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	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
2	Free electron to electride transition in dense liquid potassium. Nature Physics, 2021, 17, 955-960.	16.7	15
3	Two-state model for critical points and the negative slope of the melting curve. Physical Review B, 2021, 104, .	3.2	2
4	Raman frequencies of diamond under non-hydrostatic pressure. Applied Physics Letters, 2021, 119, 211902.	3.3	1
5	Squeezing Oil into Water under Pressure: Inverting the Hydrophobic Effect. Journal of Physical Chemistry Letters, 2020, 11, 4826-4833.	4.6	7
6	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
7	High-pressure transformations in liquid rubidium. Physical Review Materials, 2020, 4, .	2.4	10
8	Ab initio study of the LiH phase diagram at extreme pressures and temperatures. Physical Review B, 2019, 99, .	3.2	5
9	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
10	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
11	Phase diagram of oxygen at extreme pressure and temperature conditions: An ab initio study. Physical Review B, 2018, 98, .	3.2	2
12	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
13	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
14	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
15	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
16	An atomistic model of MgSiO3 perovskite and post-perovskite phases. Computational Materials Science, 2017, 126, 351-359.	3.0	3
17	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
18	Microscopic mechanisms of the pressure-induced amorphization of SiO₂. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C76-C76.	0.1	0

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19	Lightsources for Africa, the Americas and Middle East Project (LAAMP). Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1069-C1069.	0.1	0
20	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
21	Decomposition of methane hydrates at high pressure: a density-fuctional theory study. High Pressure Research, 2015, 35, 231-238.	1.2	2
22	Atomistic pathways of the pressure-induced densification of quartz. Physical Review B, 2015, 92, .	3.2	6
23	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
24	Ab-initio calculation of formation and migration energies of intrinsic defects in BaF2. Solid State Communications, 2014, 179, 25-28.	1.9	4
25	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
26	Excess electrons in ice: a density functional theory study. Physical Chemistry Chemical Physics, 2014, 16, 3103.	2.8	4
27	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
28	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
29	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
30	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
31	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
32	Ab initio parameterization of an all-atom polarizable and dissociable force field for water. Journal of Chemical Physics, 2012, 136, 114511.	3.0	26
33	High-pressure phases of crystalline tellurium: A combined Raman andab initiostudy. Physical Review B, 2012, 86, .	3.2	42
34	Titaniaâ€“Silica Interfaces. Journal of Physical Chemistry C, 2012, 116, 11062-11067.	3.1	20
35	Dislocation properties of coesite from anab-initioparametrized interatomic potential. Physical Review B, 2011, 83, .	3.2	8
36	Mixtures of planetary ices at extreme conditions. Nature Communications, 2011, 2, 185.	12.8	22

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37	Defects in ion-implanted hcp-titanium: A first-principles study of electronic structures. Solid State Communications, 2011, 151, 1889-1893.	1.9	4
38	Structural properties and phase transitions in a silica clathrate. Journal of Chemical Physics, 2011, 134, 074506.	3.0	5
39	Intrinsic defects and krypton impurity atoms in hcp titanium: A first-principles study. Physical Review B, 2011, 83, .	3.2	11
40	Far-infrared spectrum of ice Ih: A first-principles study. Physical Review B, 2011, 84, .	3.2	14
41	Material progress in Africa. Nature Physics, 2010, 6, 830-832.	16.7	4
42	Gypsum under pressure: A first-principles study. Physical Review B, 2010, 81, .	3.2	12
43	High-pressure vibrational properties of polyethylene. Journal of Chemical Physics, 2010, 133, 204502.	3.0	24
44	CCl4 dissociation on the ice Ih surface: an excess electron mediated process. Physical Chemistry Chemical Physics, 2010, 12, 13034.	2.8	8
45	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
46	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
47	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
48	Infrared absorption of MgO at high pressures and temperatures: A molecular dynamic study. Journal of Chemical Physics, 2009, 131, 014506.	3.0	15
49	Melting slope of MgO from molecular dynamics and density functional theory. Journal of Chemical Physics, 2009, 131, 124510.	3.0	16
50	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
51	Magnetism and vibrations in the phase of oxygen. Solid State Communications, 2009, 149, 160-162.	1.9	4
52	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
53	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
54	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

