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	Critical analysis of the response function in low-dimensional materials. Journal of Physics Condensed Matter, 2021, 33, 295701.	1.8	1
2	Band unfolding made simple. Journal of Physics Condensed Matter, 2020, 32, 205902.	1.8	16
3	Pressure-induced magnetism in rotated graphene bilayers. Physical Review B, 2019, 99, .	3.2	17
4	Selective Hydrogen Adsorption in Graphene Rotated Bilayers. Journal of Physical Chemistry B, 2018, 122, 595-600.	2.6	18
5	Organometallic MTCNQ films: a comparative study of CuTCNQ versus AgTCNQ. Physical Chemistry Chemical Physics, 2018, 20, 21705-21715.	2.8	10
6	Tuning the magnetic properties of pure hafnium by high pressure torsion. Acta Materialia, 2017, 123, 206-213.	7.9	14
7	Atomic-scale control of graphene magnetism by using hydrogen atoms. Science, 2016, 352, 437-441.	12.6	545
8	Theoretical study of the dynamics of atomic hydrogen adsorbed on graphene multilayers. Physical Review B, 2015, 91, .	3.2	23
9	Short range order fluctuations and itinerant ferromagnetism in Ni 3 Al. Solid State Communications, 2015, 201, 111-114.	1.9	2
10	Effect of hole doping on the magnetism of point defects in graphene: A theoretical study. Physical Review B, 2014, 90, .	3.2	18
11	Magnetism, microstructure and First Principles calculations of atomized and annealed Ni3Al. Journal of Alloys and Compounds, 2014, 615, S645-S647.	5.5	5
12	Magnetism in nanoparticles: tuning properties with coatings. Journal of Physics Condensed Matter, 2013, 25, 484006.	1.8	46
13	Electronic structure of copper nitrides as a function of nitrogen content. Thin Solid Films, 2013, 531, 588-591.	1.8	8
14	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
15	Electronic and structural characterization of divacancies in irradiated graphene. Physical Review B, 2012, 85, .	3.2	173
16	Theoretical study of magnetic moments induced by defects at the SiC(110) surface. Physical Review B, 2011, 83, .	3.2	7
17	Surface assembly of porphyrin nanorods with one-dimensional zincâ€“oxygen spinal cords. CrystEngComm, 2011, 13, 5591.	2.6	8
18	Coupling of magnetic moments with phonons and electron-phonon interaction in LaFeAsO 1-x F x. Europhysics Letters, 2011, 94, 37001.	2.0	14

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19	Stability, Adsorption, and Diffusion of <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, .	3.2	30
20	Kinetic energetics and kinetics study of H <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:msub></mml:math> in the Si clathrate hydrate. Physical Review B, 2011, .	7.8	83
21	Anomalous electron-phonon interaction in doped LaFeAsO: First-principles calculations. Physical Review B, 2009, 79, .	3.2	32
22	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
23	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
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></mml:mrow></mml:math> films epitaxially grown on Cu(001): Electronic structure and thermal stability. Physical Review B, 2008, 78, .	3.2	38
25	Formation of Gold Nanowires with Impurities: A First-Principles Molecular Dynamics Simulation. Physical Review Letters, 2007, 98, 096102.	7.8	26
26	Superconductivity and Magnetic Order inCeRhIn5: Spectra of Coexistence. Physical Review Letters, 2007, 98, 126406.	7.8	8
27	Design of molecular wires based on one-dimensional coordination polymers. Applied Physics Letters, 2007, 90, 193107.	3.3	24
28	Electronic structure of ultrathinÎ³â€²â€”Fe4N(100) films epitaxially grown on Cu(100). Physical Review B, 2007, 75, .	3.2	30
29	First-principles calculations of the diamond (110) surface: A Mott insulator. Physical Review B, 2007, 75, .	3.2	5
30	Comment on â€œMagnetism in Atomic-Size Palladium Contacts and Nanowiresâ€• Physical Review Letters, 2006, 96, 079701; author reply 079702.	7.8	32
31	Magnetism of two-dimensional defects in Pd: Stacking faults, twin boundaries, and surfaces. Physical Review B, 2006, 74, .	3.2	43
32	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
33	Low-energy quantum dynamics of atoms at defects; interstitial oxygen in silicon. Journal of Physics Condensed Matter, 1997, 9, 3107-3116.	1.8	11
34	Interstitial oxygen in germanium and silicon. Physical Review B, 1997, 56, 3820-3833.	3.2	55
35	Surface electronic structure of metastable FeSi(CsCl)(111) epitaxially grown on Si(111). Physical Review B, 1997, 55, R16065-R16068.	3.2	12
36	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

