Sandro Scandolo

List of Publications by Year
in descending order

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147	25,383	53794	10734
papers	citations	45 h-index	138 g-index

148	148	148	25159
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
2	Synthesis of Novel Transition Metal NitridesIrN2andOsN2. Physical Review Letters, 2006, 96, 155501.	7.8	481
3	Superionic and Metallic States of Water and Ammonia at Giant Planet Conditions. Science, 1999, 283, 44-46.	12.6	432
4	Physics of Iron at Earth's Core Conditions. Science, 2000, 287, 1027-1030.	12.6	341
5	X-ray Diffraction and Computation Yield the Structure of Alkanethiols on Gold(111). Science, 2008, 321, 943-946.	12.6	279
6	Nonparabolicity and a sum rule associated with bound-to-bound and bound-to-continuum intersubband transitions in quantum wells. Physical Review B, 1994, 50, 8663-8674.	3.2	271
7	Carbon Phase Diagram fromAb InitioMolecular Dynamics. Physical Review Letters, 2005, 95, 185701.	7.8	206
8	Structure of aCH3SMonolayer on Au(111) Solved by the Interplay between Molecular Dynamics Calculations and Diffraction Measurements. Physical Review Letters, 2007, 98, 016102.	7.8	204
9	An ab initio parametrized interatomic force field for silica. Journal of Chemical Physics, 2002, 117, 8898-8904.	3.0	200
10	Metal Work-Function Changes Induced by Organic Adsorbates: A Combined Experimental and Theoretical Study. Physical Review Letters, 2005, 95, 046804.	7.8	196
11	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	177
12	Pressure-Induced Transformation Path of Graphite to Diamond. Physical Review Letters, 1995, 74, 4015-4018.	7.8	175
13	Liquid-liquid phase transition in compressed hydrogen from first-principles simulations. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 3051-3053.	7.1	158
14	Amorphous silica-like carbon dioxide. Nature, 2006, 441, 857-860.	27.8	153
15	Dissociation of Methane into Hydrocarbons at Extreme (Planetary) Pressure and Temperature. Science, 1997, 275, 1288-1290.	12.6	140
16	First-principle-constant pressure molecular dynamics. Journal of Physics and Chemistry of Solids, 1995, 56, 501-505.	4.0	132
17	Pressure-Induced Solid Carbonates from Molecular CO2 by Computer Simulation. Science, 1999, 284, 788-790.	12.6	127
18	Interstitial dinitrogen makesPtN2an insulating hard solid. Physical Review B, 2006, 73, .	3.2	125

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19	Interchain electron states in polyethylene. Physical Review B, 2000, 62, 4389-4393.	3.2	111
20	Thermal conductivity of solid argon from molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 3765-3769.	3.0	109
21	How well do Carâ€“Parrinello simulations reproduce the Bornâ€“Oppenheimer surface? Theory and examples. Journal of Chemical Physics, 2002, 116, 14.	3.0	107
22	High-pressure polymeric phases of carbon dioxide. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6077-6081.	7.1	104
23	Solid Molecular Hydrogen: The Broken Symmetry Phase. Physical Review Letters, 1997, 78, 2783-2786.	7.8	94
24	Pressure-Induced Structural Changes in LiquidSiO2fromAb InitioSimulations. Physical Review Letters, 2002, 89, 245504.	7.8	91
25	Mechanical strength and coordination defects in compressed silica glass: Molecular dynamics simulations. Physical Review B, 2007, 75, .	3.2	91
26	Dispersion relations and sum rules in nonlinear optics. Physical Review B, 1991, 44, 8446-8453.	3.2	90
27	OsN2: Crystal structure and electronic properties. Applied Physics Letters, 2007, 90, 011909.	3.3	87
28	Surface States and Negative Electron Affinity in Polyethylene. Physical Review Letters, 2001, 87, 076802.	7.8	86
29	Pressure-Induced Magnetic Collapse and Metallization of Molecular Oxygen: TheÎ¶-O2Phase. Physical Review Letters, 1998, 80, 5160-5163.	7.8	79
30	Decomposition and Polymerization of Solid Carbon Monoxide under Pressure. Physical Review Letters, 1998, 81, 2092-2095.	7.8	76
31	Charge-density waves and surface Mott insulators for adlayer structures on semiconductors: Extended Hubbard modeling. Physical Review B, 1999, 59, 1891-1901.	3.2	76
32	Thermal conductivity of crystalline quartz from classical simulations. Physical Review B, 2004, 70, .	3.2	71
33	Electronic properties of metalâ€“moleculeâ€“metal systems at zero bias: A periodic density functional study. Journal of Chemical Physics, 2003, 119, 6729-6735.	3.0	65
34	Partially collapsed cristobalite structure in the non molecular phase V in CO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5176-5179.	7.1	63
35	A Dynamic Landscape from Femtoseconds to Minutes for Excess Electrons at Iceâ^'Metal Interfaces. Journal of Physical Chemistry C, 2009, 113, 979-988.	3.1	61
36	Interfacial Electrostatics of Self-Assembled Monolayers of Alkane Thiolates on Au(111):Â Work Function Modification and Molecular Level Alignments. Journal of Physical Chemistry B, 2006, 110, 10862-10872.	2.6	57

