

# Fabrizio Cleri

## List of Publications by Citations

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140  
papers

3,713  
citations

27  
h-index

59  
g-index

156  
ext. papers

3,962  
ext. citations

3.2  
avg, IF

5.46  
L-index

#	Paper	IF	Citations
140	Tight-binding potentials for transition metals and alloys. <i>Physical Review B</i> , <b>1993</b> , 48, 22-33	3.3	1625
139	Turning carbon nanotubes from exceptional heat conductors into insulators. <i>Physical Review Letters</i> , <b>2009</b> , 102, 105901	7.4	249
138	Atomic-Scale Mechanism of Crack-Tip Plasticity: Dislocation Nucleation and Crack-Tip Shielding. <i>Physical Review Letters</i> , <b>1997</b> , 79, 1309-1312	7.4	94
137	Atomic scale origin of crack resistance in brittle fracture. <i>Physical Review Letters</i> , <b>2005</b> , 95, 115501	7.4	71
136	Thermal conductivity from approach-to-equilibrium molecular dynamics. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 033525	2.5	68
135	On the electrical activity of sp <sup>2</sup> -bonded grain boundaries in nanocrystalline diamond. <i>Europhysics Letters</i> , <b>1999</b> , 46, 671-677	1.6	56
134	Atomistic Simulations of Materials Fracture and the Link between Atomic and Continuum Length Scales. <i>Journal of the American Ceramic Society</i> , <b>2005</b> , 81, 501-516	3.8	55
133	Thermal boundary resistance at silicon-silica interfaces by molecular dynamics simulations. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 131906	3.4	52
132	Contact resistance in percolating networks. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	52
131	Atomic hydrogen adsorption on a Stone-Wales defect in graphite. <i>Surface Science</i> , <b>2002</b> , 496, 33-38	1.8	50
130	On the Nature of Grain Boundaries in Nanocrystalline Diamond. <i>MRS Bulletin</i> , <b>1998</b> , 23, 36-41	3.2	48
129	Elasticity of flexible and semiflexible polymers with extensible bonds in the Gibbs and Helmholtz ensembles. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 154906	3.9	39
128	Role of surface chemistry in hydrogen adsorption in single-wall carbon nanotubes. <i>Chemical Physics Letters</i> , <b>2003</b> , 371, 476-482	2.5	39
127	Molecular dynamics simulation of the recrystallization of amorphous Si layers: Comprehensive study of the dependence of the recrystallization velocity on the interatomic potential. <i>Journal of Applied Physics</i> , <b>2007</b> , 101, 123506	2.5	38
126	Interaction of benzene thiol and thiolate with small gold clusters. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 10062-8	3.9	38
125	Representation of mechanical loads in molecular dynamics simulations. <i>Physical Review B</i> , <b>2001</b> , 65,	3.3	38
124	Surface-induced optimal packing of two-dimensional molecular networks. <i>Physical Review Letters</i> , <b>2015</b> , 114, 066101	7.4	37

