Fabrizio Cleri

List of Publications by Year in Descending Order

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	Bragg's additivity rule and core and bond model studied by real-time TDDFT electronic stopping simulations: The case of water vapor. *Radiation Physics and Chemistry*, **2022**, 193, 109961	2.5	0
139	Radiation Environment and Doses on Mars at Oxia Planum and Mawrth Vallis: Support for Exploration at Sites With High Biosignature Preservation Potential. *Journal of Geophysical Research E: Planets*, **2021**, 126, e2020JE006488	4.1	3
138	A stochastic force model for the ballistic-diffusive transition of heat conduction. *Physica Scripta*, **2020**, 95, 075703	2.6	1
137	Detection of single DNA mismatches by force spectroscopy in short DNA hairpins. *Journal of Chemical Physics*, **2020**, 152, 074204	3.9	5
136	Agent-based model of multicellular tumor spheroid evolution including cell metabolism. *European Physical Journal E*, **2019**, 42, 112	1.5	3
135	Interface thermal behavior in nanomaterials by thermal grating relaxation. *International Journal of Heat and Mass Transfer*, **2019**, 131, 932-943	4.9	7
134	On the occurrence of size effects in the calculation of thermal conductivity by first-principles molecular dynamics: The case of glassy GeTe4. *Journal of Non-Crystalline Solids*, **2018**, 498, 190-193	3.9	12
133	Mechanical evolution of DNA double-strand breaks in the nucleosome. *PLoS Computational Biology*, **2018**, 14, e1006224	5	9
132	Thermal conductivity of deca-nanometric patterned Si membranes by multiscale simulations. *International Journal of Heat and Mass Transfer*, **2018**, 126, 830-835	4.9	4
131	Deformation Localization in Molecular Layers Constrained between Self-Assembled Au Nanoparticles. *Langmuir*, **2017**, 33, 2677-2687	4	2
130	Stability of radiation-damaged DNA after multiple strand breaks. *Physical Chemistry Chemical Physics*, **2017**, 19, 14641-14651	3.6	6
129	Thermal conductivity of glassy GeTe by first-principles molecular dynamics. *Physical Chemistry Chemical Physics*, **2017**, 19, 9729-9732	3.6	27
128	Fourier-like conduction and finite one-dimensional thermal conductivity in long silicon nanowires by approach-to-equilibrium molecular dynamics. *Physical Review B*, **2017**, 95,	3.3	8
127	Supramolecular self-assembly on the B-Si(111)-(√3x√3) R30° surface: From single molecules to multicomponent networks. *Surface Science Reports*, **2017**, 72, 316-349	12.9	19
126	Approach-to-Equilibrium Molecular Dynamics **2017**, 191-205		
125	Nano systems and devices for applications in biology and nanotechnology. *Solid-State Electronics*, **2016**, 115, 66-73	1.7	3
124	Characteristic lengths in natural bundle assemblies arising from fiber-matrix energy competition: A floquet-based homogenization theory. *European Journal of Mechanics, A/Solids*, **2016**, 60, 145-165	3.7	3

123	Of Limbs, Wings and Fins. *Undergraduate Lecture Notes in Physics*, **2016**, 423-473	0.1	
122	Thermodynamics for Living Systems. *Undergraduate Lecture Notes in Physics*, **2016**, 9-59	0.1	
121	Entropic Forces in the Cell. *Undergraduate Lecture Notes in Physics*, **2016**, 159-203	0.1	
120	Bioelectricity, Hearts and Brains. *Undergraduate Lecture Notes in Physics*, **2016**, 253-316	0.1	
119	The Materials of the Living. *Undergraduate Lecture Notes in Physics*, **2016**, 367-421	0.1	
118	Tunneling mechanism and contact mechanics of colloidal nanoparticle assemblies. *Nanotechnology*, **2016**, 27, 475502	3.4	2
117	A biophysical model of cell evolution after cytotoxic treatments: Damage, repair and cell response. *Journal of Theoretical Biology*, **2016**, 389, 146-58	2.3	5
116	On the ability of molecular dynamics simulation and continuum electrostatics to treat interfacial water molecules in protein-protein complexes. *Scientific Reports*, **2016**, 6, 38259	4.9	7
115	Real-time mechanical characterization of DNA degradation under therapeutic X-rays and its theoretical modeling. *Microsystems and Nanoengineering*, **2016**, 2, 16062	7.7	20
114	Shapes of the Living. *Undergraduate Lecture Notes in Physics*, **2016**, 475-526	0.1	
113	The Hidden Mathematics of Living Systems. *Undergraduate Lecture Notes in Physics*, **2016**, 527-572	0.1	
112	Energy, Information, and The Origins of Life. *Undergraduate Lecture Notes in Physics*, **2016**, 61-111	0.1	
111	Energy Production and Storage for Life. *Undergraduate Lecture Notes in Physics*, **2016**, 113-158	0.1	
110	Molecular Motors in the Cell. *Undergraduate Lecture Notes in Physics*, **2016**, 205-252	0.1	0
109	Molecular Mechanics of the Cell. *Undergraduate Lecture Notes in Physics*, **2016**, 317-366	0.1	
108	The Physics of Living Systems. *Undergraduate Lecture Notes in Physics*, **2016**,	0.1	5
107	Length dependence of thermal conductivity by approach-to-equilibrium molecular dynamics. *Physical Review B*, **2016**, 94,	3.3	32
106	Surface-induced optimal packing of two-dimensional molecular networks. *Physical Review Letters*, **2015**, 114, 066101	7.4	37

