Felix Yndurain MuÃ±oz

List of Publications by Year
in descending order

127 papers	3,994 citations	147801 31 h-index	133252 59 g-index
129 all docs	129 docs citations	129 times ranked	3762 citing authors

#	Article	IF	Citations
1	Atomic-scale control of graphene magnetism by using hydrogen atoms. Science, 2016, 352, 437-441.	12.6	545
2	Unraveling the Intrinsic and Robust Nature of van Hove Singularities in Twisted Bilayer Graphene by Scanning Tunneling Microscopy and Theoretical Analysis. Physical Review Letters, 2012, 109, 196802.	7.8	345
3	Electronic and structural characterization of divacancies in irradiated graphene. Physical Review B, 2012, 85, .	3.2	173
4	"Cluster-Bethe-lattice" method: Electronic density of states of amorphous and crystalline homopolar solids. Physical Review B, 1974, 10, 5164-5174.	3.2	166
5	Experimental and theoretical study of Co adsorbed at the surface of Cu: Reconstructions, charge-density waves, surface magnetism, and oxygen adsorption. Physical Review B, 1981, 24, 3245-3254.	3.2	134
6	Proposal for symmetric dimers at the Si(100)-2Ã—1 surface. Physical Review Letters, 1989, 62, 2491-2494.	7.8	118
7	Model calculation of the electronic structure of a (111) surface in a diamond-structure solid. Journal of Physics C: Solid State Physics, 1975, 8, 147-157.	1.5	102
8	Theory of binary alloys including short-range order properties. Physical Review B, 1975, 12, 5664-5675.	3.2	90
9	Metal-semiconductor junction for (110) surfaces of zinc-blende compounds. Physical Review B, 1976, 13, 4408-4418.	3.2	85
10	Stability, Adsorption, and Diffusion of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>,<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>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>2</mml:mn></mml:msu	7.8	83
11	Theoretical study of the electronic structure ofSiOx. Physical Review B, 1981, 24, 5718-5725.	3.2	76
12	New theoretical method to study densities of states of tetrahedrally coordinated solids. Solid State Communications, 1974, 15, 617-620.	1.9	68
13	Electronic structure, defect states, and optical absorption of amorphousSi1â^'xNx[0â‰¤x/(1-x)â‰¤2]. Physical Review B, 1987, 35, 9683-9692.	3.2	58
14	Interstitial oxygen in germanium and silicon. Physical Review B, 1997, 56, 3820-3833.	3.2	55
15	"Clusterâ€"Bethe-lattice" method: The electronic density of states of heteropolar systems. Physical Review B, 1975, 11, 2957-2964.	3.2	53
16	Magnetic exchange splitting of one layer of cobalt deposited on top of the (111) surface of copper. Physical Review B, 1982, 25, 527-530.	3.2	51
17	Effects of the local configuration on the lattice dynamics of group-IV semiconductors. Physical Review B, 1976, 14, 531-537.	3.2	50
18	Density of states and barrier height of metal-Si contacts. Journal of Physics C: Solid State Physics, 1971, 4, 2849-2858.	1.5	47

