3	17
100	Interface elasticity in nanostructured silicon. Physical Review B, 2009, 80, .	3.2	8
101	Nonlinear elasticity of composite materials. European Physical Journal B, 2009, 68, 89-101.	1.5	24
102	Atomistic simulations of the sliding friction of graphene flakes. European Physical Journal B, 2009, 70, 449-459.	1.5	102
103	Large-Area Synthesis of High-Quality and Uniform Graphene Films on Copper Foils. Science, 2009, 324, 1312-1314.	12.6	10,000
104	Nonlinear Elasticity of Monolayer Graphene. Physical Review Letters, 2009, 102, 235502.	7.8	390
105	First-principles study of the structural and elastic properties of zirconia. Physical Review B, 2009, 79, .	3.2	79
106	Atomistic fracture: QFM vs. MD. Engineering Fracture Mechanics, 2008, 75, 1794-1803.	4.3	20
107	Effective permittivity of materials containing graded ellipsoidal inclusions. European Physical Journal B, 2008, 66, 29-35.	1.5	20
108	Nonlinear elastic Landau coefficients in heterogeneous materials. Europhysics Letters, 2008, 83, 66003.	2.0	15

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109	Interface structure and defects of silicon nanocrystals embedded into a-SiO2. Applied Physics Letters, 2008, 93, 153109.	3.3	27
110	Crystallization kinetics of mixed amorphous-crystalline nanosystems. Physical Review B, 2008, 78, .	3.2	18
111	Elastic properties of solids containing elliptic cracks. Physical Review B, 2008, 77, .	3.2	8
112	Interfacial elastic properties betweena-Siandc-Si. Physical Review B, 2008, 78, .	3.2	9
113	Atomistic modeling of brittleness in covalent materials. Physical Review B, 2007, 76, .	3.2	35
114	Local elastic fields around cracks and their stress density of states. Physical Review B, 2007, 76, .	3.2	8
115	Nonuniform Growth of Embedded Silicon Nanocrystals in an Amorphous Matrix. Physical Review Letters, 2007, 99, 205501.	7.8	19
116	Effects of the Orientational Distribution of Cracks in Solids. Physical Review Letters, 2007, 98, 055503.	7.8	28
117	Failure strength of brittle materials containing nanovoids. Physical Review B, 2007, 75, .	3.2	13
118	Efficient particle labeling in atomistic simulations. Journal of Chemical Physics, 2007, 126, 121102.	3.0	35
119	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
120	Effects of the orientational distribution of cracks in isotropic solids. Engineering Fracture Mechanics, 2007, 74, 1983-2003.	4.3	14
121	Depth resolved study of impurity sites in low energy ion implanted As in Si. Journal of Applied Physics, 2007, 102, 043524.	2.5	15
122	Atomic scale simulations of vapor cooled carbon clusters. Applied Physics A: Materials Science and Processing, 2007, 86, 275-281.	2.3	18
123	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
124	Defect-induced homogeneous amorphization of silicon: the role of defect structure and population. Journal of Physics Condensed Matter, 2006, 18, 2077-2088.	1.8	6
125	Role of lattice discreteness on brittle fracture: Atomistic simulations versus analytical models. Physical Review B, 2006, 73, .	3.2	45
126	Atomistic simulation of ion channeling in heavily doped Si:As. Nuclear Instruments & Methods in Physics Research B, 2005, 230, 112-117.	1.4	8

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127	Channeling characterization of defects in silicon: an atomistic approach. Nuclear Instruments & Methods in Physics Research B, 2005, 230, 185-192.	1.4	15
128	Investigation of heavily damaged ion implanted Si by atomistic simulation of Rutherford backscattering channeling spectra. Nuclear Instruments & Methods in Physics Research B, 2005, 230, 613-618.	1.4	6
129	Crack-tip stress shielding by a hard fiber in Î²-SiC: an atomistic study. Computer Physics Communications, 2005, 169, 40-43.	7.5	0
130	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
131	Classical versus ab initio structural relaxation: electronic excitations and optical properties of Ge nanocrystals embedded in an SiC matrix. Journal of Physics Condensed Matter, 2005, 17, 643-651.	1.8	1
