Gianni Profeta

List of Publications by Year
in descending order

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111 papers	4,211 citations	136885 32 h-index	118793 62 g-index
111 all docs	111 docs citations	111 times ranked	3611 citing authors

#	Article	IF	Citations
1	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
2	Prediction of ambient-pressure superconductivity in ternary hydride PdCuHx. Journal of Applied Physics, 2022, 131, .	1.1	9
3	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
4	Clarifying the apparent flattening of the graphene band near the van Hove singularity. Physical Review B, 2022, 105, .	1.1	6
5	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
6	Electron-phonon coupling origin of the graphene Ï€* -band kink via isotope effect. Physical Review B, 2021, 103, .	1.1	3
7	Origin of the Flat Band in Heavily Cs-Doped Graphene. ACS Nano, 2020, 14, 1055-1069.	7.3	28
8	A perspective on conventional high-temperature superconductors at high pressure: Methods and materials. Physics Reports, 2020, 856, 1-78.	10.3	304
9	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
10	Superconductivity in tin selenide under pressure. Physical Review Materials, 2019, 3, .	0.9	10
11	Boron-Doped Graphene Nanoribbons: Electronic Structure and Raman Fingerprint. ACS Nano, 2018, 12, 7571-7582.	7.3	38
12	Ab initio study of the (2 Ã— 2) phase of barium on graphene. European Physical Journal B, 2018, 91, 1.	0.6	5
13	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 50 252 Td (stretchy="false"> Letters, 2018, 120, 196402.	7.9	15
14	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
15	Origin of the critical temperature discontinuity in superconducting sulfur under high pressure. Physical Review B, 2017, 95, .	1.1	19
16	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
17	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
18	Ru doping in iron-based pnictides: The â€œunfoldedâ€•dominant role of structural effects for superconductivity. Physical Review B, 2017, 95, .	1.1	11

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19	Alloyed surfaces: New substrates for graphene growth. Surface Science, 2017, 665, 28-31.	0.8	2
20	Electronic properties of superconducting FeS. Physical Review B, 2017, 95, .	1.1	10
21	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
22	Interplay between structure and superconductivity: Metastable phases of phosphorus under pressure. Physical Review Materials, 2017, 1, .	0.9	48
23	Effective band structure of Ru-doped BaFe₂As₂. Journal of Physics: Conference Series, 2016, 689, 012027.	0.3	6
24	Evolution of electronic structure of few-layer phosphorene from angle-resolved photoemission spectroscopy of black phosphorous. Physical Review B, 2016, 94, .	1.1	44
25	Environmental control of electronâ€“phonon coupling in barium doped graphene. 2D Materials, 2016, 3, 045003.	2.0	14
26	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. Physical Review B, 2016, 93, .	1.1	125
27	42214 layered Fe-based superconductors: Anab initiostudy of their structural, magnetic, and electronic properties. Physical Review B, 2016, 93, .	1.1	3
28	Fermi-Surface Topological Phase Transition and Horizontal Order-Parameter Nodes in CaFe2As2 Under Pressure. Scientific Reports, 2016, 6, 26394.	1.6	16
29	First-principles and angle-resolved photoemission study of lithium doped metallic black phosphorous. 2D Materials, 2016, 3, 025031.	2.0	21
30	Electronic and geometric structure of graphene/SiC(0001) decoupled by lithium intercalation. Physical Review B, 2015, 91, .	1.1	56
31	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
32	Atomically precise semiconductorâ€”graphene and hBN interfaces by Ge intercalation. Scientific Reports, 2015, 5, 17700.	1.6	24
33	Strain effects in monolayer iron-chalcogenide superconductors. 2D Materials, 2015, 2, 015001.	2.0	15
34	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>â^’</mml:mtext><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi 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
35	Superconducting pairing mediated by spin fluctuations from first principles. Physical Review B, 2014, 90, .	1.1	46
36	Theoretical investigation of FeTe magnetic ordering under hydrostatic pressure. Physical Review B, 2013, 87, .	1.1	17

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37	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
38	van der Waals interaction in iron-chalcogenide superconductors. Physical Review B, 2013, 87, .	1.1	23
39	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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55	Mn doping in model amorphous Si and Ge: A theoretical investigation. Journal of Physics: Conference Series, 2010, 200, 032014.	0.3	2
56	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I. Electronic and dynamical properties under pressure. Physical Review B, 2010, 81, .	1.1	47
57	Static and dynamical susceptibility ofLaO1â^'xFxFeAs. Physical Review B, 2010, 81, .	1.1	6
58	First-principles investigation ofBaFe2As2(001). Physical Review B, 2010, 82, .	1.1	7
59	Adiabatic and nonadiabatic phonon dispersion in a Wannier function approach. Physical Review B, 2010, 82, .	1.1	108
60	Electronic, vibrational, and superconducting properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mtext>CaBeSi</mml:mtext></mml:mrow></mml:mrow></mml:math>: First-principles calculations. Physical Review B, 2009, 79, .	1.1	32
61	Multiband superconductivity in Pb, H under pressure and CaBeSi fromab initiocalculations. Journal of Physics Condensed Matter, 2009, 21, 164209.	0.7	10
62	The role of Coulomb interaction in the superconducting properties of CaC₆and H under pressure. Superconductor Science and Technology, 2009, 22, 034006.	1.8	32
63	Low temperature phases of Pb/Si(111) and related surfaces. Surface Science, 2008, 602, 747-754.	0.8	12
64	The optical phonon spectrum of SmFeAsO. Europhysics Letters, 2008, 84, 67013.	0.7	27
65	Role of oxygen defects in diluted Mn:Ge. Physical Review B, 2008, 78, .	1.1	10
66	AbÂInitioDescription of High-Temperature Superconductivity in Dense Molecular Hydrogen. Physical Review Letters, 2008, 100, 257001.	2.9	199
67	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
68	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
69	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
70	Competition of Charge-Density Waves and Superconductivity in Sulfur. Physical Review Letters, 2007, 99, 155505.	2.9	46
71	Triangular Mott-Hubbard Insulator Phases ofSn/Si(111)andSn/Ge(111)Surfaces. Physical Review Letters, 2007, 98, 086401.	2.9	72
72	Anisotropic gap of superconductingCaC6: A first-principles density functional calculation. Physical Review B, 2007, 75, .	1.1	101