#	Article	IF	Citations
19	Magnetism in nanoparticles: tuning properties with coatings. Journal of Physics Condensed Matter, 2013, 25, 484006.	1.8	46
20	Electronic structure of the Bi(111) surface. Physical Review B, 1986, 33, 4352-4355.	3.2	45
21	Magnetism of two-dimensional defects in Pd: Stacking faults, twin boundaries, and surfaces. Physical Review B, 2006, 74, .	3.2	43
22	Atomic oxygen in silicon: The formation of the Siâ€”Oâ€”Si bond. Physical Review B, 1987, 36, 8043-8048.	3.2	41
23	Electronic surface structure of a tetrahedrally coordinated covalent solid with a simple four-state Hamiltonian. Journal of Physics C: Solid State Physics, 1975, 8, 1563-1570.	1.5	39
24	Nonmagnetic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>Î³</mml:mi><mml:mo>â€³</mml:mo></mml:msup><mml:mtext>-FeN</mml:mtext> films epitaxially grown on Cu(001): Electronic structure and thermal stability. Physical Review B, 2008, 78, .	3.2	38
25	Electronic density of states of group-IV semiconductors: A cluster-Bethe lattice approach for realistic Hamiltonians. Solid State Communications, 1976, 20, 309-312.	1.9	36
26	Optical absorption in plasmaâ€deposited silicon oxynitride films. Applied Physics Letters, 1992, 60, 1399-1401.	3.3	35
27	First Principles Calculation of Localized Surface Phonons and Electron-Phonon Interaction at Pb(111) Thin Films. Physical Review Letters, 2008, 100, 205501.	7.8	34
28	Surface states calculation for the (100), (110) and (111) faces of Si. Surface Science, 1972, 29, 540-554.	1.9	33
29	Theory of Vibrational Properties of Amorphous Alloys: Application toSixGe1â^'x. Physical Review Letters, 1976, 37, 1062-1065.	7.8	33
30	Coexistence of charge-density waves and magnetic order. Physical Review B, 1980, 21, 5267-5271.	3.2	33
31	Electron states at planar and stepped semiconductor surfaces. Physical Review B, 1977, 16, 1542-1551.	3.2	32
32	Comment on â€œMagnetism in Atomic-Size Palladium Contacts and Nanowiresâ€• Physical Review Letters, 2006, 96, 079701; author reply 079702.	7.8	32
33	Anomalous electron-phonon interaction in doped LaFeAsO: First-principles calculations. Physical Review B, 2009, 79, .	3.2	32
34	Theoretical study of oxygen in silicon: Breaking of the Siâ€”Si bond. Physical Review B, 1987, 35, 788-791.	3.2	31
35	1D Lattice Distortions as the Origin of the(2Ã—2)p4gmReconstruction inÎ³â€²â^'Fe4N(100): A Magnetism-Induced Surface Reconstruction. Physical Review Letters, 2005, 95, 136102.	7.8	31
36	New approach to the study of binary alloys. Physical Review B, 1976, 13, 4387-4395.	3.2	30

#	Article	IF	Citations
37	Spin polarization and dimer buckling at the Si(100)-2Ã—1 surface. Physical Review B, 1990, 42, 11310-11316.	3.2	30
38	Electronic structure of ultrathinÎ³â€²â€”Fe4N(100) films epitaxially grown on Cu(100). Physical Review B, 2007, 75, .	3.2	30
39	Ab initioenergetics and kinetics study of H<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>and CH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>in the SI clathrate hydrate. Physical Review B, 2011, 84, .	3.2	30
40	Geometry and quantum delocalization of interstitial oxygen in silicon. Physical Review B, 1995, 51, 7862-7865.	3.2	28
41	Effects of impurities on charge-density waves: A mean-field calculation. Physical Review B, 1984, 29, 4459-4467.	3.2	26
42	Formation of Gold Nanowires with Impurities: A First-Principles Molecular Dynamics Simulation. Physical Review Letters, 2007, 98, 096102.	7.8	26
43	Absence of Surface States in Oxidized Si. Physical Review Letters, 1971, 26, 138-140.	7.8	25
44	Magnetic exchange splitting of a quasi two-dimensional hexagonal close packed layer of cobalt. Surface Science, 1982, 117, 319-329.	1.9	24
45	Nonparametrized tight-binding method for local and extended defects in homopolar semiconductors. Physical Review B, 1991, 44, 6169-6187.	3.2	24
46	Nonparametrized calculation of the electronic and vibrational structure of amorphousSiOx. Physical Review B, 1991, 43, 4552-4555.	3.2	24
47	Design of molecular wires based on one-dimensional coordination polymers. Applied Physics Letters, 2007, 90, 193107.	3.3	24
48	Theoretical study of the dynamics of atomic hydrogen adsorbed on graphene multilayers. Physical Review B, 2015, 91, .	3.2	23
49	New theory of binary alloys with short-range order properties. Solid State Communications, 1975, 17, 1545-1548.	1.9	22
50	Electronic Structure of Stacking Faults in Transition Metals: Nickel. Physical Review Letters, 1976, 37, 928-930.	7.8	21
51	Theory of off-center impurities in semiconductors. Physical Review B, 1986, 34, 6038-6040.	3.2	21
52	Atomic configuration of H-based complexes in silicon. Solid State Communications, 1989, 72, 393-396.	1.9	21
53	Electronic surface structure of a tetrahedrally coordinated binary compound. Journal of Physics C: Solid State Physics, 1975, 8, 1571-1580.	1.5	19
54	One-electron properties of the metal-semiconductor junction for zincblende compounds. Journal of Physics C: Solid State Physics, 1973, 6, L465-L469.	1.5	18