132	Atomic Scale Origin of Crack Resistance in Brittle Fracture. Physical Review Letters, 2005, 95, 115501.	7.8	83
133	Interaction of doping impurities with the 30Â° partial dislocations in SiC: Anab initioinvestigation. Physical Review B, 2005, 72, .	3.2	16
134	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
135	Diffusion of small self-interstitial clusters in silicon: Temperature-accelerated tight-binding molecular dynamics simulations. Physical Review B, 2005, 71, .	3.2	29
136	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
137	Atomistic study of the dissolution of small boron interstitial clusters in c-Si. Applied Physics Letters, 2005, 87, 191912.	3.3	24
138	Fracture toughness of nanostructured silicon carbide. Applied Physics Letters, 2005, 87, 141912.	3.3	17
139	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
140	Neutral boron-interstitial clusters in crystalline silicon. Physical Review B, 2004, 69, .	3.2	19
141	Elastic moduli of nanostructured carbon films. Physical Review B, 2004, 70, .	3.2	7
142	Classical versus ab initio structural relaxation: electronic excitations and optical properties of Ge nanocrystals embedded in a SiC matrix. Materials Research Society Symposia Proceedings, 2004, 832, 313.	0.1	0
143	Energetics of native point defects in cubic silicon carbide. European Physical Journal B, 2004, 38, 437-444.	1.5	22
144	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

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145	Boron ripening during solid-phase epitaxy of amorphous silicon. Physical Review B, 2004, 69, .	3.2	67
146	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
147	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
148	Atomic-scale model ofcâ^'Si/a-Si:H interfaces. Physical Review B, 2004, 69, .	3.2	17
149	Atomistic study of the interaction between a microcrack and a hard inclusion inÎ²â^'SiC. Physical Review B, 2004, 70, .	3.2	26
150	Boron ripening in amorphous silicon by large scale molecular dynamics simulations. Computational Materials Science, 2004, 30, 143-149.	3.0	2
151	Combined atomistic and continuum methods to map electric properties of nanostructured carbon films. Computational Materials Science, 2004, 30, 150-154.	3.0	0
152	Modeling of time-dependent damage in structural wall of inertial fusion reactors and new tight binding model for SiC. Fusion Engineering and Design, 2003, 69, 795-801.	1.9	0
153	Atomic scale computer aided design for novel semiconductor devices. Computational Materials Science, 2003, 27, 10-15.	3.0	6
154	On the solid-phase epitaxy of the a-Si:B/c-Si interface. Europhysics Letters, 2003, 62, 862-868.	2.0	6
155	Time-Dependent Neutronics in Structural Materials of Inertial Fusion Reactors and Simulation of Defect Accumulation in Pulsed Fe and SiC. Fusion Science and Technology, 2003, 43, 384-392.	1.1	3
156	Atomistic Study of Boron Clustering in Silicon. Solid State Phenomena, 2002, 82-84, 163-170.	0.3	0
157	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
158	Self-interstitial trapping by carbon complexes in crystalline silicon. Physical Review B, 2002, 66, .	3.2	45
159	Insight into the materials choice for inertial fusion energy reactors considering radiation damage: Neutron irradiation intensities and basic knowledge from multiscale modeling. Laser and Particle Beams, 2002, 20, 627-631.	1.0	1
160	Nanofriction Behavior of Cluster-Assembled Carbon Films. Journal of Nanoscience and Nanotechnology, 2002, 2, 637-643.	0.9	5
161	Microstructure evolution at a triple junction in polycrystalline silicon. Journal of Physics Condensed Matter, 2002, 14, 13003-13008.	1.8	7
162	Tight-Binding Theory of Native Point Defects in Silicon. Annual Review of Materials Research, 2002, 32, 271-295.	9.3	30

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163	Microstructure evolution from the atomic scale up. Computational Materials Science, 2002, 24, 21-27.	3.0	13
164	Atomistic simulations and the requirements of process simulator for novel semiconductor devices. Computational Materials Science, 2002, 24, 213-222.	3.0	2