123	Theory and Monte Carlo simulations for the stretching of flexible and semiflexible single polymer chains under external fields. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 244907	3.9	35
122	Chemisorption of atomic hydrogen in graphite and carbon nanotubes. <i>Surface Science</i> , <b>2003</b> , 544, 24-34	1.8	35
121	Experimental and theoretical investigation of the order-disorder transformation in Ni <sub>3</sub> Al. <i>Journal of Materials Research</i> , <b>1993</b> , 8, 2504-2509	2.5	35
120	Atomic-scale modeling of the interaction between short polypeptides and carbon surfaces. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 12105-12	3.4	32
119	Correlation between atomic structure and localized gap states in silicon grain boundaries. <i>Physical Review B</i> , <b>1998</b> , 57, 6247-6250	3.3	32
118	Length dependence of thermal conductivity by approach-to-equilibrium molecular dynamics. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	32
117	Solid-liquid interface velocity and diffusivity in laser-melt amorphous silicon. <i>Applied Physics Letters</i> , <b>2000</b> , 77, 2337-2339	3.4	31
116	Two-state theory of single-molecule stretching experiments. <i>Physical Review E</i> , <b>2013</b> , 87,	2.4	28
115	Thermal conductivity of glassy GeTe by first-principles molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 9729-9732	3.6	27
114	On the equivalence of thermodynamics ensembles for flexible polymer chains. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2014</b> , 395, 154-170	3.3	27
113	Atomic Scale Modeling of Two-Dimensional Molecular Self-Assembly on a Passivated Si Surface. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 12817-12825	3.8	26
112	A stochastic grain growth model based on a variational principle for dissipative systems. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2000</b> , 282, 339-354	3.3	25
111	Atomistic study of the interaction between a microcrack and a hard inclusion in BiC. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	22
110	Order-disorder transition in Cu <sub>3</sub> Au: A combined molecular-dynamics and cluster-variation-method approach. <i>Physical Review B</i> , <b>1993</b> , 47, 14541-14544	3.3	22
109	Lattice dynamics of ordered and disordered Cu <sub>3</sub> Au with a tight-binding potential model. <i>Philosophical Magazine Letters</i> , <b>1993</b> , 67, 369-378	1	22
108	Atomistic Simulations of Intergranular Fracture in Symmetric-Tilt Grain Boundaries. <i>Journal of Materials Science</i> , <b>1999</b> , 7, 45-55		21
107	Real-time mechanical characterization of DNA degradation under therapeutic X-rays and its theoretical modeling. <i>Microsystems and Nanoengineering</i> , <b>2016</b> , 2, 16062	7.7	20
106	Supramolecular self-assembly on the B-Si(111)-(√3×√3) R30° surface: From single molecules to multicomponent networks. <i>Surface Science Reports</i> , <b>2017</b> , 72, 316-349	12.9	19

105	Interface structure of silicon nanocrystals embedded in an amorphous silica matrix. <i>Solid State Sciences</i> , <b>2010</b> , 12, 163-171	3.4	18
104	Atomic and electronic structure of high-energy grain boundaries in silicon and carbon. <i>Computational Materials Science</i> , <b>2001</b> , 20, 351-362	3.2	18
103	Molecular dynamics of ionic self-diffusion at an MgO grain boundary. <i>Journal of Materials Science</i> , <b>2015</b> , 50, 2502-2509	4.3	17
102	Scaling shift in multicroaked fiber bundles. <i>Physical Review Letters</i> , <b>2014</b> , 113, 255501	7.4	17
101	Triple junctions and elastic stability of polycrystalline silicon. <i>Physical Review B</i> , <b>2000</b> , 63,	3.3	17
100	Lattice instability analysis of a prototype intermetallic system under stress. <i>Journal of Applied Physics</i> , <b>1995</b> , 77, 1449-1458	2.5	17
99	Atomistic simulation of dislocation nucleation and motion from a crack tip. <i>Acta Materialia</i> , <b>1997</b> , 45, 4993-5003	8.4	16
98	Exceptional plasticity of silicon nanobridges. <i>Nanotechnology</i> , <b>2011</b> , 22, 355704	3.4	15
97	Synthesis and Characterization of a Polycrystalline Ionic Thin Film by Large-Scale Molecular-Dynamics Simulation. <i>Journal of Materials Science</i> , <b>1999</b> , 7, 15-31		15
96	Fracture toughness of nanostructured silicon carbide. <i>Applied Physics Letters</i> , <b>2005</b> , 87, 141912	3.4	14
95	Analysis of Sample and Fuel Pin Irradiation Experiments in Phix for Basic Nuclear Data Validation. <i>Nuclear Science and Engineering</i> , <b>1990</b> , 105, 244-255	1.2	14
94	High Conductance Ratio in Molecular Optical Switching of Functionalized Nanoparticle Self-Assembled Nanodevices. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 21173-21183	3.8	13
93	Localization and quantization in covalently bonded carbon nanotube junctions. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	13
92	On the occurrence of size effects in the calculation of thermal conductivity by first-principles molecular dynamics: The case of glassy GeTe4. <i>Journal of Non-Crystalline Solids</i> , <b>2018</b> , 498, 190-193	3.9	12
91	Structure and mechanical characterization of DNA i-motif nanowires by molecular dynamics simulation. <i>Biophysical Journal</i> , <b>2013</b> , 105, 2820-31	2.9	12
90	Microstructure evolution from the atomic scale up. <i>Computational Materials Science</i> , <b>2002</b> , 24, 21-27	3.2	12
89	Response to "Comment on "Elasticity of flexible and semiflexible polymers with extensible bonds in the Gibbs and Helmholtz ensembles"[J. Chem. Phys. 138, 157101 (2013)]. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 157102	3.9	11
88	Point-defect recombination efficiency at grain boundaries in irradiated SiC. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	11

