Vincenzo Fiorentini

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

144 papers	10,155 citations	45 h-index	99 g-index
152 ext. papers	10,964 ext. citations	3.6 avg, IF	6.12 L-index

#	Paper	IF	Citations
144	Efficient thermoelectricity in Sr2Nb2O7 with energy-dependent relaxation times. *Physical Review Materials*, **2020**, 4,	3.2	5
143	A three-order-parameter bistable magnetoelectric multiferroic metal. *Nature Communications*, **2020**, 11, 4922	17.4	4
142	Influence of thermal conductivity and of non-constant relaxation time on thermoelectricity in Mg3Sb2. *Journal of Physics: Conference Series*, **2019**, 1226, 012010	0.3	2
141	The electronic structure of □Ga2O3. *APL Materials*, **2019**, 7, 022522	5.7	33
140	Singling out the effect of quenched disorder in the phase diagram of cuprates. *Journal of Physics Condensed Matter*, **2019**, 31, 184002	1.8	1
139	High thermoelectric figure of merit and thermopower in layered perovskite oxides. *Physical Review Materials*, **2019**, 3,	3.2	7
138	Theory of thermoelectricity in MgSb with an energy- and temperature-dependent relaxation time. *Journal of Physics Condensed Matter*, **2019**, 31, 065702	1.8	8
137	Meta-screening and permanence of polar distortion in metallized ferroelectrics. *Physical Review B*, **2018**, 97,	3.3	24
136	Ab initio thermal conductivity of thermoelectric Mg3Sb2: Evidence for dominant extrinsic effects. *Physical Review B*, **2018**, 98,	3.3	14
135	Prediction of a native ferroelectric metal. *Nature Communications*, **2016**, 7, 11211	17.4	48
134	Theoretical and experimental investigation of optical absorption anisotropy in □Ga2O3. *Journal of Physics Condensed Matter*, **2016**, 28, 224005	1.8	46
133	Properties of (Ga1-x In x)2O3 over the whole x range. *Journal of Physics Condensed Matter*, **2016**, 28, 224001	1.8	8
132	Phase diagram and polarization of stable phases of (Ga1□Inx)2O3. *Applied Physics Express*, **2016**, 9, 041102	2.4	81
131	Topological multiferroics. *Phase Transitions*, **2015**, 88, 953-961	1.3	4
130	Intrinsic origin of two-dimensional electron gas at the (001) surface of SrTiO3. *Physical Review B*, **2015**, 91,	3.3	24
129	Vibrational stability of graphene under combined shear and axial strains. *Physical Review B*, **2015**, 92,	3.3	1
128	Giant oscillating thermopower at oxide interfaces. *Nature Communications*, **2015**, 6, 6678	17.4	52

127	Low In solubility and band offsets in the small-x□Ga2O3/(Ga1□Inx)2O3system. *Applied Physics Express*, **2015**, 8, 021102	2.4	18
126	Doping-dependent band structure of LaAlO3/SrTiO3 interfaces by soft x-ray polarization-controlled resonant angle-resolved photoemission. *Physical Review B*, **2014**, 89,	3.3	61
125	Structure and gap of low-x(Ga1-xInx)2O3alloys. *Journal of Physics: Conference Series*, **2014**, 566, 012016	0.3	9
124	Multigap absorption in CaCu3Ti4O12 and the prediction capability of ab initio methods. *Physical Review B*, **2014**, 90,	3.3	2
123	Impurity-vacancy complexes and ferromagnetism in doped sesquioxides. *Physical Review B*, **2014**, 89,	3.3	7
122	Multiferroicity in vanadium-doped La2Ti2O7: insights from first principles. *European Physical Journal B*, **2013**, 86, 1	1.2	10
121	Surface antiferromagnetism and incipient metal-insulator transition in strained manganite films. *Physical Review B*, **2013**, 87,	3.3	8
120	Giant electroresistance and tunable magnetoelectricity in a multiferroic junction. *Physical Review B*, **2013**, 88,	3.3	3
119	Large band offset as driving force of two-dimensional electron confinement: The case of SrTiO3/SrZrO3 interface. *Physical Review B*, **2013**, 88,	3.3	22
118	Doping-induced dimensional crossover and thermopower burst in Nb-doped SrTiO3 superlattices. *Physical Review B*, **2013**, 88,	3.3	34
117	Multiferroicity in V-doped PbTiO3. *Journal of Physics: Conference Series*, **2013**, 470, 012013	0.3	3
116	Magnetism and unusual Cu valency in quadruple perovskites. *European Physical Journal B*, **2012**, 85, 1	1.2	9
115	Ferromagnetism and orbital order in a topological ferroelectric. *Physical Review Letters*, **2012**, 109, 217202	7.4	19
114	Thermopower in oxide heterostructures: The importance of being multiple-band conductors. *Physical Review B*, **2012**, 86,	3.3	43
113	Ordering and multiple phase transitions in ultrathin nickelate superlattices. *Physical Review B*, **2012** , 86,	3.3	34
112	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods. *Physical Review B*, **2011**, 84,	3.3	53
111	Spontaneous 2-dimensional carrier confinement at the n-type SrTiO3/LaAlO3 interface. *Physical Review Letters*, **2011**, 106, 166807	7.4	170
110	Bound states of the Fe impurity in wurtzite GaN from hybrid density-functional calculations. *Physical Review B*, **2011**, 84,	3.3	16