165	Atomic scale characterization of nanostructured a-C:H films. European Physical Journal B, 2002, 27, 335-340.	1.5	3
166	Nanofriction Behavior of Cluster-Assembled Carbon Films. Journal of Nanoscience and Nanotechnology, 2002, 2, 637-643.	0.9	1
167	Atomic-scale characterization of boron diffusion in silicon. Physical Review B, 2001, 64, .	3.2	43
168	A theoretical study of the smallest tetrahedral carbon schwarzites. Europhysics Letters, 2001, 53, 559-559.	2.0	0
169	Role of defects in the electronic properties of amorphous/crystalline Si interface. Physical Review B, 2001, 64, .	3.2	11
170	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
171	Simulation of atomic force microscopy of fractal nanostructured carbon films. Europhysics Letters, 2001, 54, 72-76.	2.0	11
172	Multiscale Modeling of Radiation Damage of Metals and SIC in Inertial Fusion Reactors. Fusion Science and Technology, 2001, 39, 579-584.	0.6	2
173	Coupled atomistic-mesoscopic model of polycrystalline plasticity. Materials Research Society Symposia Proceedings, 2001, 677, 761.	0.1	0
174	A multi-scale atomistic study of the interstitials agglomeration in crystalline Si. Nuclear Instruments & Methods in Physics Research B, 2001, 178, 154-159.	1.4	7
175	Triple Junctions in Polycrystalline Silicon: A Numerical Study Based upon Atomistic Simulations. Key Engineering Materials, 2001, 221-222, 307-314.	0.4	1
176	From Point to Extended Defects in Silicon: A Theoretical Study. Solid State Phenomena, 2001, 85-86, 177-202.	0.3	2
177	Self-Interstitial Kinetics and Transient Phenomena in Si Crystals. Solid State Phenomena, 2001, 82-84, 171-176.	0.3	1
178	Low-energy recoils in crystalline silicon: Quantum simulations. Physical Review B, 2001, 63, .	3.2	21
179	Silicon self-diffusion constants by tight-binding molecular dynamics. Physical Review B, 2001, 64, .	3.2	21
180	Local lattice distortion inSi1â^'xâ^'yGexCyepitaxial layers from x-ray absorption fine structure. Physical Review B, 2001, 63, .	3.2	11

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181	Interstitial Cluster Evolution and Transient Phenomena in Si-crystal. , 2001, , 120-123.		0
182	Covalent Cluster-Assembled Carbon Solids. , 2001, , 89-126.		4
183	Identification of tetrahedrally coordinated atoms in supercooled liquid silicon. Materials Research Society Symposia Proceedings, 2000, 638, 1.	0.1	0
184	Parallel tight-binding molecular dynamics simulations on symmetric multi-processing platforms. Computer Physics Communications, 2000, 128, 108-117.	7.5	16
185	Molecular dynamics simulation of defect production in irradiated Î²-SiC. Journal of Nuclear Materials, 2000, 283-287, 794-798.	2.7	18
186	Triple junctions and elastic stability of polycrystalline silicon. Physical Review B, 2000, 63, .	3.2	17
187	Lattice-strain field induced by{311}self-interstitial defects in silicon. Physical Review B, 2000, 62, 1815-1820.	3.2	27
188	Laser-induced melting of silicon: A tight-binding molecular dynamics simulation. Physical Review B, 2000, 61, 8233-8237.	3.2	28
189	Solidâ€“liquid interface velocity and diffusivity in laser-melt amorphous silicon. Applied Physics Letters, 2000, 77, 2337-2339.	3.3	33
190	Evolution of energetics and bonding of compact self-interstitial clusters in Si. Europhysics Letters, 2000, 50, 608-614.	2.0	45
191	On the electrical activity of sp 2 -bonded grain boundaries in nanocrystalline diamond. Europhysics Letters, 1999, 46, 671-677.	2.0	62
192	Growth of Nanostructured Carbon Films by Cluster Assembly. Physical Review Letters, 1999, 83, 776-779.	7.8	82
193	Role of Extended Vacancy-Vacancy Interaction on the Ripening of Voids in Silicon. Physical Review Letters, 1999, 82, 1720-1723.	7.8	45
194	Native defects and their interactions in silicon. Physica B: Condensed Matter, 1999, 273-274, 458-462.	2.7	21
195	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
196	On the effect of quench rate on the structure of amorphous carbon. Computational Materials Science, 1998, 10, 67-74.	3.0	8