105	Stochastic mechanical degradation of multi-cracked fiber bundles with elastic and viscous interactions. *European Physical Journal E*, **2015**, 38, 131	1.5	5
104	High Conductance Ratio in Molecular Optical Switching of Functionalized Nanoparticle Self-Assembled Nanodevices. *Journal of Physical Chemistry C*, **2015**, 119, 21173-21183	3.8	13
103	Molecular dynamics of ionic self-diffusion at an MgO grain boundary. *Journal of Materials Science*, **2015**, 50, 2502-2509	4.3	17
102	Kinetic proofreading of chromatin remodeling: from gene activation to gene repression and back. *AIMS Biophysics*, **2015**, 2, 398-411	0.8	3
101	Atomic Scale Modeling of Two-Dimensional Molecular Self-Assembly on a Passivated Si Surface. *Journal of Physical Chemistry C*, **2014**, 118, 12817-12825	3.8	26
100	Scaling shift in multicracked fiber bundles. *Physical Review Letters*, **2014**, 113, 255501	7.4	17
99	DNA i-motif provides steel-like tough ends to chromosomes. *Materials Research Society Symposia Proceedings*, **2014**, 1621, 135-141		
98	On the equivalence of thermodynamics ensembles for flexible polymer chains. *Physica A: Statistical Mechanics and Its Applications*, **2014**, 395, 154-170	3.3	27
97	Structure and mechanical characterization of DNA i-motif nanowires by molecular dynamics simulation. *Biophysical Journal*, **2013**, 105, 2820-31	2.9	12
96	Thermal conductivity from approach-to-equilibrium molecular dynamics. *Journal of Applied Physics*, **2013**, 114, 033525	2.5	68
95	Two-state theory of single-molecule stretching experiments. *Physical Review E*, **2013**, 87,	2.4	28
94	Response to "Comment on SElasticity of flexible and semiflexible polymers with extensible bonds in the Gibbs and Helmholtz ensembles"S[J. Chem. Phys. 138, 157101 (2013)]. *Journal of Chemical Physics*, **2013**, 138, 157102	3.9	11
93	Silicon Nanotweezers with a microfluidic cavity for the real time characterization of DNA damage under therapeutic radiation beams. *Annual International Conference of the IEEE Engineering in Medicine and Biology Society IEEE Engineering in Medicine and Biology Society Annual International Conference*, **2013**, 2013, 6820	0.9	2
92	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	3.9	35
91	A two-phase model of large-strain plasticity in covalent nanostructures. *International Journal of Plasticity*, **2012**, 37, 31-52	7.6	6
90	Elasticity of flexible and semiflexible polymers with extensible bonds in the Gibbs and Helmholtz ensembles. *Journal of Chemical Physics*, **2012**, 136, 154906	3.9	39
89	Thermal boundary resistance at silicon-silica interfaces by molecular dynamics simulations. *Applied Physics Letters*, **2012**, 100, 131906	3.4	52
88	Monte Carlo simulations of single polymer force-extension relations. *Journal of Physics: Conference Series*, **2012**, 383, 012016	0.3	6