87	Mechanical Instability of Oxidized Metal Clusters. <i>Physical Review Letters</i> , <b>1996</b> , 77, 2495-2498	7.4	10
86	Mechanical evolution of DNA double-strand breaks in the nucleosome. <i>PLoS Computational Biology</i> , <b>2018</b> , 14, e1006224	5	9
85	Atomistic simulation of plasticity in silicon nanowires. <i>Applied Physics Letters</i> , <b>2010</b> , 97, 153106	3.4	9
84	Microscopic mechanics of biomolecules in living cells. <i>Scientific Modeling and Simulation SMNS</i> , <b>2008</b> , 15, 339-362		9
83	A molecular dynamics simulation of the effects of excess free volume on the diffusion in metallic glasses. <i>Journal of Non-Crystalline Solids</i> , <b>1992</b> , 144, 187-195	3.9	9
82	Fourier-like conduction and finite one-dimensional thermal conductivity in long silicon nanowires by approach-to-equilibrium molecular dynamics. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	8
81	Surface ordering of molecular structures by dispersion forces. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	8
80	Evolution of dislocation cell structures in plastically deformed metals. <i>Computer Physics Communications</i> , <b>2005</b> , 169, 44-49	4.2	7
79	Vibrational modes of graphitic fragments and the nucleation of carbon nanotubes. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 3308-3314	3.9	7
78	Microstructure evolution at a triple junction in polycrystalline silicon. <i>Journal of Physics Condensed Matter</i> , <b>2002</b> , 14, 13003-13008	1.8	7
77	Multiscale Modeling of Composite Materials by a Multifield Finite Element Approach. <i>International Journal for Multiscale Computational Engineering</i> , <b>2005</b> , 3, 463-480	2.4	7
76	On the ability of molecular dynamics simulation and continuum electrostatics to treat interfacial water molecules in protein-protein complexes. <i>Scientific Reports</i> , <b>2016</b> , 6, 38259	4.9	7
75	Interface thermal behavior in nanomaterials by thermal grating relaxation. <i>International Journal of Heat and Mass Transfer</i> , <b>2019</b> , 131, 932-943	4.9	7
74	Stability of radiation-damaged DNA after multiple strand breaks. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 14641-14651	3.6	6
73	A two-phase model of large-strain plasticity in covalent nanostructures. <i>International Journal of Plasticity</i> , <b>2012</b> , 37, 31-52	7.6	6
72	Monte Carlo simulations of single polymer force-extension relations. <i>Journal of Physics: Conference Series</i> , <b>2012</b> , 383, 012016	0.3	6
71	Experimental and Theoretical Characterization of the 3D-Dopants Bias on the H Desorption of Mg Hydrides. <i>Materials Science Forum</i> , <b>2007</b> , 555, 349-354	0.4	6
70	Phase stability of NiAl solid solutions. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , <b>1993</b> , 68, 845-851		6