197	A source code for tight-binding molecular dynamics simulations. Computational Materials Science, 1998, 12, 278-287.	3.0	29
198	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

#	Article	IF	Citations
199	Formation and annihilation of a bond defect in silicon: Anab initioquantum-mechanical characterization. Physical Review B, 1998, 57, 170-177.	3.2	73
200	Parallel tight-binding molecular dynamics code based on integration of HPF and optimized parallel libraries. Lecture Notes in Computer Science, 1998, , 104-111.	1.3	0
201	Structural and binding properties of vacancy clusters in silicon. Europhysics Letters, 1998, 43, 695-700.	2.0	65
202	A theoretical study of the smallest tetrahedral carbon schwarzites. Europhysics Letters, 1998, 44, 525-530.	2.0	26
203	Structure and chemical order of bulkSi1â^'xCxamorphous alloys. Physical Review B, 1998, 58, 10357-10362.	3.2	34
204	Interaction between a monovacancy and a vacancy cluster in silicon. Physical Review B, 1998, 57, 8767-8769.	3.2	33
205	Correlation between atomic structure and localized gap states in silicon grain boundaries. Physical Review B, 1998, 57, 6247-6250.	3.2	38
206	The Role of Cluster Size and Topology on the Ripening of Defect Aggregates in Crystalline Si. Materials Research Society Symposia Proceedings, 1998, 538, 241.	0.1	1
207	Understanding Structure and Electronic Properties of Extended Self-Interstitial Defects in Silicon. Materials Research Society Symposia Proceedings, 1998, 538, 353.	0.1	0
208	Silicon Self-Interstitial Clusters. Materials Research Society Symposia Proceedings, 1998, 538, 413.	0.1	1
209	Modelling Point Defects Diffusion and Interaction in Silicon: The Tight-Binding Molecular Dynamics Approach. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 1211-1214.	0.9	0
210	Structural Disorder and Localized Gap States in Silicon Grain Boundaries from a Tight-Binding Model. Materials Research Society Symposia Proceedings, 1997, 491, 513.	0.1	0
211	Migration of Atomic and Molecular Hydrogen in SiO₂: A Molecular Dynamics Study. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 1229-1231.	0.9	1
212	Formation and Binding Energies of Vacancy Clusters in Silicon. Materials Research Society Symposia Proceedings, 1997, 469, 205.	0.1	2
213	Large Scale Atomistic Simulations using the Tight Binding Approach. Materials Research Society Symposia Proceedings, 1997, 491, 481.	0.1	0
214	Carbon Schwarzites: Properties and Growth Simulation from Fullerene Fragments. Materials Research Society Symposia Proceedings, 1997, 491, 529.	0.1	0
215	Prediction of newsp2andsp2/sp3hollow carbon crystals. Journal of Chemical Physics, 1997, 106, 2311-2316.	3.0	16
216	Routes to carbon schwarzites from fullerene fragments. Europhysics Letters, 1997, 39, 269-274.	2.0	29

#	Article	IF	Citations
217	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
218	Structural properties of silica surface: a classical molecular dynamics study. Journal of Non-Crystalline Solids, 1997, 220, 164-168.	3.1	21
219	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
220	A theoretical investigation on the chemical bonding of interstitial and vacancy defects in silicon during their migration. Nuclear Instruments & Methods in Physics Research B, 1997, 127-128, 235-238.	1.4	2
221	Hydrogen diffusion in crystalline SiO2. Chemical Physics Letters, 1997, 264, 435-440.	2.6	16
222	Quantum Mechanical Simulations in Semiconductor Materials Science:. , 1997, , 79-85.		0
223	Hydrogen bonding and migration in amorphous silicon. Europhysics Letters, 1996, 36, 295-300.	2.0	18
224	Hollow Diamonds from Fullerenes. Materials Science Forum, 1996, 232, 247-274.	0.3	24
225	Elastic constants in defected and amorphous silicon by tight-binding molecular dynamics. , 1996, , 189-192.		1
226	Bonding and diffusion in hydrogenated amorphous silicon by tight-binding molecular dynamics. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1996, 36, 264-267.	3.5	0