109	Variational pseudo-self-interaction-corrected density functional approach to the ab initio description of correlated solids and molecules. *Physical Review B*, **2011**, 84,	3.3	71
108	First-principles calculation of electronic and structural properties of YBa2Cu3O6+y. *Physical Review B*, **2010**, 82,	3.3	15
107	Reorientable dipolar CuCa antisite and anomalous screening in CaCu3Ti4O12. *Physical Review B*, **2010**, 81,	3.3	10
106	Multiferroicity and orbital ordering in Pr0.5Ca0.5MnO3 from first principles. *Physical Review B*, **2010**, 82,	3.3	13
105	Band alignment at Cu2O/La0.7Sr0.3MnO3 interface: A combined experimental-theoretical determination. *Applied Physics Letters*, **2010**, 97, 032115	3.4	11
104	Indium on Cu(100) from first principles: Energetics, complex formation, and diffusion of adsorbates and vacancies on terraces and at steps. *Physical Review B*, **2009**, 79,	3.3	2
103	Dielectric and vibrational properties of bixbyite sesquioxides. *Physical Review B*, **2009**, 80,	3.3	6
102	Fermi-surface pockets in YBa2Cu3O6.5: Comparison of ab initio techniques. *Physical Review B*, **2009**, 79,	3.3	9
101	Modeling of Alternative High-k Dielectrics for Memory Based Applications. *ECS Transactions*, **2009**, 25, 131-145	1	3
100	Fermi-surface pockets in magnetic underdoped cuprates from first principles. *Europhysics Letters*, **2009**, 88, 67009	1.6	2
99	Magnetic couplings vs. stress and strain in epitaxial (La, Sr)MnO3. *European Physical Journal B*, **2009**, 70, 343-346	1.2	4
98	A practical first-principles band-theory approach to the study of correlated materials. *European Physical Journal B*, **2009**, 71, 139-183	1.2	40
97	Jahn-Teller stabilization of magnetic and orbital ordering in rocksalt CuO. *Physical Review B*, **2009**, 80,	3.3	21
96	Te-induced modulation of the Mo□HfO2 interface effective work function. *Applied Physics Letters*, **2008**, 92, 113504	3.4	13
95	Chain metallicity and competition between paramagnetism and antiferromagnetism in underdoped YBa2Cu3O6+x: A first principles description. *Physical Review B*, **2008**, 78,	3.3	12
94	Interplay of strain and magnetism in La1□SrxMnO3 from first principles. *Physical Review B*, **2008**, 78,	3.3	33
93	Metal-insulator transitions and singlet polarons in one-dimensional Ca2+xY2□Cu5O10. *Physical Review B*, **2008**, 77,	3.3	9
92	Dielectric constant boost in amorphous sesquioxides. *Applied Physics Letters*, **2008**, 92, 172903	3.4	14