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37	High-pressure crystalline polyethylene studied by x-ray diffraction andab initiosimulations. Physical Review B, 2007, 75, .	3.2	56
38	Infrared and Raman spectra of silica polymorphs from anab initioparametrized polarizable force field. Journal of Chemical Physics, 2006, 125, 194524.	3.0	54
39	SC4: A metallic phase of carbon at terapascal pressures. Physical Review B, 1996, 53, 5051-5054.	3.2	53
40	Ab initiopseudopotential study of vacancies and self-interstitials in hcp titanium. Philosophical Magazine, 2009, 89, 1629-1645.	1.6	50
41	Structure and Dynamics of Low-Density and High-Density Liquid Water at High Pressure. Journal of Physical Chemistry Letters, 2014, 5, 235-240.	4.6	50
42	Mixed Threefold and Fourfold Carbon Coordination in Compressed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 100, 163002.	7.8	48
43	Dipole-Quadrupole Interactions and the Nature of Phase III of Compressed Hydrogen. Physical Review Letters, 1999, 83, 4097-4100.	7.8	46
44	Surface Trapped Excess Electrons on Ice. Physical Review Letters, 2005, 95, 176801.	7.8	46
45	Competition of Charge-Density Waves and Superconductivity in Sulfur. Physical Review Letters, 2007, 99, 155505.	7.8	46
46	The mechanism for the 3Ã—3 distortion of Sn/Ge(111). Surface Science, 2000, 454-456, 172-177.	1.9	43
47	High-pressure phases of crystalline tellurium: A combined Raman andab initiostudy. Physical Review B, 2012, 86, .	3.2	42
48	First-principles study of density, viscosity, and diffusion coefficients of liquid MgSiO3at conditions of the Earth's deep mantle. Journal of Geophysical Research, 2007, 112, .	3.3	40
49	Trapping of excitons at chemical defects in polyethylene. Journal of Chemical Physics, 2004, 121, 6478-6484.	3.0	39
50	Far-infrared absorption of water clusters by first-principles molecular dynamics. Journal of Chemical Physics, 2008, 128, 214506.	3.0	39
51	Ab initio theory of planetary materials. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	37
52	Disproportionation Phenomena on Free and StrainedSn/Ge(111)andSn/Si(111)Surfaces. Physical Review Letters, 2002, 89, 126803.	7.8	36
53	Tuning Oxygen Packing in Silica by Nonhydrostatic Pressure. Physical Review Letters, 2007, 99, 215504.	7.8	34
54	Self-trapping vs. non-trapping of electrons and holes in organic insulators: polyethylene. Chemical Physics Letters, 2002, 360, 487-493.	2.6	33