#	Article	IF	Citations
55	Effect of hole doping on the magnetism of point defects in graphene: A theoretical study. Physical Review B, 2014, 90, .	3.2	18
56	Selective Hydrogen Adsorption in Graphene Rotated Bilayers. Journal of Physical Chemistry B, 2018, 122, 595-600.	2.6	18
57	New interpretation of the electronic structure of SiO2. Solid State Communications, 1978, 27, 75-80.	1.9	17
58	Pressure-induced magnetism in rotated graphene bilayers. Physical Review B, 2019, 99, .	3.2	17
59	Surface states and ionicity. Physica Status Solidi (B): Basic Research, 1973, 57, 175-186.	1.5	16
60	Lattice vibrations at (111) surfaces and stacking faults in transition metals: Ni. Surface Science, 1979, 85, 107-124.	1.9	16
61	Correlation between electronic structure and local ordering in hydrogenated amorphous silicon. Physical Review B, 1989, 40, 12416-12422.	3.2	16
62	Interplay between electron-phonon superconductivity and magnetic order in high Tc superconductors. Solid State Communications, 1992, 81, 939-942.	1.9	16
63	Band unfolding made simple. Journal of Physics Condensed Matter, 2020, 32, 205902.	1.8	16
64	Electron states at steps in transition metal surfaces: A cluster-Bethe lattice approximation. Journal of Physics F: Metal Physics, 1978, 8, 873-881.	1.6	15
65	Electronic surface states in Ge. Journal of Physics C: Solid State Physics, 1972, 5, L146-L150.	1.5	14
66	Effects of the 2 Ã— 1 reconstruction on the electronic structure of the (111) surface of Si and Ge. Solid State Communications, 1975, 17, 855-859.	1.9	14
67	Vibrational properties of alloys: Study ofSixGe1â^'x. Physical Review B, 1978, 18, 2876-2883.	3.2	14
68	Theoretical study of a-SiNxHy alloys. Journal of Non-Crystalline Solids, 1991, 137-138, 891-894.	3.1	14
69	Coupling of magnetic moments with phonons and electron-phonon interaction in LaFeAsO 1-x F x. Europhysics Letters, 2011, 94, 37001.	2.0	14
70	Tuning the magnetic properties of pure hafnium by high pressure torsion. Acta Materialia, 2017, 123, 206-213.	7.9	14
71	Study of the electronic local density of states using the cluster-Bethe-lattice method: Application to amorphous III-V semiconductors. Physical Review B, 1976, 14, 3569-3577.	3.2	13
72	Electronic structure of H chemisorbed on Si(111) surfaces. Solid State Communications, 1978, 25, 439-441.	1.9	13

