Gianni Profeta

List of Publications by Year
in descending order

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111 papers	4,211 citations	136740 32 h-index	118652 62 g-index
111 all docs	111 docs citations	111 times ranked	3611 citing authors

#	Article	IF	Citations
1	Phonon-mediated superconductivity in graphene by lithium deposition. Nature Physics, 2012, 8, 131-134.	6.5	431
2	Ab initiotheory of superconductivity. I. Density functional formalism and approximate functionals. Physical Review B, 2005, 72, .	1.1	314
3	A perspective on conventional high-temperature superconductors at high pressure: Methods and materials. Physics Reports, 2020, 856, 1-78.	10.3	304
4	Ab initiotheory of superconductivity. II. Application to elemental metals. Physical Review B, 2005, 72, .	1.1	261
5	AbÂInitioDescription of High-Temperature Superconductivity in Dense Molecular Hydrogen. Physical Review Letters, 2008, 100, 257001.	2.9	199
6	Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study. Physical Review Letters, 2006, 96, 047003.	2.9	159
7	Superconducting Properties ofMgB2from First Principles. Physical Review Letters, 2005, 94, 037004.	2.9	137
8	Electronic and structural properties of superconductingMgB2,CaSi2,and related compounds. Physical Review B, 2001, 64, .	1.1	135
9	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. Physical Review B, 2016, 93, .	1.1	125
10	Adiabatic and nonadiabatic phonon dispersion in a Wannier function approach. Physical Review B, 2010, 82, .	1.1	108
11	Anisotropic gap of superconductingCaC6: A first-principles density functional calculation. Physical Review B, 2007, 75, .	1.1	101
12	Intercalant and Intermolecular Phonon Assisted Superconductivity in K-Doped Picene. Physical Review Letters, 2011, 107, 137006.	2.9	79
13	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
14	Triangular Mott-Hubbard Insulator Phases ofSn/Si(111)andSn/Ge(111)Surfaces. Physical Review Letters, 2007, 98, 086401.	2.9	72
15	Electronic and geometric structure of graphene/SiC(0001) decoupled by lithium intercalation. Physical Review B, 2015, 91, .	1.1	56
16	Phonon and electron-phonon renormalization in Al-dopedMgB2. Physical Review B, 2003, 68, .	1.1	53
17	Transition metal impurities in Ge: Chemical trends and codoping studied by electronic structure calculations. Physical Review B, 2006, 73, .	1.1	52
18	X-ray absorption spectroscopy in MnxGe1â^'x diluted magnetic semiconductor: Experiment and theory. Applied Physics Letters, 2005, 86, 062501.	1.5	48