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55	A many-body interatomic potential for ionic systems: Application to MgO. Journal of Chemical Physics, 2003, 119, 9673-9685.	3.0	33
56	Kramers-Kronig relations and sum rules for the second-harmonic susceptibility. Physical Review B, 1995, 51, 6925-6927.	3.2	32
57	Dynamical and thermal properties of polyethylene by ab initio simulation. Chemical Physics Letters, 2000, 331, 339-345.	2.6	32
58	SiC(0001):â€‚â€‚A surface Mott-Hubbard insulator. Physical Review B, 2000, 61, 1752-1755.	3.2	32
59	Noncolinear spin polarization from frustrated antiferromagnetism: A possible scenario for molecular oxygen at high pressure. Physical Review B, 2000, 61, 6145-6149.	3.2	31
60	Thermal conductivity of solid argon at high pressure and high temperature:â€‚A molecular dynamics study. Journal of Chemical Physics, 2004, 121, 11177.	3.0	31
61	Finite-Temperature Effects on the Stability and Infrared Spectra of HCl(H₂O)₆ Clusters. Journal of Physical Chemistry A, 2007, 111, 12810-12815.	2.5	31
62	Computational materials science meets geophysics: dislocations and slip planes of MgO. Computer Physics Communications, 2005, 169, 24-27.	7.5	30
63	Exciton self-trapping in bulk polyethylene. Journal of Physics Condensed Matter, 2005, 17, 4621-4627.	1.8	27
64	Polarizable interatomic force field for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> using density functional theory. Physical Review B, 2010, 81, .	3.2	27
65	Thermodynamic stability of layered structures in compressed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2009, 79, .	3.2	26
66	Ab initio parameterization of an all-atom polarizable and dissociable force field for water. Journal of Chemical Physics, 2012, 136, 114511.	3.0	26
67	Elasticity and mechanical instabilities of diamond at megabar stresses: Implications for diamond-anvil-cell research. Applied Physics Letters, 1999, 75, 487-488.	3.3	25
68	Atomic and electronic structure of ideal and reconstructedÎ±-Sn (100) surfaces. Physical Review B, 1998, 58, 13698-13711.	3.2	24
69	High-pressure vibrational properties of polyethylene. Journal of Chemical Physics, 2010, 133, 204502.	3.0	24
70	Dimerization of CO2 at High Pressure and Temperature. ChemPhysChem, 2005, 6, 1752-1756.	2.1	22
71	Mixtures of planetary ices at extreme conditions. Nature Communications, 2011, 2, 185.	12.8	22
72	Nonlinear sum rules: The three-level and the anharmonic-oscillator models. Physical Review B, 1992, 45, 13257-13261.	3.2	21

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73	Metallic charge density waves and surface Mott insulators for adlayer structures on semiconductors: extended Hubbard modeling. Surface Science, 1998, 402-404, 802-807.	1.9	21
74	First principles calculations of charge and spin density waves of -adsorbates on semiconductors. Surface Science, 1998, 402-404, 808-812.	1.9	21
75	3Ã—3R30Â°versus adatomâ€“rest-atom phases on (111) semiconductor surfaces. Physical Review B, 2000, 61, R13345-R13348.	3.2	21
76	Collective spin 1 singlet phase in high-pressure oxygen. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10427-10432.	7.1	21
77	Millerâ€™s rule and the static limit for second-harmonic generation. Physical Review B, 1995, 51, 6928-6931.	3.2	20
78	Titaniaâ€“Silica Interfaces. Journal of Physical Chemistry C, 2012, 116, 11062-11067.	3.1	20
79	Connecting the Water Phase Diagram to the Metastable Domain: High-Pressure Studies in the Supercooled Regime. Journal of Physical Chemistry Letters, 2014, 5, 3804-3809.	4.6	20
80	Temperature-induced densification of compressed SiO₂glass: A molecular dynamics study. High Pressure Research, 2008, 28, 35-44.	1.2	19
81	First-principles investigation of the electron-phonon interaction in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Os</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: Theoretical prediction of superconductivity mediated by N-N covalent bonds. Physical Review B, 2008, 77, .	3.2	17
82	SixC1â^'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	1.9	16
83	Melting slope of MgO from molecular dynamics and density functional theory. Journal of Chemical Physics, 2009, 131, 124510.	3.0	16
84	Pressure Dependence of Hydrogen-Bond Dynamics in Liquid Water Probed by Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 3579-3584.	4.6	16
85	Infrared absorption of MgO at high pressures and temperatures: A molecular dynamic study. Journal of Chemical Physics, 2009, 131, 014506.	3.0	15
86	Free electron to electride transition in dense liquid potassium. Nature Physics, 2021, 17, 955-960.	16.7	15
87	Far-infrared spectrum of ice Ih: A first-principles study. Physical Review B, 2011, 84, .	3.2	14
88	A Molecular Dynamics Study of the Role of Adatoms in SAMs of Methylthiolate on Au(111): A New Force Field Parameterized from Ab Initio Calculations. Journal of Physical Chemistry C, 2012, 116, 14883-14891.	3.1	14
89	Interband nearâ€infrared secondâ€harmonic generation with very large â€–Ï‡(2)(2Ï‰)â€– in AlSb/GaSbâ€InAsSb/AlSb asymmetric quantum wells. Applied Physics Letters, 1993, 62, 3138-3140.	3.3	13
90	Organic molecular crystals in electric fields. Surface Science, 2004, 566-568, 644-649.	1.9	13