91	Conservation of dielectric constant upon amorphization in perovskite oxides. *Physical Review B*, **2007**, 76,	3.3	10
90	Self-interaction-free density-functional band theory for magnetic cuprates. *Journal of Magnetism and Magnetic Materials*, **2007**, 310, 1648-1650	2.8	5
89	Cation charge anomalies and high-□dielectric behavior in DyScO3: Ab initio density-functional and self-interaction-corrected calculations. *Physical Review B*, **2007**, 75,	3.3	31
88	Magnetism of La0.625Sr0.375MnO3 under high pressure from first principles. *Physical Review B*, **2007**, 76,	3.3	29
87	Magnetic ordering under strain and spin-Peierls dimerization in GeCuO3. *Physical Review Letters*, **2007**, 98, 196403	7.4	15
86	A Theoretical View on the Dielectric Properties of Crystalline and Amorphous High-□Materials and Films **2007**, 269-292		1
85	Electronic Structure of Bulk and Defected CaCu3Ti4O12. *ECS Transactions*, **2006**, 3, 291-297	1	5
84	Double-exchange driven ferromagnetic metal-paramagnetic insulator transition in Mn-doped CuO. *Physical Review B*, **2006**, 74,	3.3	24
83	Large fluorine-vacancy clusters in Si and their capture efficiency for self-interstitials. *Applied Physics Letters*, **2006**, 89, 092113	3.4	13
82	Comment on "ab initio calculations to model anomalous fluorine behavior". *Physical Review Letters*, **2006**, 96, 039601; discussion 039602	7.4	8
81	Dielectric properties and long-wavelength optical modes of the high-□oxide LaAlO3. *Physical Review B*, **2005**, 71,	3.3	61
80	Coexistence of ionic and metallic bonding in noble-metal oxides. *Physical Review B*, **2005**, 72,	3.3	61
79	Magnetic ordering in CuO from first principles: a cuprate antiferromagnet with fully three-dimensional exchange interactions. *Physical Review Letters*, **2005**, 95, 086405	7.4	82
78	Theoretical electron affinities of PAHs and electronic absorption spectra of their mono-anions. *Astronomy and Astrophysics*, **2005**, 432, 585-594	5.1	50
77	Dielectric properties of two phases of crystalline lutetium oxide. *Microelectronics Reliability*, **2005**, 45, 831-833	1.2	15
76	Fluorine in Si: Native-defect complexes and the suppression of impurity diffusion. *Physical Review B* , **2005**, 72,	3.3	48
75	Influence of point defects injection on the stability of a supersaturated Ga-Si solid solution. *Physical Review B*, **2005**, 71,	3.3	6
74	Comparison between experimental and theoretical determination of the local structure of the GaAs1-□Ny dilute nitride alloy. *Physical Review B*, **2005**, 71,	3.3	10

73	Dielectric properties of high-kappa oxides: theory and experiment for Lu2O3. *Physical Review Letters*, **2005**, 94, 027602	7.4	54
72	Tunable variation of the electron effective mass and exciton radius in hydrogenated GaAs1−xNx. *Physical Review B*, **2004**, 69,	3.3	38
71	Complexes, clustering, and native-defect-assisted diffusion of aluminum in silicon. *Physical Review B*, **2004**, 70,	3.3	7
70	Lattice constant, effective mass, and gap recovery in hydrogenated GaAs1−xNx. *Physical Review B*, **2004**, 69,	3.3	8
69	Structure, energetics, and extrinsic levels of small self-interstitial clusters in silicon. *Physical Review B*, **2004**, 69,	3.3	42
68	Energetics of transient enhanced diffusion of boron in Ge and SiGe. *Physical Review B*, **2004**, 69,	3.3	30
67	Structure and stability of rare-earth and transition-metal oxides. *Physical Review B*, **2004**, 69,	3.3	110
66	Tuning of the electron effective mass and exciton wavefunction size in GaAs1−xNx. *Physica E: Low-Dimensional Systems and Nanostructures*, **2004**, 21, 747-751	3	1
65	Anomalous energetics and defect-assisted diffusion of Ga in silicon. *Applied Physics Letters*, **2004**, 85, 4902-4904	3.4	15
64	Vibrational modes of three-membered self-interstitial clusters in silicon. *Journal of Physics Condensed Matter*, **2003**, 15, 7851-7857	1.8	7
63	Electronics and sensors based on pyroelectric AlGaN/GaN heterostructures. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2003**, 1878-1907		56
62	Origin of the efficient light emission from inversion domain boundaries in GaN. *Applied Physics Letters*, **2003**, 82, 1182-1184	3.4	26
61	Ordered versus disordered growth of copper quantum wires on Mo and W vicinal surfaces. *Physical Review B*, **2003**, 67,	3.3	3
60	Nonlinear Behavior of Spontaneous and Piezoelectric Polarization in III–V Nitride Alloys. *Physica Status Solidi A*, **2002**, 190, 65-73		39
59	Stability of Ge-related point defects and complexes in Ge-doped SiO2. *Physical Review B*, **2002**, 66,	3.3	15
58	Theoretical evaluation of zirconia and hafnia as gate oxides for si microelectronics. *Physical Review Letters*, **2002**, 89, 266101	7.4	158
57	Evidence for nonlinear macroscopic polarization in III–V nitride alloy heterostructures. *Applied Physics Letters*, **2002**, 80, 1204-1206	3.4	607
56	First-principles calculation of the piezoelectric tensor d? of III–V nitrides. *Applied Physics Letters*, **2002**, 80, 4145-4147	3.4	107