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19	Interplay between structure and superconductivity: Metastable phases of phosphorus under pressure. Physical Review Materials, 2017, 1, .	0.9	48
20	The amplification of the superconducting T c by combined effect of tuning of the Fermi level and the tensile micro-strain in Al 1 â^' x Mg x B 2. Europhysics Letters, 2002, 58, 278-284.	0.7	47
21	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I. Electronic and dynamical properties under pressure. Physical Review B, 2010, 81, .	1.1	47
22	Competition of Charge-Density Waves and Superconductivity in Sulfur. Physical Review Letters, 2007, 99, 155505.	2.9	46
23	Superconducting properties of MgB2 from first principles. Physica C: Superconductivity and Its Applications, 2007, 456, 45-53.	0.6	46
24	Evidence for Gap Anisotropy in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CaC</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:math>from Directional Point-Contact Spectroscopy. Physical Review Letters, 2008, 100, 207004.	2.9	46
25	Superconducting pairing mediated by spin fluctuations from first principles. Physical Review B, 2014, 90, .	1.1	46
26	Structural and magnetic properties of CaFe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>As<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mro	1.1	44
27	Evolution of electronic structure of few-layer phosphorene from angle-resolved photoemission spectroscopy of black phosphorous. Physical Review B, 2016, 94, .	1.1	44
28	Ab initioprediction of pressure-induced superconductivity in potassium. Physical Review B, 2006, 73, .	1.1	41
29	Retention of the Tetragonal to Orthorhombic Structural Transition in F-Substituted SmFeAsO: A New Phase Diagram for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>SmFeAs</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:msub><mml:mi) Tj ETQq1 1 0.784314 rgBT	2.9	38
30	Boron-Doped Graphene Nanoribbons: Electronic Structure and Raman Fingerprint. ACS Nano, 2018, 12, 7571-7582.	7.3	38
31	Disproportionation Phenomena on Free and StrainedSn/Ge(111)andSn/Si(111)Surfaces. Physical Review Letters, 2002, 89, 126803.	2.9	36
32	Common effect of chemical and external pressures on the magnetic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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37	Structural and electronic properties of theSn/Si(111)3Ã—3R30Â°surface. Physical Review B, 2000, 62, 1556-1559.	1.1	26
38	Room-temperature ferromagnetism in Mn-implanted amorphous Ge. Physical Review B, 2011, 83, .	1.1	25
39	Atomically precise semiconductorâ€"graphene and hBN interfaces by Ge intercalation. Scientific Reports, 2015, 5, 17700.	1.6	24
40	van der Waals interaction in iron-chalcogenide superconductors. Physical Review B, 2013, 87, .	1.1	23
41	First-principles and angle-resolved photoemission study of lithium doped metallic black phosphorous. 2D Materials, 2016, 3, 025031.	2.0	21
42	Transition metal doping and clustering in Ge. Applied Physics Letters, 2006, 89, 202510.	1.5	20
43	Origin of the critical temperature discontinuity in superconducting sulfur under high pressure. Physical Review B, 2017, 95, .	1.1	19
44	Weakly-Correlated Nature of Ferromagnetism in Nonsymmorphic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CrO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Revealed by Bulk-Sensitive Soft-X-Ray ARPES. Physical Review X, 2017, 7, .	2.8	19
45	MgB2andBeB2:â€ƒA comparative study of their electronic and superconducting properties. Physical Review B, 2001, 65, .	1.1	18
46	Theoretical investigation of optical conductivity in Ba(Fe1â^'xCox)2As2. Physical Review B, 2011, 83, .	1.1	18
47	Theoretical and experimental investigation of magnetotransport in iron chalcogenides. Science and Technology of Advanced Materials, 2012, 13, 054402.	2.8	18
48	Role of structural relaxations and chemical substitutions on piezoelectric fields and potential lineup inGaN/Aljunctions. Physical Review B, 2002, 65, .	1.1	17
49	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, .	1.1	17
50	Hopping-resolved electron-phonon coupling in bilayer graphene. Physical Review B, 2012, 85, .	1.1	17
51	Theoretical investigation of FeTe magnetic ordering under hydrostatic pressure. Physical Review B, 2013, 87, .	1.1	17
52	Effects of strain on ferroelectric polarization and magnetism in orthorhombic HoMnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, .	1.1	17
53	Short-range order in two-dimensional binary alloys. Physical Review B, 2003, 67, .	1.1	16
54	Effects of nonhydrostatic pressure on the structural and magnetic properties of BaFe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>As<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mro	1.1	16