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91	Stability of Diamond at Megabar Pressures. Physica Status Solidi (B): Basic Research, 1996, 198, 447-453.	1.5	12
92	Theoretical Evidence for a Reentrant Phase Diagram in Ortho-Para Mixtures of SolidH2at High Pressure. Physical Review Letters, 2005, 94, 125503.	7.8	12
93	Gypsum under pressure: A first-principles study. Physical Review B, 2010, 81, .	3.2	12
94	Interchain states and the negative electron affinity of polyethylene. , 0, , .		11
95	Intrinsic defects and krypton impurity atoms in hcp titanium: A first-principles study. Physical Review B, 2011, 83, .	3.2	11
96	A computational study of elastic properties of disordered systems with voids. Journal of Non-Crystalline Solids, 2006, 352, 4283-4286.	3.1	10
97	Ab Initio Simulations of Copper Oxide Nanowires and Clusters on TiO₂ (101) Anatase Surface. Journal of Physical Chemistry C, 2017, 121, 20359-20365.	3.1	10
98	AbÂinitio Determination of the Phase Diagram of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> at High Pressures and Temperatures. Physical Review Letters, 2020, 124, 095701.	7.8	10
99	High-pressure transformations in liquid rubidium. Physical Review Materials, 2020, 4, .	2.4	10
100	Sum Rules for Nonlinear Optical Susceptibilities. Physica Status Solidi (B): Basic Research, 1992, 173, 263-270.	1.5	9
101	Atomic and electronic structure of ideal and reconstructed Î±-Sn (111) surface. Physical Review B, 1996, 54, 11769-11776.	3.2	9
102	Universal constraints for the third-harmonic generation susceptibility. Journal of Physics Condensed Matter, 1996, 8, 6997-7004.	1.8	9
103	Optical Bistability Induced by Charge Separation in Asymmetric Quantum Wells. Physica Status Solidi (B): Basic Research, 1992, 173, 453-458.	1.5	8
104	CCl4 dissociation on the ice Ih surface: an excess electron mediated process. Physical Chemistry Chemical Physics, 2010, 12, 13034.	2.8	8
105	Dislocation properties of coesite from anab-initioparametrized interatomic potential. Physical Review B, 2011, 83, .	3.2	8
106	Probing the structure of iron at extreme conditions by X-ray absorption near-edge structure calculations. High Pressure Research, 2013, 33, 119-123.	1.2	7
107	Multiple pathways in pressure-induced phase transition of coesite. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12894-12899.	7.1	7
108	Squeezing Oil into Water under Pressure: Inverting the Hydrophobic Effect. Journal of Physical Chemistry Letters, 2020, 11, 4826-4833.	4.6	7