55	Pyroelectric properties of Al(In)GaN/GaN hetero- and quantum well structures. *Journal of Physics Condensed Matter*, **2002**, 14, 3399-3434	1.8	689
54	Multiscale approaches for metal thin film growth. *Computational Materials Science*, **2002**, 24, 58-65	3.2	12
53	First-principles prediction of structure, energetics, formation enthalpy, elastic constants, polarization, and piezoelectric constants of AlN, GaN, and InN: Comparison of local and gradient-corrected density-functional theory. *Physical Review B*, **2001**, 64,	3.3	366
52	Roughening of close-packed singular surfaces. *Physical Review B*, **2001**, 63,	3.3	2
51	Nonlinear macroscopic polarization in III-V nitride alloys. *Physical Review B*, **2001**, 64,	3.3	238
50	Accurate calculation of polarization-related quantities in semiconductors. *Physical Review B*, **2001**, 63,	3.3	146
49	Proof of the thermodynamical stability of the EQcenter in SiO2. *Physical Review Letters*, **2001**, 86, 3064-7	7.4	45
48	Stress and reconstruction on (001) transition-metal surfaces. *Computational Materials Science*, **2001**, 20, 423-428	3.2	3
47	Polarization fields in nitride nanostructures: 10 points to think about. *Applied Surface Science*, **2000**, 166, 23-29	6.7	63
46	Doping screening of polarization fields in nitride heterostructures. *Applied Physics Letters*, **2000**, 76, 3950-3952	3.4	50
45	Incorporation, diffusion, and electrical activity of Li in GaN. *Physical Review B*, **2000**, 61, 12598-12601	3.3	7
44	Band offsets and stability of BeTe/ZnSe (100) heterojunctions. *Physical Review B*, **2000**, 62, R16302-R16305	3.3	14
43	Connection between charge transfer and alloying core-level shifts based on density-functional calculations. *Physical Review B*, **2000**, 61, 5229-5236	3.3	26
42	Theory and applications of the stress density. *Physical Review B*, **2000**, 61, 8433-8442	3.3	109
41	Theoretical evidence for the semi-insulating character of AlN. *Journal of Applied Physics*, **1999**, 85, 2001-2003	2.5	47
40	Atomistic modeling of large-scale metal film growth fronts. *Physical Review B*, **1999**, 59, R7856-R7859	3.3	21
39	Free-carrier screening of polarization fields in wurtzite GaN/InGaN laser structures. *Applied Physics Letters*, **1999**, 74, 2002-2004	3.4	233
38	Quasiharmonic versus exact surface free energies of Al: A systematic study employing a classical interatomic potential. *Physical Review B*, **1999**, 60, 5055-5064	3.3	44