87	Interacting Lewis-X carbohydrates in condensed phase: a first-principles molecular dynamics study. *Journal of Physical Chemistry B*, **2011**, 115, 12599-606	3.4	2
86	Exceptional plasticity of silicon nanobridges. *Nanotechnology*, **2011**, 22, 355704	3.4	15
85	Metallographic and Numerical Studies of the Role of Catalyst Particles of MgH2-Mg System. *Defect and Diffusion Forum*, **2010**, 297-301, 263-268	0.7	
84	Atomistic simulation of plasticity in silicon nanowires. *Applied Physics Letters*, **2010**, 97, 153106	3.4	9
83	Interface structure of silicon nanocrystals embedded in an amorphous silica matrix. *Solid State Sciences*, **2010**, 12, 163-171	3.4	18
82	Surface ordering of molecular structures by dispersion forces. *Physical Review B*, **2009**, 80,	3.3	8
81	Atomic-scale modeling of the interaction between short polypeptides and carbon surfaces. *Journal of Physical Chemistry B*, **2009**, 113, 12105-12	3.4	32
80	Turning carbon nanotubes from exceptional heat conductors into insulators. *Physical Review Letters*, **2009**, 102, 105901	7.4	249
79	Energy band and vacuum level alignment at a semiconductor-molecule-metal interface. *Applied Physics Letters*, **2008**, 92, 103112	3.4	5
78	Hydrogen Storage in MgH2 Matrices: An Ab-Initio Study of Mg-MgH2 Interface. *Solid State Phenomena*, **2008**, 139, 23-28	0.4	2
77	Metallographic and numerical characterization of MgH2-Mg system. *Materials Research Society Symposia Proceedings*, **2008**, 1127, 1		
76	Microscopic mechanics of biomolecules in living cells. *Scientific Modeling and Simulation SMNS*, **2008** , 15, 339-362		9
75	Microscopic mechanics of biomolecules in living cells. *Lecture Notes in Computational Science and Engineering*, **2008**, 339-362	0.3	
74	Molecular dynamics simulation of the recrystallization of amorphous Si layers: Comprehensive study of the dependence of the recrystallization velocity on the interatomic potential. *Journal of Applied Physics*, **2007**, 101, 123506	2.5	38
73	Experimental and Theoretical Characterization of the 3D-Dopants Bias on the H Desorption of Mg Hydrides. *Materials Science Forum*, **2007**, 555, 349-354	0.4	6
72	Multiscale modelling of molecular monolayers adsorbed on silicon. *Applied Physics A: Materials Science and Processing*, **2007**, 86, 293-300	2.6	3
71	A Multiscale Approach for Composite Materials as Multifield Continua. *Materials Science Forum*, **2007**, 539-543, 2551-2556	0.4	1
70	Diffusion of boron in silicon: Compatibility of empirical molecular dynamics with continuum simulations. *Europhysics Letters*, **2006**, 76, 842-848	1.6	5

69	Point-defect recombination efficiency at grain boundaries in irradiated SiC. *Physical Review B*, **2006**, 73,	3.3	11
68	Screening and surface states in molecular monolayers adsorbed on silicon. *Journal of Physical Chemistry B*, **2006**, 110, 11496-503	3.4	3
67	What's so special about nanocrystalline semiconductors?. *International Journal of Computational Science and Engineering*, **2006**, 2, 242	0.4	2
66	Phonon instability in nanocrystalline silicon carbide. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 3311-3315	1.3	
65	Atomic-Scale Investigation on Fracture Toughness in Nanocomposite Silicon Carbide **2006**, 41-42		
64	Fracture toughness of nanostructured silicon carbide. *Applied Physics Letters*, **2005**, 87, 141912	3.4	14
63	Crack-tip stress shielding by a hard fiber in β-SiC: an atomistic study. *Computer Physics Communications*, **2005**, 169, 40-43	4.2	
62	Evolution of dislocation cell structures in plastically deformed metals. *Computer Physics Communications*, **2005**, 169, 44-49	4.2	7
61	Atomistic Simulations of Materials Fracture and the Link between Atomic and Continuum Length Scales. *Journal of the American Ceramic Society*, **2005**, 81, 501-516	3.8	55
60	Atomic scale origin of crack resistance in brittle fracture. *Physical Review Letters*, **2005**, 95, 115501	7.4	71
59	Multiscale Modeling of Composite Materials by a Multifield Finite Element Approach. *International Journal for Multiscale Computational Engineering*, **2005**, 3, 463-480	2.4	7
58	Localization and quantization in covalently bonded carbon nanotube junctions. *Physical Review B*, **2004**, 69,	3.3	13
57	Contact resistance in percolating networks. *Physical Review B*, **2004**, 69,	3.3	52
56	Atomistic study of the interaction between a microcrack and a hard inclusion in β-SiC. *Physical Review B*, **2004**, 70,	3.3	22
55	Interaction of benzene thiol and thiolate with small gold clusters. *Journal of Chemical Physics*, **2004**, 120, 10062-8	3.9	38
54	Role of surface chemistry in hydrogen adsorption in single-wall carbon nanotubes. *Chemical Physics Letters*, **2003**, 371, 476-482	2.5	39
53	Chemisorption of atomic hydrogen in graphite and carbon nanotubes. *Surface Science*, **2003**, 544, 24-34	1.8	35
52	Quantum Dots from Carbon Nanotube Junctions. *Materials Research Society Symposia Proceedings*, **2003**, 789, 217		1