69	Low-energy photon scattering simulations with the Monte Carlo code ACCEPT. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , <b>1990</b> , 295, 231-240	1.2	6
68	On the validity of the Hartree approximation and the effect of short-range correlations in $\bar{n}$ -condensation in finite nuclei. <i>Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics</i> , <b>1984</b> , 141, 33-36	4.2	6
67	Stochastic mechanical degradation of multi-cracked fiber bundles with elastic and viscous interactions. <i>European Physical Journal E</i> , <b>2015</b> , 38, 131	1.5	5
66	Detection of single DNA mismatches by force spectroscopy in short DNA hairpins. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 074204	3.9	5
65	A biophysical model of cell evolution after cytotoxic treatments: Damage, repair and cell response. <i>Journal of Theoretical Biology</i> , <b>2016</b> , 389, 146-58	2.3	5
64	Energy band and vacuum level alignment at a semiconductor-molecule-metal interface. <i>Applied Physics Letters</i> , <b>2008</b> , 92, 103112	3.4	5
63	Diffusion of boron in silicon: Compatibility of empirical molecular dynamics with continuum simulations. <i>Europhysics Letters</i> , <b>2006</b> , 76, 842-848	1.6	5
62	Molecular dynamics calculation of the Zr(Ni) enthalpy of mixing. <i>Applied Physics Letters</i> , <b>1996</b> , 69, 1701-1703	3.4	5
61	The Physics of Living Systems. <i>Undergraduate Lecture Notes in Physics</i> , <b>2016</b> ,	0.1	5
60	Thermal conductivity of deca-nanometric patterned Si membranes by multiscale simulations. <i>International Journal of Heat and Mass Transfer</i> , <b>2018</b> , 126, 830-835	4.9	4
59	Nano systems and devices for applications in biology and nanotechnology. <i>Solid-State Electronics</i> , <b>2016</b> , 115, 66-73	1.7	3
58	Agent-based model of multicellular tumor spheroid evolution including cell metabolism. <i>European Physical Journal E</i> , <b>2019</b> , 42, 112	1.5	3
57	Characteristic lengths in natural bundle assemblies arising from fiber-matrix energy competition: A floquet-based homogenization theory. <i>European Journal of Mechanics, A/Solids</i> , <b>2016</b> , 60, 145-165	3.7	3
56	Multiscale modelling of molecular monolayers adsorbed on silicon. <i>Applied Physics A: Materials Science and Processing</i> , <b>2007</b> , 86, 293-300	2.6	3
55	Screening and surface states in molecular monolayers adsorbed on silicon. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 11496-503	3.4	3
54	Kinetic proofreading of chromatin remodeling: from gene activation to gene repression and back. <i>AIMS Biophysics</i> , <b>2015</b> , 2, 398-411	0.8	3
53	Radiation Environment and Doses on Mars at Oxia Planum and Mawrth Vallis: Support for Exploration at Sites With High Biosignature Preservation Potential. <i>Journal of Geophysical Research E: Planets</i> , <b>2021</b> , 126, e2020JE006488	4.1	3
52	Deformation Localization in Molecular Layers Constrained between Self-Assembled Au Nanoparticles. <i>Langmuir</i> , <b>2017</b> , 33, 2677-2687	4	2