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55	Ab initiopseudopotential study of vacancies and self-interstitials in hcp titanium. Philosophical Magazine, 2009, 89, 1629-1645.	1.6	50
56	X-ray Diffraction and Computation Yield the Structure of Alkanethiols on Gold(111). Science, 2008, 321, 943-946.	12.6	279
57	Temperature-induced densification of compressed SiO₂glass: A molecular dynamics study. High Pressure Research, 2008, 28, 35-44.	1.2	19
58	Far-infrared absorption of water clusters by first-principles molecular dynamics. Journal of Chemical Physics, 2008, 128, 214506.	3.0	39
59	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>.	7.8	48
60	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
61	Competition of Charge-Density Waves and Superconductivity in Sulfur. Physical Review Letters, 2007, 99, 155505.	7.8	46
62	Tuning Oxygen Packing in Silica by Nonhydrostatic Pressure. Physical Review Letters, 2007, 99, 215504.	7.8	34
63	Mechanical strength and coordination defects in compressed silica glass: Molecular dynamics simulations. Physical Review B, 2007, 75, .	3.2	91
64	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
65	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
66	OsN2: Crystal structure and electronic properties. Applied Physics Letters, 2007, 90, 011909.	3.3	87
67	SixC1â^'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	1.9	16
68	High-pressure crystalline polyethylene studied by x-ray diffraction andab initiosimulations. Physical Review B, 2007, 75, .	3.2	56
69	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
70	Infrared and Raman spectra of silica polymorphs from anab initioparametrized polarizable force field. Journal of Chemical Physics, 2006, 125, 194524.	3.0	54
71	Synthesis of Novel Transition Metal NitridesIrN2andOsN2. Physical Review Letters, 2006, 96, 155501.	7.8	481
72	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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73	A computational study of elastic properties of disordered systems with voids. Journal of Non-Crystalline Solids, 2006, 352, 4283-4286.	3.1	10
74	Amorphous silica-like carbon dioxide. Nature, 2006, 441, 857-860.	27.8	153
75	Interstitial dinitrogen makesPtN2an insulating hard solid. Physical Review B, 2006, 73, .	3.2	125
76	Carbon Phase Diagram fromAb InitioMolecular Dynamics. Physical Review Letters, 2005, 95, 185701.	7.8	206
77	An Effective Pseudopotential for Modeling Gold Surface Slabs for Ab Initio Simulations. ChemPhysChem, 2005, 6, 1756-1760.	2.1	6
78	Dimerization of CO2 at High Pressure and Temperature. ChemPhysChem, 2005, 6, 1752-1756.	2.1	22
79	Computational materials science meets geophysics: dislocations and slip planes of MgO. Computer Physics Communications, 2005, 169, 24-27.	7.5	30
80	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
81	Theoretical Evidence for a Reentrant Phase Diagram in Ortho-Para Mixtures of SolidH2at High Pressure. Physical Review Letters, 2005, 94, 125503.	7.8	12
82	Surface Trapped Excess Electrons on Ice. Physical Review Letters, 2005, 95, 176801.	7.8	46
83	Exciton self-trapping in bulk polyethylene. Journal of Physics Condensed Matter, 2005, 17, 4621-4627.	1.8	27
84	Metal Work-Function Changes Induced by Organic Adsorbates: A Combined Experimental and Theoretical Study. Physical Review Letters, 2005, 95, 046804.	7.8	196
85	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	177
86	Ab initio theory of planetary materials. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	37
87	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
88	Thermal conductivity of solid argon from molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 3765-3769.	3.0	109
89	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
90	Trapping of excitons at chemical defects in polyethylene. Journal of Chemical Physics, 2004, 121, 6478-6484.	3.0	39

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91	Organic molecular crystals in electric fields. Surface Science, 2004, 566-568, 644-649.	1.9	13
92	Thermal conductivity of crystalline quartz from classical simulations. Physical Review B, 2004, 70, .	3.2	71
93	Back to square one for superfluidity. Physics World, 2004, 17, 18-19.	0.0	0
94	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
95	A many-body interatomic potential for ionic systems: Application to MgO. Journal of Chemical Physics, 2003, 119, 9673-9685.	3.0	33
96	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
97	The Centers of Planets. American Scientist, 2003, 91, 516.	0.1	7
98	Disproportionation Phenomena on Free and StrainedSn/Ge(111)andSn/Si(111)Surfaces. Physical Review Letters, 2002, 89, 126803.	7.8	36
99	Molecular simulations break the ice. Physics World, 2002, 15, 25-26.	0.0	1
100	Pressure-Induced Structural Changes in LiquidSiO2fromAb InitioSimulations. Physical Review Letters, 2002, 89, 245504.	7.8	91
101	How well do Carâ€“Parrinello simulations reproduce the Bornâ€“Oppenheimer surface? Theory and examples. Journal of Chemical Physics, 2002, 116, 14.	3.0	107
102	An ab initio parametrized interatomic force field for silica. Journal of Chemical Physics, 2002, 117, 8898-8904.	3.0	200
103	Self-trapping vs. non-trapping of electrons and holes in organic insulators: polyethylene. Chemical Physics Letters, 2002, 360, 487-493.	2.6	33
104	Surface charge density waves and the Mott insulators for adlayers on semiconductor surfaces. Computational Materials Science, 2001, 20, 343-350.	3.0	4
105	Spatial-dispersion and relativistic effects in the optical sum rules. European Physical Journal B, 2001, 23, 319-323.	1.5	4
106	Surface States and Negative Electron Affinity in Polyethylene. Physical Review Letters, 2001, 87, 076802.	7.8	86
107	Diamonds in the sky?. Physics World, 2000, 13, 31-36.	0.0	5
108	Dynamical and thermal properties of polyethylene by ab initio simulation. Chemical Physics Letters, 2000, 331, 339-345.	2.6	32