51	ab-initio modelling of Mg:H interstitial solid solutions. *Materials Research Society Symposia Proceedings*, **2003**, 801, 120		
50	Microstructure evolution at a triple junction in polycrystalline silicon. *Journal of Physics Condensed Matter*, **2002**, 14, 13003-13008	1.8	7
49	Multiphase microstructure evolution model including dislocation plasticity. *Journal of Materials Research*, **2002**, 17, 1932-1940	2.5	1
48	Atomic hydrogen adsorption on a Stone□Wales defect in graphite. *Surface Science*, **2002**, 496, 33-38	1.8	50
47	Microstructure evolution from the atomic scale up. *Computational Materials Science*, **2002**, 24, 21-27	3.2	12
46	Dedicated hardware for linearly-scaling algorithms in condensed-matter physics. *Computer Physics Communications*, **2001**, 139, 20-33	4.2	
45	Triple Junctions in Polycrystalline Silicon: A Numerical Study Based upon Atomistic Simulations. *Key Engineering Materials*, **2001**, 221-222, 307-314	0.4	1
44	Vibrational modes of graphitic fragments and the nucleation of carbon nanotubes. *Journal of Chemical Physics*, **2001**, 115, 3308-3314	3.9	7
43	Representation of mechanical loads in molecular dynamics simulations. *Physical Review B*, **2001**, 65,	3.3	38
42	Atomic and electronic structure of high-energy grain boundaries in silicon and carbon. *Computational Materials Science*, **2001**, 20, 351-362	3.2	18
41	A molecular dynamics investigation on grain disappearance at a triple junction in polycrystalline silicon. *Materials Research Society Symposia Proceedings*, **2001**, 677, 171		
40	Ab-initio modelling of atomic and molecular Hydrogen adsorption in graphite. *Materials Research Society Symposia Proceedings*, **2001**, 677, 471		1
39	Coupled atomistic-mesoscopic model of polycrystalline plasticity. *Materials Research Society Symposia Proceedings*, **2001**, 677, 761		
38	Vibrational modes of graphitic fragments and the nucleation of carbon nanotubes. *Materials Research Society Symposia Proceedings*, **2000**, 633, 1341		2
37	Defect energetics, thermal stability and localized electronic states in carbon nanotubes. *Materials Research Society Symposia Proceedings*, **2000**, 633, 1481		2
36	Identification of tetrahedrally coordinated atoms in supercooled liquid silicon. *Materials Research Society Symposia Proceedings*, **2000**, 638, 1		
35	Atomistic models of triple junctions and the origin of topological changes in microstructural evolution. *Materials Research Society Symposia Proceedings*, **2000**, 652, 1		
34	A microstructure evolution model including dislocation plasticity. *Materials Research Society Symposia Proceedings*, **2000**, 652, 1		