51	Tunneling mechanism and contact mechanics of colloidal nanoparticle assemblies. <i>Nanotechnology</i> , <b>2016</b> , 27, 475502	3.4	2
50	Silicon Nanotweezers with a microfluidic cavity for the real time characterization of DNA damage under therapeutic radiation beams. <i>Annual International Conference of the IEEE Engineering in Medicine and Biology Society IEEE Engineering in Medicine and Biology Society Annual International Conference</i> , <b>2013</b> , 2013, 6820	0.9	2
49	Interacting Lewis-X carbohydrates in condensed phase: a first-principles molecular dynamics study. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 12599-606	3.4	2
48	Hydrogen Storage in MgH <sub>2</sub> Matrices: An Ab-Initio Study of Mg-MgH <sub>2</sub> Interface. <i>Solid State Phenomena</i> , <b>2008</b> , 139, 23-28	0.4	2
47	What's so special about nanocrystalline semiconductors?. <i>International Journal of Computational Science and Engineering</i> , <b>2006</b> , 2, 242	0.4	2
46	Vibrational modes of graphitic fragments and the nucleation of carbon nanotubes. <i>Materials Research Society Symposia Proceedings</i> , <b>2000</b> , 633, 1341		2
45	Defect energetics, thermal stability and localized electronic states in carbon nanotubes. <i>Materials Research Society Symposia Proceedings</i> , <b>2000</b> , 633, 1481		2
44	Stability of the ground state of finite nuclei against neutral pion condensation. <i>Physical Review C</i> , <b>1986</b> , 34, 1134-1136	2.7	2
43	A stochastic force model for the ballistic-diffusive transition of heat conduction. <i>Physica Scripta</i> , <b>2020</b> , 95, 075703	2.6	1
42	A Multiscale Approach for Composite Materials as Multifield Continua. <i>Materials Science Forum</i> , <b>2007</b> , 539-543, 2551-2556	0.4	1
41	Quantum Dots from Carbon Nanotube Junctions. <i>Materials Research Society Symposia Proceedings</i> , <b>2003</b> , 789, 217		1
40	Triple Junctions in Polycrystalline Silicon: A Numerical Study Based upon Atomistic Simulations. <i>Key Engineering Materials</i> , <b>2001</b> , 221-222, 307-314	0.4	1
39	Multiphase microstructure evolution model including dislocation plasticity. <i>Journal of Materials Research</i> , <b>2002</b> , 17, 1932-1940	2.5	1
38	Ab-initio modelling of atomic and molecular Hydrogen adsorption in graphite. <i>Materials Research Society Symposia Proceedings</i> , <b>2001</b> , 677, 471		1
37	Deuterium clusters in a strained palladium lattice. <i>Journal of Materials Research</i> , <b>1990</b> , 5, 2094-2099	2.5	1
36	Bragg's additivity rule and core and bond model studied by real-time TDDFT electronic stopping simulations: The case of water vapor. <i>Radiation Physics and Chemistry</i> , <b>2022</b> , 193, 109961	2.5	0
35	Molecular Motors in the Cell. <i>Undergraduate Lecture Notes in Physics</i> , <b>2016</b> , 205-252	0.1	0
34	Of Limbs, Wings and Fins. <i>Undergraduate Lecture Notes in Physics</i> , <b>2016</b> , 423-473	0.1	