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55	Fermi-Surface Topological Phase Transition and Horizontal Order-Parameter Nodes in CaFe2As2 Under Pressure. Scientific Reports, 2016, 6, 26394.	1.6	16
56	Mechanism of the short range ordering in a 2D binary alloy. Surface Science, 2002, 501, L171-L176.	0.8	15
57	First-principles study of rare-earth-doped superconducting CaFe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>As<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	15
58	Strain effects in monolayer iron-chalcogenide superconductors. 2D Materials, 2015, 2, 015001.	2.0	15
59	Chiral Spin Texture in the Charge-Density-Wave Phase of the Correlated Metallic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Pb</mml:mi><mml:mrow><mml:mo>/</mml:mo><mml:mi>Si</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 572 Td (stretchy="false Letters, 2018, 120, 196402.	7.8	15
60	Supersoft silicides:Ab initiostudy of (001)TSi surfaces and (001) Si/TSi (T=Fe, Co, and Ni) interfaces. Physical Review B, 2004, 70, .	1.1	14
61	Structural and electronic properties of the Sn/Si(111)-(2âˆš3Ã—2âˆš3)R30Â° surface revised. Surface Science, 2004, 554, 109-118.	0.8	14
62	Novel Electronically Driven Surface Phase Predicted inC/Si(111). Physical Review Letters, 2005, 95, 206801.	2.9	14
63	Far-infrared spectrum of ice Ih: A first-principles study. Physical Review B, 2011, 84, .	1.1	14
64	Environmental control of electronâ€“phonon coupling in barium doped graphene. 2D Materials, 2016, 3, 045003.	2.0	14
65	Energetics and bonding properties of the Ni /Î²-SiC (001) interface: Anabinitiostudy. Physical Review B, 2001, 64, .	1.1	13
66	Superconducting properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">K</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mtext>âˆ’</mml:mtext><mml:mi>x</mml:mi></mml:mrow mathvariant="normal">Na</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">Fe</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">As</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>under pressure. Ph	1.1	13
67	Low temperature phases of Pb/Si(111) and related surfaces. Surface Science, 2008, 602, 747-754.	0.8	12
68	Superconductivity in metalâ€coated graphene. Physica Status Solidi (B): Basic Research, 2012, 249, 2544-2548.	0.7	12
69	Ru doping in iron-based pnictides: The â€œunfoldedâ€•dominant role of structural effects for superconductivity. Physical Review B, 2017, 95, .	1.1	11
70	Electronic and dynamical properties of theMgB2surface: Implications for the superconducting properties. Physical Review B, 2002, 66, .	1.1	10
71	Two-dimensional alloying on Si(111) surface:â€, Anab initiostudy. Physical Review B, 2002, 66, .	1.1	10
72	3Ã—3R30Â°â†'3Ã—3distortion on theCâ•Si(111)surface. Physical Review B, 2004, 69, .	1.1	10

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73	Role of oxygen defects in diluted Mn:Ge. Physical Review B, 2008, 78, .	1.1	10
74	Multiband superconductivity in Pb, H under pressure and CaBeSi fromab initiocalculations. Journal of Physics Condensed Matter, 2009, 21, 164209.	0.7	10
75	Electronic properties of superconducting FeS. Physical Review B, 2017, 95, .	1.1	10
76	Superconductivity in tin selenide under pressure. Physical Review Materials, 2019, 3, .	0.9	10
77	Prediction of ambient-pressure superconductivity in ternary hydride PdCuHx. Journal of Applied Physics, 2022, 131, .	1.1	9
78	First-stage Mn adsorption on clean Ge(111). Physical Review B, 2004, 70, .	1.1	8
79	Superconducting Chevrel phase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">PbMo</mml:mi><mml:mn>6</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>8</mml:mn></mml:msub></mml:math> from first principles. Physical Review B, 2021, 103, .	1.1	8
80	Defect-induced perturbation on the Snâ€“Si(111) surface: a voltage-dependent scanning tunneling microscopy study. Surface Science, 2000, 464, 57-67.	0.8	7
81	Scanning tunneling spectroscopy investigation of the (âˆš3Ã—âˆš3)R30Â° Sn/Si(111) Î± and Î² surfaces. Surface Science, 2004, 562, 128-136.	0.8	7
82	First-principles investigation ofBaFe2As2(001). Physical Review B, 2010, 82, .	1.1	7
83	Comment on â€œElectronic Structure of SuperconductingKC8and NonsuperconductingLiC6Graphite Intercalation Compounds: Evidence for a Graphene-Sheet-Driven Superconducting Stateâ€• Physical Review Letters, 2012, 108, 149701; discussion 149702.	2.9	7
84	Static and dynamical susceptibility ofLaO1âˆ’xFxFeAs. Physical Review B, 2010, 81, .	1.1	6
85	Effective band structure of Ru-doped BaFe₂As₂. Journal of Physics: Conference Series, 2016, 689, 012027.	0.3	6
86	Compressed tetragonal phase in XFe2As2 (X=Na , K, Rb, Cs) and in the alloy Na0.5K0.5Fe2As2. Physical Review B, 2017, 95, .	1.1	6
87	Clarifying the apparent flattening of the graphene band near the van Hove singularity. Physical Review B, 2022, 105, .	1.1	6
88	Cu doping effects inMgB2. Physical Review B, 2003, 67, .	1.1	5
89	Bi incorporation in GaN andAlxGa1âˆ’xNalloys. Physical Review B, 2003, 68, .	1.1	5
90	Common effect of chemical and external pressures on the magnetic properties ofRCoPOÂ(R=La,Pr,Nd,Sm). II.. Physical Review B, 2015, 92, .	1.1	5