#	Article	IF	Citations
73	Theoretical study of intrinsic surface phonons in hydrogenated amorphous silicon. Solid State Communications, 1982, 44, 1477-1480.	1.9	13
74	Magnetic short-range order inCuO2planes of high-Tcsuperconductors. Physical Review B, 1991, 43, 3691-3694.	3.2	13
75	Density of states of tight-binding disordered systems. Journal of Physics C: Solid State Physics, 1975, 8, 434-444.	1.5	12
76	Electron states at steps in semiconductor surfaces. Solid State Communications, 1977, 22, 147-151.	1.9	12
77	Surface electronic structure of metastable FeSi(CsCl)(111) epitaxially grown on Si(111). Physical Review B, 1997, 55, R16065-R16068.	3.2	12
78	Crystallographic and electronic contribution to the apparent step height in nanometer-thin Pb(111) films grown on Cu(111). New Journal of Physics, 2009, 11, 123003.	2.9	12
79	Electronic surface properties of group V semimetals. Surface Science, 1976, 57, 375-384.	1.9	11
80	Effect of the electron-electron interaction on periodic lattice distortions: coexistence of CDW and SDW. Journal of Physics C: Solid State Physics, 1984, 17, 5539-5548.	1.5	11
81	Geometrical configuration of interstitial oxygen in silicon and in germanium. Solid State Communications, 1994, 89, 819-822.	1.9	11
82	Low-energy quantum dynamics of atoms at defects; interstitial oxygen in silicon. Journal of Physics Condensed Matter, 1997, 9, 3107-3116.	1.8	11
83	Long-range correlations in Bethe lattices. Physical Review B, 1983, 28, 3576-3578.	3.2	10
84	Minimal tight-binding Hamiltonian for semiconductors. Physical Review B, 1988, 37, 4333-4336.	3.2	10
85	Organometallic MTCNQ films: a comparative study of CuTCNQ versus AgTCNQ. Physical Chemistry Chemical Physics, 2018, 20, 21705-21715.	2.8	10
86	Exact results for the density of states of a cluster. Journal of Physics C: Solid State Physics, 1974, 7, 61-64.	1.5	9
87	Interpretation of photoemission spectra of Cu in terms of surface density of states. Solid State Communications, 1979, 29, 635-640.	1.9	9
88	Realistic model for the electronic structure of amorphous SiOx alloy. Solid State Communications, 1981, 37, 979-982.	1.9	9
89	Electronic structure of substitutional oxygen in silicon. Solid State Communications, 1989, 71, 1107-1111.	1.9	9
90	Effects of topology versus disorder on the vibrational properties of amorphous semiconductors. Physical Review B, 1977, 15, 5076-5077.	3.2	8

#	Article	IF	Citations
91	Effects of overlap and next-nearest-neighbor interactions in tight-binding calculations. Physical Review B, 1978, 17, 3063-3069.	3.2	8
92	Possibility of intrinsic Si gap states localized at the Si-SiO2interface. Physical Review B, 1982, 25, 6511-6513.	3.2	8
93	A Hartree-Fock approach to electronic structure of non-periodic systems. Journal of Non-Crystalline Solids, 1985, 72, 181-189.	3.1	8
94	Superconductivity and Magnetic Order inCeRhIn5: Spectra of Coexistence. Physical Review Letters, 2007, 98, 126406.	7.8	8
95	Surface assembly of porphyrin nanorods with one-dimensional zincâ€“oxygen spinal cords. CrystEngComm, 2011, 13, 5591.	2.6	8
96	Electronic structure of copper nitrides as a function of nitrogen content. Thin Solid Films, 2013, 531, 588-591.	1.8	8
97	Pseudo-Jahn-Teller effect and chemical rebonding: Two distinct physical phenomena. Physical Review B, 1988, 37, 1016-1018.	3.2	7
98	Model for the variation upon doping of the isotope coefficient in high-Tcsuperconductors. Physical Review B, 1995, 51, 8494-8497.	3.2	7
99	Theoretical study of magnetic moments induced by defects at the SiC(110) surface. Physical Review B, 2011, 83, .	3.2	7
100	The crystal ionicity of the zincblende and rocksalt compounds as a function of the valence band gap. Journal of Physics C: Solid State Physics, 1974, 7, L303-L307.	1.5	6
101	AmorphousSixGe1â^'xO2. I. Electronic structure. Physical Review B, 1980, 21, 3589-3596.	3.2	6
102	A consistent interpretation of the atomic and electronic structure of the Si(111)â^'7Ã—7 surface. Solid State Communications, 1981, 39, 925-928.	1.9	6
103	Local approach to calculate total energies in semiconductors beyond the Hartree-Fock approximation. Physical Review B, 1991, 44, 12794-12799.	3.2	6
104	First-Principles Calculation of the Electronic Structure of Nonperiodic Solids: Application toaâ^'Si:H. Physical Review Letters, 1986, 56, 1731-1734.	7.8	5
105	Electronic structure of amorphous semiconducting alloys. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 70, 535-546.	0.6	5
106	First-principles calculations of the diamond (110) surface: A Mott insulator. Physical Review B, 2007, 75, .	3.2	5
107	Magnetism, microstructure and First Principles calculations of atomized and annealed Ni3Al. Journal of Alloys and Compounds, 2014, 615, S645-S647.	5.5	5
108	Exact solution of the Bethe lattice with long-range interactions: Application to a Heisenberg ferromagnet. Physical Review B, 1983, 28, 2839-2844.	3.2	4