33	A stochastic grain growth model based on a variational principle for dissipative systems. *Physica A: Statistical Mechanics and Its Applications*, **2000**, 282, 339-354	3.3	25
32	Triple junctions and elastic stability of polycrystalline silicon. *Physical Review B*, **2000**, 63,	3.3	17
31	Solid□quid interface velocity and diffusivity in laser-melt amorphous silicon. *Applied Physics Letters* , **2000**, 77, 2337-2339	3.4	31
30	On the electrical activity of sp 2 -bonded grain boundaries in nanocrystalline diamond. *Europhysics Letters*, **1999**, 46, 671-677	1.6	56
29	Atomistic Simulations of Integranular Fracture in Symmetric-Tilt Grain Boundaries. *Journal of Materials Science*, **1999**, 7, 45-55		21
28	Synthesis and Characterization of a Polycrystalline Ionic Thin Film by Large-Scale Molecular-Dynamics Simulation. *Journal of Materials Science*, **1999**, 7, 15-31		15
27	Correlation between atomic structure and localized gap states in silicon grain boundaries. *Physical Review B*, **1998**, 57, 6247-6250	3.3	32
26	On the Nature of Grain Boundaries in Nanocrystalline Diamond. *MRS Bulletin*, **1998**, 23, 36-41	3.2	48
25	Atomistic Aspects of Fracture Modelling in the Framework of Continuum Mechanics. *Materials Research Society Symposia Proceedings*, **1998**, 538, 441		
24	Atomic-Scale Mechanism of Crack-Tip Plasticity: Dislocation Nucleation and Crack-Tip Shielding. *Physical Review Letters*, **1997**, 79, 1309-1312	7.4	94
23	Structural Disorder and Localized Gap States in Silicon Grain Boundaries from a Tight-Binding Model. *Materials Research Society Symposia Proceedings*, **1997**, 491, 513		
22	Large Scale Atomistic Simulations using the Tight Binding Approach. *Materials Research Society Symposia Proceedings*, **1997**, 491, 481		
21	Comparison Between Atomistic and Continuum-Mechanics Modelling of Grain-Boundary Fracture. *Materials Research Society Symposia Proceedings*, **1997**, 492, 377		
20	Atomistic simulation of dislocation nucleation and motion from a crack tip. *Acta Materialia*, **1997**, 45, 4993-5003	8.4	16
19	Molecular dynamics calculation of the Zr(Ni) enthalpy of mixing. *Applied Physics Letters*, **1996**, 69, 1701-1703	3.4	5
18	Mechanical Instability of Oxidized Metal Clusters. *Physical Review Letters*, **1996**, 77, 2495-2498	7.4	10
17	Lattice instability analysis of a prototype intermetallic system under stress. *Journal of Applied Physics*, **1995**, 77, 1449-1458	2.5	17
16	A Molecular Dynamics Study of the Terminal Zr(Ni) Solid Solutions. *Materials Research Society Symposia Proceedings*, **1995**, 400, 131		

15	Microscopic-scale simulations of macroscopic flow patterns in non-equilibrium two-dimensional systems **1994**, 17, 281-299		
14	Order-disorder transition in Cu3Au: A combined molecular-dynamics and cluster-variation-method approach. *Physical Review B*, **1993**, 47, 14541-14544	3.3	22
13	Tight-binding potentials for transition metals and alloys. *Physical Review B*, **1993**, 48, 22-33	3.3	1625
12	Experimental and theoretical investigation of the order-disorder transformation in Ni3Al. *Journal of Materials Research*, **1993**, 8, 2504-2509	2.5	35
11	Lattice dynamics of ordered and disordered Cu3 Au with a tight-binding potential model. *Philosophical Magazine Letters*, **1993**, 67, 369-378	1	22
10	Phase stability of Ni□Al solid solutions. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1993**, 68, 845-851		6
9	Atomistic Simulation of Crystal-to-Amorphous Transitions in the Intermetallic Alloys NiZr2 and Cu3Au. *Materials Research Society Symposia Proceedings*, **1992**, 278, 87		
8	Order-Disorder Transformation in Cu3Au: A Molecular Dynamics Study. *Materials Research Society Symposia Proceedings*, **1992**, 291, 531		
7	A molecular dynamics simulation of the effects of excess free volume on the diffusion in metallic glasses. *Journal of Non-Crystalline Solids*, **1992**, 144, 187-195	3.9	9
6	The Mach-1 Code for Coupled Neutron, Photon and Electron Transport by the Monte Carlo Method **1992**, 315-322		
5	Analysis of Sample and Fuel Pin Irradiation Experiments in Ph□ix for Basic Nuclear Data Validation. *Nuclear Science and Engineering*, **1990**, 105, 244-255	1.2	14
4	Low-energy photon scattering simulations with the Monte Carlo code ACCEPT. *Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, **1990**, 295, 231-240	1.2	6
3	Deuterium clusters in a strained palladium lattice. *Journal of Materials Research*, **1990**, 5, 2094-2099	2.5	1
2	Stability of the ground state of finite nuclei against neutral pion condensation. *Physical Review C*, **1986**, 34, 1134-1136	2.7	2
1	On the validity of the Hartree approximation and the effect of short-range correlations in □-condensation in finite nuclei. *Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics*, **1984**, 141, 33-36	4.2	6