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91	Atomic-scale distortions and temperature-dependent large pseudogap in thin films of the parent iron-chalcogenide superconductor Fe_{1+y}Te. Journal of Physics Condensed Matter, 2017, 29, 485002.	0.7	5
92	Ab initio study of the (2 Ã— 2) phase of barium on graphene. European Physical Journal B, 2018, 91, 1.	0.6	5
93	Magnetic properties of supersoft transition metal silicides. Journal of Magnetism and Magnetic Materials, 2004, 272-276, E233-E234.	1.0	4
94	Electronic structure of a two-dimensional alloy: Snâ€“Pbâ€“Si on Si(111). Journal of Physics Condensed Matter, 2004, 16, 3507-3516.	0.7	4
95	Transition metal doping in Ge. Journal of Magnetism and Magnetic Materials, 2007, 310, 2147-2149.	1.0	4
96	Publisherâ€™s Note:Ab initioDescription of High-Temperature Superconductivity in Dense Molecular Hydrogen [Phys. Rev. Lett.100, 257001 (2008)]. Physical Review Letters, 2008, 101, .	2.9	4
97	Origin, symmetry, and temperature dependence of the perturbation induced by Si extrinsic defects on the Sn/Si(111) Î± surface: A scanning tunneling microscopy study. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2000, 18, 1946-1949.	0.9	3
98	TESTING THE CHARGED ADATOM MODEL ONTO THE ${m Sn}_{1-x}{m Si}_x/{m Si}(111) (sqrt{3}times) Tj ETQq0 0 0 rgBT /Overlock 10 and Letters, 2002, 09, 675-679.	0.5	3
99	CORRELATION BETWEEN LOCAL OXYGEN DISORDER AND ELECTRONIC PROPERTIES IN SUPERCONDUCTING RESR2CU3O6+X(RE = Y, YB). International Journal of Modern Physics B, 2003, 17, 873-878.	1.0	3
100	MartinellietÂal.Reply:. Physical Review Letters, 2013, 110, 209702.	2.9	3
101	42214 layered Fe-based superconductors: Anab initiostudy of their structural, magnetic, and electronic properties. Physical Review B, 2016, 93, .	1.1	3
102	Electron-phonon coupling origin of the graphene Ï€* -band kink via isotope effect. Physical Review B, 2021, 103, .	1.1	3
103	Unconventional ferrimagnetism and enhanced magnetic ordering temperature in monolayer CrCl₃ by introducing O impurities and Cl vacancies. JPhys Materials, 2022, 5, 014004.	1.8	3
104	Electronic, dynamical and superconducting properties of MgB2: doping, surface and pressure effects. Superconductor Science and Technology, 2003, 16, 137-142.	1.8	2
105	First-principles investigation of Sn1â^'xSix/Si(111) and Sn1â^'xPbx/Si(111) surfaces. Surface Science, 2004, 566-568, 492-496.	0.8	2
106	Ab-initio Computation of Superconducting Properties of Elemental Superconductors and MgB2. Journal of Superconductivity and Novel Magnetism, 2005, 18, 649-652.	0.5	2
107	Mn doping in model amorphous Si and Ge: A theoretical investigation. Journal of Physics: Conference Series, 2010, 200, 032014.	0.3	2
108	Ab initiostudy of doping effects in the 42214 compounds: A new family of layered iron-based superconductors. Physical Review B, 2017, 95, .	1.1	2

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109	Alloyed surfaces: New substrates for graphene growth. Surface Science, 2017, 665, 28-31.	0.8	2
110	Direct evaluation of the isotope effect within the framework of density functional theory for superconductors. Journal of Physics Condensed Matter, 2019, 31, 334001.	0.7	2
111	Magnetic properties of Fe-pnictides superconductors as a function of pressure and doping. Materials Research Society Symposia Proceedings, 2012, 1434, 1.	0.1	0