#	Article	IF	Citations
109	Optical properties of amorphous semiconductors. Solid State Communications, 1992, 84, 217-220.	1.9	4
110	Band structure features involved in charge transfer in bonds. Physics Letters, Section A: General, Atomic and Solid State Physics, 1974, 47, 293-294.	2.1	3
111	Surface magnetic order in the Ising model: A Cayley tree approximation. Physics Letters, Section A: General, Atomic and Solid State Physics, 1977, 62, 93-94.	2.1	3
112	New Theoretical Method for Studying Elementary Excitations in Crystalline Disordered Alloys. Application to Phonons in Ni_xPt_{1â^'x}. Physica Status Solidi (B): Basic Research, 1982, 113, 697-707.	1.5	3
113	Substitutional impurities in a linear chain with Peierls instability: Single-impurity approach. Physical Review B, 1985, 31, 5086-5093.	3.2	3
114	Real space first principles calculation of the quasiparticle spectrum in semiconductors: Application to interstitial O in Si. Solid State Communications, 1995, 94, 335-340.	1.9	3
115	A charge density wave model for reconstructed monolayers of Co on Cu(100). Solid State Communications, 1981, 38, 317-320.	1.9	2
116	Coexistence of spiral spin-density waves and superconductivity: Ground-state properties. Physical Review B, 1990, 41, 2540-2542.	3.2	2
117	Short range order fluctuations and itinerant ferromagnetism in Ni 3 Al. Solid State Communications, 2015, 201, 111-114.	1.9	2
118	A rigorous proof of the existence of band tails in disordered magnetic insulators. Solid State Communications, 1974, 14, 1065-1068.	1.9	1
119	Moments and averages of the electronic density of states of amorphous and crystalline homopolar solids. Physics Letters, Section A: General, Atomic and Solid State Physics, 1975, 51, 79-80.	2.1	1
120	Calculation of the infrared spectra of hydrogenated and fluorinated amorphous Si. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1983, 117-118, 935-937.	0.9	1
121	Local approach to study densities of states in random alloys. Solid State Communications, 1983, 46, 823-826.	1.9	1
122	Weakening of bonds: Discussion of two different mechanisms. Solid State Communications, 1987, 62, 113-115.	1.9	1
123	Critical analysis of the response function in low-dimensional materials. Journal of Physics Condensed Matter, 2021, 33, 295701.	1.8	1
124	Electronic structure of amorphous SixGe1â^'xO2. Journal of Non-Crystalline Solids, 1980, 35-36, 71.	3.1	0
125	Itinerant magnetism in metallic glasses. Solid State Communications, 1984, 51, 753-756.	1.9	0
126	First principles calculation of the electronic structure of hydrogenated amorphous silicon. Journal of Non-Crystalline Solids, 1985, 77-78, 63-66.	3.1	0

#	Article	IF	Citations
127	ELECTRONIC STRUCTURE OF AMORPHOUS SiOx. Journal De Physique Colloque, 1981, 42, C4-1021-C4-1024.	0.2	0