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109	Physics of Iron at Earth's Core Conditions. Science, 2000, 287, 1027-1030.	12.6	341
110	Optimal basis set for electronic structure calculations in periodic systems. Physical Review B, 2000, 62, 15499-15504.	3.2	4
111	Interchain electron states in polyethylene. Physical Review B, 2000, 62, 4389-4393.	3.2	111
112	3Ã—3R30Â°versus adatomâ€“rest-atom phases on (111) semiconductor surfaces. Physical Review B, 2000, 61, R13345-R13348.	3.2	21
113	The mechanism for the 3Ã—3 distortion of Sn/Ge(111). Surface Science, 2000, 454-456, 172-177.	1.9	43
114	Spectroscopic fingerprints of a surface Mottâ€“Hubbard insulator: the case of SiC(0001). Surface Science, 2000, 454-456, 534-538.	1.9	3
115	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
116	SiC(0001):â€‚â€‚A surface Mott-Hubbard insulator. Physical Review B, 2000, 61, 1752-1755.	3.2	32
117	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
118	Dipole-Quadrupole Interactions and the Nature of Phase III of Compressed Hydrogen. Physical Review Letters, 1999, 83, 4097-4100.	7.8	46
119	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
120	Superionic and Metallic States of Water and Ammonia at Giant Planet Conditions. Science, 1999, 283, 44-46.	12.6	432
121	Pressure-Induced Solid Carbonates from Molecular CO2 by Computer Simulation. Science, 1999, 284, 788-790.	12.6	127
122	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
123	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
124	First principles calculations of charge and spin density waves of -adsorbates on semiconductors. Surface Science, 1998, 402-404, 808-812.	1.9	21
125	Atomic and electronic structure of ideal and reconstructedÎ±-Sn (100) surfaces. Physical Review B, 1998, 58, 13698-13711.	3.2	24
126	Pressure-Induced Magnetic Collapse and Metallization of Molecular Oxygen: TheÎ¶-O2Phase. Physical Review Letters, 1998, 80, 5160-5163.	7.8	79

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127	Decomposition and Polymerization of Solid Carbon Monoxide under Pressure. Physical Review Letters, 1998, 81, 2092-2095.	7.8	76
128	Solid Molecular Hydrogen: The Broken Symmetry Phase. Physical Review Letters, 1997, 78, 2783-2786.	7.8	94
129	Solid molecular phases of Hydrogen via constant-pressure first-principles Molecular Dynamics. Materials Research Society Symposia Proceedings, 1997, 499, 329.	0.1	1
130	Dissociation of Methane into Hydrocarbons at Extreme (Planetary) Pressure and Temperature. Science, 1997, 275, 1288-1290.	12.6	140
131	Stability of Diamond at Megabar Pressures. Physica Status Solidi (B): Basic Research, 1996, 198, 447-453.	1.5	12
132	Atomic and electronic structure of ideal and reconstructed Î±-Sn (111) surface. Physical Review B, 1996, 54, 11769-11776.	3.2	9
133	Universal constraints for the third-harmonic generation susceptibility. Journal of Physics Condensed Matter, 1996, 8, 6997-7004.	1.8	9
134	SC4: A metallic phase of carbon at terapascal pressures. Physical Review B, 1996, 53, 5051-5054.	3.2	53
135	First-principle-constant pressure molecular dynamics. Journal of Physics and Chemistry of Solids, 1995, 56, 501-505.	4.0	132
136	Pressure-Induced Transformation Path of Graphite to Diamond. Physical Review Letters, 1995, 74, 4015-4018.	7.8	175
137	Millerâ€™s rule and the static limit for second-harmonic generation. Physical Review B, 1995, 51, 6928-6931.	3.2	20
138	Kramers-Kronig relations and sum rules for the second-harmonic susceptibility. Physical Review B, 1995, 51, 6925-6927.	3.2	32
139	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
140	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
141	Very large |x(2)(2w)| in the near infrared in AlSb/GaSb-InAsSb/AlSb asymmetric quantum wells. , 1993, , .		0
142	Tuning heterojunction band offsets by interface Î´-doping. , 1993, , .		2
143	Nonlinear sum rules: The three-level and the anharmonic-oscillator models. Physical Review B, 1992, 45, 13257-13261.	3.2	21
144	Sum Rules for Nonlinear Optical Susceptibilities. Physica Status Solidi (B): Basic Research, 1992, 173, 263-270.	1.5	9

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145	Optical Bistability Induced by Charge Separation in Asymmetric Quantum Wells. Physica Status Solidi (B): Basic Research, 1992, 173, 453-458.	1.5	8
146	Dispersion relations and sum rules in nonlinear optics. Physical Review B, 1991, 44, 8446-8453.	3.2	90
147	Interchain states and the negative electron affinity of polyethylene. , 0, , .		11