227	Elastic constants in defected and amorphous silicon by tight-binding molecular dynamics. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1996, 37, 189-192.	3.5	3
228	A parallel implementation of tight-binding molecular dynamics. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1996, 37, 228-231.	3.5	5
229	Calculation of elastic constants in defected and amorphous silicon by quantum simulations. Physical Review B, 1996, 54, 11857-11860.	3.2	21
230	TIGHT-BINDING MOLECULAR DYNAMICS. , 1996, , 147-183.		19
231	Large Scale Simulations Using Tight Binding Molecular Dynamics. , 1996, , 495-510.		1
232	Structure, energetics, clustering and migration of point-defects in silicon. Physica Scripta, 1996, T66, 207-211.	2.5	2
233	Bonding and diffusion in hydrogenated amorphous silicon by tight-binding molecular dynamics. , 1996, , 264-267.		0
234	Tight-Binding Molecular Dynamics Simulations on Point Defects Diffusion and Interactions in Crystalline Silicon. Materials Research Society Symposia Proceedings, 1995, 396, 33.	0.1	3

#	Article	IF	Citations
235	A Parallel Implementation of Tight-Binding Molecular Dynamics Based on Reordering of Atoms and the Lanczos Eigen-Solver. Materials Research Society Symposia Proceedings, 1995, 408, 107.	0.1	1
236	Hydrogen Diffusion in Quartz: A Molecular Dynamics Investigation. Materials Research Society Symposia Proceedings, 1995, 408, 515.	0.1	1
237	Amorphization of fullerite crystals. Chemical Physics Letters, 1995, 238, 281-285.	2.6	9
238	A first-principles derived parametrization for the adiabatic bond charge model. Solid State Communications, 1995, 96, 49-52.	1.9	8
239	Phonon properties and Raman response of (113) GaAs/AlAs corrugated superlattices. Physical Review B, 1995, 51, 1647-1652.	3.2	17
240	Electronic states in one-dimensional polymeric superlattices: A tight-binding approach. Physical Review B, 1995, 51, 1624-1630.	3.2	18
241	Solidâ€toâ€liquid phase change and fragmentation in C60. Journal of Chemical Physics, 1995, 102, 2151-2155.	3.0	18
242	Defect-Induced Amorphization in Silicon. Europhysics Letters, 1995, 29, 623-628.	2.0	22
243	Hydrogen diffusion in crystalline silicon: A tight-binding molecular dynamics study. Phase Transitions, 1994, 52, 137-149.	1.3	5
244	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
245	Confinement effects on the phonon spectrum of thin InAs/InP strained single quantum wells. Semiconductor Science and Technology, 1994, 9, 256-262.	2.0	5
246	Tight-binding molecular dynamics in liquid III-V compounds. I. Potential generation. Journal of Physics Condensed Matter, 1994, 6, 5243-5254.	1.8	18
247	Lattice dynamics and Raman response of (113) GaAs/AlAs superlattices. Physical Review B, 1994, 49, 10362-10372.	3.2	21
248	Hydrogen Diffusion in Silicon from Tight-Binding Molecular Dynamics. Physical Review Letters, 1994, 73, 1636-1639.	7.8	72
249	Study of vibrational properties of InGaAsP by farâ€infrared reflectivity. Journal of Applied Physics, 1994, 75, 3085-3088.	2.5	4
250	Barrier height versus confinement efficiency for the optical phonons in GaAs/AlxGa1â^'xAs heterostructures. Physical Review B, 1994, 50, 11684-11686.	3.2	3
251	Structure and properties of amorphous gallium arsenide by tight-binding molecular dynamics. Physical Review B, 1994, 50, 4371-4377.	3.2	47
252	Pre-fragmentation dynamics of C60. A molecular dynamics investigation. Chemical Physics Letters, 1994, 225, 191-195.	2.6	20

#	Article	IF	Citations
253	Growth and structural characterization of thin Ge films by molecular dynamic simulation. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1994, 26, 61-65.	3.5	0
254	Efficient Linear Scaling Algorithm for Tight-Binding Molecular Dynamics. Physical Review Letters, 1994, 73, 122-125.	7.8	412
255	Structure, Stability and Properties of Covalent C₃₄, C₂₀, and C₂₂ Crystals. Materials Research Society Symposia Proceedings, 1994, 359, 157.	0.1	2
256	Structural and Electronic Properties of Damaged Fullerite Crystals. Materials Research Society Symposia Proceedings, 1994, 359, 475.	0.1	0