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73	Superconducting properties of MgB2 from first principles. Physica C: Superconductivity and Its Applications, 2007, 456, 45-53.	0.6	46
74	Transition metal doping in Ge. Journal of Magnetism and Magnetic Materials, 2007, 310, 2147-2149.	1.0	4
75	Ab initioprediction of pressure-induced superconductivity in potassium. Physical Review B, 2006, 73, .	1.1	41
76	Transition metal impurities in Ge: Chemical trends and codoping studied by electronic structure calculations. Physical Review B, 2006, 73, .	1.1	52
77	Transition metal doping and clustering in Ge. Applied Physics Letters, 2006, 89, 202510.	1.5	20
78	Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study. Physical Review Letters, 2006, 96, 047003.	2.9	159
79	Ab-initio Computation of Superconducting Properties of Elemental Superconductors and MgB2. Journal of Superconductivity and Novel Magnetism, 2005, 18, 649-652.	0.5	2
80	Superconducting Properties ofMgB2from First Principles. Physical Review Letters, 2005, 94, 037004.	2.9	137
81	Novel Electronically Driven Surface Phase Predicted inC/Si(111). Physical Review Letters, 2005, 95, 206801.	2.9	14
82	X-ray absorption spectroscopy in MnxGe1â^'x diluted magnetic semiconductor: Experiment and theory. Applied Physics Letters, 2005, 86, 062501.	1.5	48
83	Ab initiotheory of superconductivity. II. Application to elemental metals. Physical Review B, 2005, 72, .	1.1	261
84	Ab initiotheory of superconductivity. I. Density functional formalism and approximate functionals. Physical Review B, 2005, 72, .	1.1	314
85	First-stage Mn adsorption on clean Ge(111). Physical Review B, 2004, 70, .	1.1	8
86	3Ã—3R30Â°â†'3Ã—3distortion on theCâ^•Si(111)surface. Physical Review B, 2004, 69, .	1.1	10
87	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
88	Scanning tunneling spectroscopy investigation of the (â^š3Ã—â^š3)R30Â° Sn/Si(111) Î± and Î³ surfaces. Surface Science, 2004, 562, 128-136.	0.8	7
89	Magnetic properties of supersoft transition metal silicides. Journal of Magnetism and Magnetic Materials, 2004, 272-276, E233-E234.	1.0	4
90	Structural and electronic properties of the Sn/Si(111)-(2â^š3Ã—2â^š3)R30Â° surface revised. Surface Science, 2004, 554, 109-118.	0.8	14

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91	First-principles investigation of Sn1â^'xSix/Si(111) and Sn1â^'xPbx/Si(111) surfaces. Surface Science, 2004, 566-568, 492-496.	0.8	2
92	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
93	Cu doping effects inMgB2. Physical Review B, 2003, 67, .	1.1	5
94	Bi incorporation in GaN andAlxGa1â^'xNalloys. Physical Review B, 2003, 68, .	1.1	5
95	Phonon and electron-phonon renormalization in Al-dopedMgB2. Physical Review B, 2003, 68, .	1.1	53
96	Short-range order in two-dimensional binary alloys. Physical Review B, 2003, 67, .	1.1	16
97	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
98	Electronic, dynamical and superconducting properties of MgB2: doping, surface and pressure effects. Superconductor Science and Technology, 2003, 16, 137-142.	1.8	2
99	Disproportionation Phenomena on Free and StrainedSn/Ge(111)andSn/Si(111)Surfaces. Physical Review Letters, 2002, 89, 126803.	2.9	36
100	Electronic and dynamical properties of theMgB2surface: Implications for the superconducting properties. Physical Review B, 2002, 66, .	1.1	10
101	Two-dimensional alloying on Si(111) surface:â€, Anab initiostudy. Physical Review B, 2002, 66, .	1.1	10
102	Role of structural relaxations and chemical substitutions on piezoelectric fields and potential lineup inGaN/Aljunctions. Physical Review B, 2002, 65, .	1.1	17
103	TESTING THE CHARGED ADATOM MODEL ONTO THE ${m Sn}_{1-x}{m Si}_x/{m Si}(111) (sqrt{3}imes) Tj ETQq1 1 0.784314 rgBT /Ov and Letters, 2002, 09, 675-679.	0.5	3
104	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
105	Mechanism of the short range ordering in a 2D binary alloy. Surface Science, 2002, 501, L171-L176.	0.8	15
106	Electronic and structural properties of superconductingMgB2,CaSi2,and related compounds. Physical Review B, 2001, 64, .	1.1	135
107	MgB2andBeB2:â€ƒA comparative study of their electronic and superconducting properties. Physical Review B, 2001, 65, .	1.1	18
108	Energetics and bonding properties of the Ni /Î²-SiC (001) interface: Anabinitiostudy. Physical Review B, 2001, 64, .	1.1	13

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109	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
110	Structural and electronic properties of theSn/Si(111)3Ã—3R30Â°surface. Physical Review B, 2000, 62, 1556-1559.	1.1	26
111	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