- 33 Thermodynamics for Living Systems. *Undergraduate Lecture Notes in Physics*, **2016**, 9-59 0.1
- 32 Entropic Forces in the Cell. *Undergraduate Lecture Notes in Physics*, **2016**, 159-203 0.1
- 31 Bioelectricity, Hearts and Brains. *Undergraduate Lecture Notes in Physics*, **2016**, 253-316 0.1
- 30 The Materials of the Living. *Undergraduate Lecture Notes in Physics*, **2016**, 367-421 0.1
- 29 DNA i-motif provides steel-like tough ends to chromosomes. *Materials Research Society Symposia Proceedings*, **2014**, 1621, 135-141
- 28 Metallographic and Numerical Studies of the Role of Catalyst Particles of MgH<sub>2</sub>-Mg System. *Defect and Diffusion Forum*, **2010**, 297-301, 263-268 0.7
- 27 Structural Disorder and Localized Gap States in Silicon Grain Boundaries from a Tight-Binding Model. *Materials Research Society Symposia Proceedings*, **1997**, 491, 513
- 26 Large Scale Atomistic Simulations using the Tight Binding Approach. *Materials Research Society Symposia Proceedings*, **1997**, 491, 481
- 25 Comparison Between Atomistic and Continuum-Mechanics Modelling of Grain-Boundary Fracture. *Materials Research Society Symposia Proceedings*, **1997**, 492, 377
- 24 Metallographic and numerical characterization of MgH<sub>2</sub>-Mg system. *Materials Research Society Symposia Proceedings*, **2008**, 1127, 1
- 23 Phonon instability in nanocrystalline silicon carbide. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 3311-3315 1.3
- 22 ab-initio modelling of Mg:H interstitial solid solutions. *Materials Research Society Symposia Proceedings*, **2003**, 801, 120
- 21 Crack-tip stress shielding by a hard fiber in SiC: an atomistic study. *Computer Physics Communications*, **2005**, 169, 40-43 4.2
- 20 Dedicated hardware for linearly-scaling algorithms in condensed-matter physics. *Computer Physics Communications*, **2001**, 139, 20-33 4.2
- 19 Identification of tetrahedrally coordinated atoms in supercooled liquid silicon. *Materials Research Society Symposia Proceedings*, **2000**, 638, 1
- 18 Atomistic models of triple junctions and the origin of topological changes in microstructural evolution. *Materials Research Society Symposia Proceedings*, **2000**, 652, 1
- 17 A microstructure evolution model including dislocation plasticity. *Materials Research Society Symposia Proceedings*, **2000**, 652, 1
- 16 A molecular dynamics investigation on grain disappearance at a triple junction in polycrystalline silicon. *Materials Research Society Symposia Proceedings*, **2001**, 677, 171



- 15 Coupled atomistic-mesoscopic model of polycrystalline plasticity. *Materials Research Society Symposia Proceedings*, **2001**, 677, 761
- 14 Atomistic Aspects of Fracture Modelling in the Framework of Continuum Mechanics. *Materials Research Society Symposia Proceedings*, **1998**, 538, 441
- 13 Microscopic-scale simulations of macroscopic flow patterns in non-equilibrium two-dimensional systems **1994**, 17, 281-299
- 12 A Molecular Dynamics Study of the Terminal Zr(Ni) Solid Solutions. *Materials Research Society Symposia Proceedings*, **1995**, 400, 131
- 11 Atomistic Simulation of Crystal-to-Amorphous Transitions in the Intermetallic Alloys NiZr<sub>2</sub> and Cu<sub>3</sub>Au. *Materials Research Society Symposia Proceedings*, **1992**, 278, 87
- 10 Order-Disorder Transformation in Cu<sub>3</sub>Au: A Molecular Dynamics Study. *Materials Research Society Symposia Proceedings*, **1992**, 291, 531
- 9 Atomic-Scale Investigation on Fracture Toughness in Nanocomposite Silicon Carbide **2006**, 41-42
- 8 Microscopic mechanics of biomolecules in living cells. *Lecture Notes in Computational Science and Engineering*, **2008**, 339-362 0.3
- 7 The Mach-1 Code for Coupled Neutron, Photon and Electron Transport by the Monte Carlo Method **1992**, 315-322
- 6 Approach-to-Equilibrium Molecular Dynamics **2017**, 191-205
- 5 Shapes of the Living. *Undergraduate Lecture Notes in Physics*, **2016**, 475-526 0.1
- 4 The Hidden Mathematics of Living Systems. *Undergraduate Lecture Notes in Physics*, **2016**, 527-572 0.1
- 3 Energy, Information, and The Origins of Life. *Undergraduate Lecture Notes in Physics*, **2016**, 61-111 0.1
- 2 Energy Production and Storage for Life. *Undergraduate Lecture Notes in Physics*, **2016**, 113-158 0.1
- 1 Molecular Mechanics of the Cell. *Undergraduate Lecture Notes in Physics*, **2016**, 317-366 0.1