37	Anomalous relaxations and chemical trends at III-V semiconductor nitride nonpolar surfaces. *Physical Review B*, **1999**, 59, 8026-8031	3.3	56
36	Faceting and stress of missing-row reconstructed transition-metal (110) surfaces. *Physical Review B*, **1999**, 60, 14366-14371	3.3	15
35	Spontaneous versus Piezoelectric Polarization in III□V Nitrides: Conceptual Aspects and Practical Consequences. *Physica Status Solidi (B): Basic Research*, **1999**, 216, 391-398	1.3	241
34	Effects of macroscopic polarization in III-V nitride multiple quantum wells. *Physical Review B*, **1999**, 60, 8849-8858	3.3	432
33	Ionicity and Relaxation Anomalies at III□V Nitride Surfaces. *Physica Status Solidi A*, **1998**, 170, 265-269		8
32	Macroscopic polarization and band offsets at nitride heterojunctions. *Physical Review B*, **1998**, 57, R9427-R9430	3.3	340
31	Extracting convergent surface formation energies from slab calculations. *Journal of Physics Condensed Matter*, **1998**, 10, 895-895	1.8	14
30	Electronic dielectric constants of insulators calculated by the polarization method. *Physical Review B*, **1998**, 58, 15292-15295	3.3	71
29	No In-Plane Reconstruction of Cu(001). *Physical Review Letters*, **1998**, 81, 4278-4278	7.4	8
28	Theoretical evidence for efficient p-type doping of GaN using beryllium. *Applied Physics Letters*, **1997**, 70, 2990-2992	3.4	95
27	Polarization-Based Calculation of the Dielectric Tensor of Polar Crystals. *Physical Review Letters*, **1997**, 79, 3958-3961	7.4	210
26	Reconstructions of Ir(110) and (100): an ab initio study. *Surface Science*, **1997**, 377-379, 112-116	1.8	45
25	Ab initio study of oxygen vacancies in □quartz. *Journal of Non-Crystalline Solids*, **1997**, 221, 89-96	3.9	30
24	Spontaneous polarization and piezoelectric constants of III-V nitrides. *Physical Review B*, **1997**, 56, R10024-R10027	3.3	2529
23	Extracting convergent surface energies from slab calculations. *Journal of Physics Condensed Matter*, **1996**, 8, 6525-6529	1.8	259
22	Offsets and Polarization at Strained AlN/GaN Polar Interfaces. *Materials Research Society Symposia Proceedings*, **1996**, 449, 923		7
21	Inhibited Al Diffusion and Growth Roughening of Ga-Coated Al(100). *Physical Review Letters*, **1996**, 77, 695-698	7.4	8
20	Homoepitaxial Growth of Metals and the Role of Surfactants **1996**, 219-231		

19	Effective-mass single and double acceptor spectra in GaAs. *Physical Review B*, **1995**, 51, 10161-10163	3.3	10
18	Dielectric scaling of the self-energy scissor operator in semiconductors and insulators. *Physical Review B*, **1995**, 51, 17196-17198	3.3	119
17	Local norm-conserving pseudo-Hamiltonians. *Physical Review A*, **1995**, 52, 236-257	2.6	47
16	Towards an understanding of surfactant action in the epitaxial growth of metals: The case of Sb on Ag (111). *Applied Physics A: Materials Science and Processing*, **1995**, 60, 399-402	2.6	19
15	Structure and Quasiparticle Energies of Cubic, Wurtzite and Hexagonal BN. *Materials Research Society Symposia Proceedings*, **1995**, 395, 429		5
14	Simulated Thermal Effects on Structural and Electronic Properties of GaN. *Materials Research Society Symposia Proceedings*, **1995**, 395, 435		
13	Hydrogen, Acceptors, and H-Acceptor Complexes in GaN. *Materials Research Society Symposia Proceedings*, **1995**, 395, 503		20
12	Structural and Electronic Properties of AlN, GaN And InN, and Band Offsets at AlN/GaN (1010) and (0001) Interfaces. *Materials Research Society Symposia Proceedings*, **1995**, 395, 515		8
11	Formation Energy, Stress, and Relaxations of Low-Index Rhodium Surfaces. *Materials Research Society Symposia Proceedings*, **1995**, 408, 457		3
10	Electronic and structural properties of GaN by the full-potential linear muffin-tin orbitals method: The role of the d electrons. *Physical Review B*, **1993**, 47, 13353-13362	3.3	177
9	Theory of adsorption and surfactant effect of Sb on Ag(111). *Physical Review Letters*, **1993**, 71, 2437-2440	7.4	123
8	Surface Alloying and Surfactant Action of Sb ON Ag (111). *Materials Research Society Symposia Proceedings*, **1993**, 317, 323		1
7	Reconstruction mechanism of fcc transition metal (001) surfaces. *Physical Review Letters*, **1993**, 71, 1051-1054	7.4	249
6	Semiempirical self-energy corrections to LDA bands of semiconductors, and a scaling law for the scissor operator. *Journal of Physics Condensed Matter*, **1992**, 4, 5967-5976	1.8	25
5	Semiconductor band structures at zero pressure. *Physical Review B*, **1992**, 46, 2086-2091	3.3	54
4	A note on AB INITIO semiconductor band structures. *Solid State Communications*, **1992**, 83, 871-875	1.6	2
3	Self-consistent DFT calculations of electronic states in superlattices and quantum wells with arbitrary compositional and doping profiles. *Semiconductor Science and Technology*, **1990**, 5, 211-217	1.8	2
2	Interpretation of double acceptor spectra in Ge. *Solid State Communications*, **1989**, 69, 953-958	1.6	9

1 Dielectric Properties of Rare-Earth Oxides: General Trends from Theory225-246 2