257	Computer Simulation of Thermal Annealing Effects on Self Implanted Silicon. Materials Research Society Symposia Proceedings, 1994, 373, 463.	0.1	0
258	Simulation of the Amorphous-Silicon Properties and Their Dependence on Sample Preparation. Europhysics Letters, 1993, 22, 107-112.	2.0	64
259	Structural Properties of Liquid and Amorphous GaAs by Tight-Binding Molecular Dynamics. Europhysics Letters, 1993, 24, 659-664.	2.0	30
260	Structural and electronic properties of strained Si/GaAs heterostructures. Physical Review B, 1993, 48, 12047-12052.	3.2	19
261	Band offsets engineering at semiconductor heterojunctions. , 1993, , .		1
262	Defect Induced Amortization in Silicon: A Tight Binding Molecular Dynamics Simulation. Materials Research Society Symposia Proceedings, 1993, 316, 223.	0.1	1
263	Preparation, Structure, And Electronic Properties Of Amorphous Gaas By Tight-Binding Molecular Dynamics. Materials Research Society Symposia Proceedings, 1993, 321, 135.	0.1	0
264	Defect Induced Amortization in Silicon: A Tight Binding Molecular Dynamics Simulation. Materials Research Society Symposia Proceedings, 1993, 321, 423.	0.1	2
265	Influence of Interface Disorder on the Raman Response of {113}-Oriented Superlattices. Materials Research Society Symposia Proceedings, 1993, 326, 199.	0.1	0
266	Compositional Disorder in AlGaAs Superlattices: Bond Charge Model Calculations of Vibrational Features and Optical Spectra. , 1993, , 279-311.		0
267	Chemistry, interface features and strain: how do they affect the valence band offset at Si/Ge interfaces?. Physica Scripta, 1992, T45, 181-185.	2.5	0
268	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
269	Quantum Simulation of Amorphous Silicon: Preparation, Structure and Properties. Materials Research Society Symposia Proceedings, 1992, 291, 61.	0.1	1
270	Raman response of GaAs/AlAs superlattices with AlxGa1â^'xAs intralayers. Superlattices and Microstructures, 1992, 12, 523-525.	3.1	3

#	Article	IF	Citations
271	Dynamical effects of biaxial strain in thin Cu/Ni(111) superlattices. Journal of Applied Physics, 1991, 70, 2079-2085.	2.5	7
272	Valence-band offsets at strained Si/Ge interfaces. Physical Review B, 1991, 44, 5572-5579.	3.2	177
273	Order-disorder interplay in AlÏ‡Ga1â^'Ï‡As superlattices: Calculation of infrared and Raman spectra. Superlattices and Microstructures, 1991, 10, 153-156.	3.1	2
274	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
275	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
276	Geometric construction of large dynamical matrices: Applications to reconstructed surfaces, superlattices and mixed crystals. Superlattices and Microstructures, 1990, 7, 139-146.	3.1	14
277	Absolute deformation potentials in semiconductors. Physical Review B, 1990, 41, 12358-12361.	3.2	49
278	Lattice dynamics of homopolar/heteropolar semiconductor superlattices: Ge/GaAs and Ge/AlAs. Surface Science, 1990, 234, 169-180.	1.9	3
279	Interplanar force constants in GaAs and Ge: Bond-Charge-Model vs.ab-initiocalculations. Physica Scripta, 1989, 40, 238-241.	2.5	6
280	A planar approach to the lattice dynamics of polar semiconductor superlattices. Surface Science, 1989, 221, 486-512.	1.9	15
281	Infrared characterization of silicon dioxide films obtained by chemical vapour deposition. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1988, 10, 1487-1496.	0.4	0
282	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
283	Surface phonons in Si(111) + H(1Ã—1). Physical Review B, 1988, 38, 3305-3310.	3.2	68
284	Phonon calculations in superperiodic structures: The surface Green-function matching approach. Physical Review B, 1988, 38, 3172-3179.	3.2	20
285	Surface phonon calculation for Si(111): H(1Ã—1). Physica Scripta, 1988, 37, 768-772.	2.5	45
286	Electric-field effects on the infra-red absorption of H in a SiO2 film. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1986, 7, 87-97.	0.4	1
287	The Calculation of Free-Energiesin Semiconductors: Defects, Transitionsand Phase Diagrams. , 0, , 115-140.		1