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109	The Centers of Planets. American Scientist, 2003, 91, 516.	0.1	7
110	An Effective Pseudopotential for Modeling Gold Surface Slabs for Ab Initio Simulations. ChemPhysChem, 2005, 6, 1756-1760.	2.1	6
111	Ab initio study of Kr in hcp Ti: Diffusion, formation and stability of small Krâ€“vacancy clusters. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 2991-2994.	1.4	6
112	Atomistic pathways of the pressure-induced densification of quartz. Physical Review B, 2015, 92, .	3.2	6
113	Diamonds in the sky?. Physics World, 2000, 13, 31-36.	0.0	5
114	Structural properties and phase transitions in a silica clathrate. Journal of Chemical Physics, 2011, 134, 074506.	3.0	5
115	Titaniaâ€“silica mixed oxides investigated with density functional theory and molecular dynamics simulations. Physica Status Solidi (B): Basic Research, 2017, 254, 1600510.	1.5	5
116	Density Functional Theory Study of Water Photo-Oxidation at Copper Oxide Nanostructures on the Anatase (101) Surface. Journal of Physical Chemistry C, 2018, 122, 16765-16771.	3.1	5
117	Ab initio study of the LiH phase diagram at extreme pressures and temperatures. Physical Review B, 2019, 99, .	3.2	5
118	Optimal basis set for electronic structure calculations in periodic systems. Physical Review B, 2000, 62, 15499-15504.	3.2	4
119	Surface charge density waves and the Mott insulators for adlayers on semiconductor surfaces. Computational Materials Science, 2001, 20, 343-350.	3.0	4
120	Spatial-dispersion and relativistic effects in the optical sum rules. European Physical Journal B, 2001, 23, 319-323.	1.5	4
121	Magnetism and vibrations in the phase of oxygen. Solid State Communications, 2009, 149, 160-162.	1.9	4
122	Material progress in Africa. Nature Physics, 2010, 6, 830-832.	16.7	4
123	Defects in ion-implanted hcp-titanium: A first-principles study of electronic structures. Solid State Communications, 2011, 151, 1889-1893.	1.9	4
124	Theoretical X-ray absorption near-edge structure signatures of solid and liquid phases of iron at extreme conditions. High Pressure Research, 2014, 34, 250-258.	1.2	4
125	Ab-initio calculation of formation and migration energies of intrinsic defects in BaF2. Solid State Communications, 2014, 179, 25-28.	1.9	4
126	Excess electrons in ice: a density functional theory study. Physical Chemistry Chemical Physics, 2014, 16, 3103.	2.8	4

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127	Machine learning provides realistic model of complex phase transition. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10204-10205.	7.1	4
128	Spectroscopic fingerprints of a surface Mottâ€“Hubbard insulator: the case of SiC(0001). Surface Science, 2000, 454-456, 534-538.	1.9	3
129	An atomistic model of MgSiO3 perovskite and post-perovskite phases. Computational Materials Science, 2017, 126, 351-359.	3.0	3
130	How to determine solubility in binary mixtures from neutron scattering data: The case of methane and water. Journal of Chemical Physics, 2022, 156, 054502.	3.0	3
131	Tuning heterojunction band offsets by interface Î´-doping. , 1993, , .		2
132	Orientational Ordering of orthoâ€“para Mixtures of Crystals of Homonuclear Diatomic Molecules: Theoretical Evidence for Reentrance. Journal of Low Temperature Physics, 2005, 139, 753-763.	1.4	2
133	Decomposition of methane hydrates at high pressure: a density-fuctional theory study. High Pressure Research, 2015, 35, 231-238.	1.2	2
134	Phase diagram of oxygen at extreme pressure and temperature conditions: An ab initio study. Physical Review B, 2018, 98, .	3.2	2
135	Two-state model for critical points and the negative slope of the melting curve. Physical Review B, 2021, 104, .	3.2	2
136	Solid molecular phases of Hydrogen via constant-pressure first-principles Molecular Dynamics. Materials Research Society Symposia Proceedings, 1997, 499, 329.	0.1	1
137	Molecular simulations break the ice. Physics World, 2002, 15, 25-26.	0.0	1
138	Growing Materials Science in Africa â€“ The Case of the African School for Electronic Structure Methods and Applications (ASESMA). MRS Advances, 2018, 3, 2183-2201.	0.9	1
139	Raman frequencies of diamond under non-hydrostatic pressure. Applied Physics Letters, 2021, 119, 211902.	3.3	1
140	Very large |x(2)(2w)| in the near infrared in AlSb/GaSb-InAsSb/AlSb asymmetric quantum wells. , 1993, , .		0
141	Theory of the 2 x 2 and 3 x 3 reconstructions of the Î±-sn(111) surface. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1998, 20, 1013-1018.	0.4	0
142	Back to square one for superfluidity. Physics World, 2004, 17, 18-19.	0.0	0
143	Oxides under pressure: from densified silica to the rheology of the Earth's mantle. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c55-c55.	0.3	0
144	First-Principles Molecular Dynamics and Applications in Planetary Science. NATO Science for Peace and Security Series B: Physics and Biophysics, 2010, , 353-356.	0.3	0

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145	Microscopic mechanisms of the pressure-induced amorphization of SiO₂. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C76-C76.	0.1	0
146	Lightsources for Africa, the Americas and Middle East Project (LAAMP). Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1069-C1069.	0.1	0
147	FAST training programme at synchrotron facilities by IUPAPâ€“IUCr LAAAMP project. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e169-e169.	0.1	0