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37	Model for the variation upon doping of the isotope coefficient in high-Tcsuperconductors. Physical Review B, 1995, 51, 8494-8497.	3.2	7
38	Geometry and quantum delocalization of interstitial oxygen in silicon. Physical Review B, 1995, 51, 7862-7865.	3.2	28
39	Geometrical configuration of interstitial oxygen in silicon and in germanium. Solid State Communications, 1994, 89, 819-822.	1.9	11
40	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
41	Optical absorption in plasmaâ€deposited silicon oxynitride films. Applied Physics Letters, 1992, 60, 1399-1401.	3.3	35
42	Optical properties of amorphous semiconductors. Solid State Communications, 1992, 84, 217-220.	1.9	4
43	Interplay between electron-phonon superconductivity and magnetic order in high Tc superconductors. Solid State Communications, 1992, 81, 939-942.	1.9	16
44	Theoretical study of a-SiNxHy alloys. Journal of Non-Crystalline Solids, 1991, 137-138, 891-894.	3.1	14
45	Nonparametrized tight-binding method for local and extended defects in homopolar semiconductors. Physical Review B, 1991, 44, 6169-6187.	3.2	24
46	Local approach to calculate total energies in semiconductors beyond the Hartree-Fock approximation. Physical Review B, 1991, 44, 12794-12799.	3.2	6
47	Nonparametrized calculation of the electronic and vibrational structure of amorphousSiOx. Physical Review B, 1991, 43, 4552-4555.	3.2	24
48	Magnetic short-range order inCuO2planes of high-Tcsuperconductors. Physical Review B, 1991, 43, 3691-3694.	3.2	13
49	Coexistence of spiral spin-density waves and superconductivity: Ground-state properties. Physical Review B, 1990, 41, 2540-2542.	3.2	2
50	Spin polarization and dimer buckling at the Si(100)-2Ã—1 surface. Physical Review B, 1990, 42, 11310-11316.	3.2	30
51	Correlation between electronic structure and local ordering in hydrogenated amorphous silicon. Physical Review B, 1989, 40, 12416-12422.	3.2	16
52	Proposal for symmetric dimers at the Si(100)-2Ã—1 surface. Physical Review Letters, 1989, 62, 2491-2494.	7.8	118
53	Atomic configuration of H-based complexes in silicon. Solid State Communications, 1989, 72, 393-396.	1.9	21
54	Electronic structure of substitutional oxygen in silicon. Solid State Communications, 1989, 71, 1107-1111.	1.9	9

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55	Minimal tight-binding Hamiltonian for semiconductors. Physical Review B, 1988, 37, 4333-4336.	3.2	10
56	Pseudo-Jahn-Teller effect and chemical rebonding: Two distinct physical phenomena. Physical Review B, 1988, 37, 1016-1018.	3.2	7
57	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
58	Atomic oxygen in silicon: The formation of the Siâ€"Oâ€"Si bond. Physical Review B, 1987, 36, 8043-8048.	3.2	41
59	Theoretical study of oxygen in silicon: Breaking of the Siâ€"Si bond. Physical Review B, 1987, 35, 788-791.	3.2	31
60	Weakening of bonds: Discussion of two different mechanisms. Solid State Communications, 1987, 62, 113-115.	1.9	1
61	First-Principles Calculation of the Electronic Structure of Nonperiodic Solids: Application toaâ^'Si:H. Physical Review Letters, 1986, 56, 1731-1734.	7.8	5
62	Electronic structure of the Bi(111) surface. Physical Review B, 1986, 33, 4352-4355.	3.2	45
63	Theory of off-center impurities in semiconductors. Physical Review B, 1986, 34, 6038-6040.	3.2	21
64	Substitutional impurities in a linear chain with Peierls instability: Single-impurity approach. Physical Review B, 1985, 31, 5086-5093.	3.2	3
65	A Hartree-Fock approach to electronic structure of non-periodic systems. Journal of Non-Crystalline Solids, 1985, 72, 181-189.	3.1	8
66	First principles calculation of the electronic structure of hydrogenated amorphous silicon. Journal of Non-Crystalline Solids, 1985, 77-78, 63-66.	3.1	0
67	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
68	Effects of impurities on charge-density waves: A mean-field calculation. Physical Review B, 1984, 29, 4459-4467.	3.2	26
69	Itinerant magnetism in metallic glasses. Solid State Communications, 1984, 51, 753-756.	1.9	0
70	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
71	Local approach to study densities of states in random alloys. Solid State Communications, 1983, 46, 823-826.	1.9	1
72	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

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73	Long-range correlations in Bethe lattices. Physical Review B, 1983, 28, 3576-3578.	3.2	10
74	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
75	Possibility of intrinsic Si gap states localized at the Si-SiO2interface. Physical Review B, 1982, 25, 6511-6513.	3.2	8
76	Magnetic exchange splitting of a quasi two-dimensional hexagonal close packed layer of cobalt. Surface Science, 1982, 117, 319-329.	1.9	24
77	Theoretical study of intrinsic surface phonons in hydrogenated amorphous silicon. Solid State Communications, 1982, 44, 1477-1480.	1.9	13
78	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
79	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
80	A charge density wave model for reconstructed monolayers of Co on Cu(100). Solid State Communications, 1981, 38, 317-320.	1.9	2
81	Realistic model for the electronic structure of amorphous SiOx alloy. Solid State Communications, 1981, 37, 979-982.	1.9	9
82	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
83	Theoretical study of the electronic structure ofSiOx. Physical Review B, 1981, 24, 5718-5725.	3.2	76
84	ELECTRONIC STRUCTURE OF AMORPHOUS SiOx. Journal De Physique Colloque, 1981, 42, C4-1021-C4-1024.	0.2	0
85	Coexistence of charge-density waves and magnetic order. Physical Review B, 1980, 21, 5267-5271.	3.2	33
86	AmorphousSixGe1â^'xO2. I. Electronic structure. Physical Review B, 1980, 21, 3589-3596.	3.2	6
87	Electronic structure of amorphous SixGe1â^'xO2. Journal of Non-Crystalline Solids, 1980, 35-36, 71.	3.1	0
88	Interpretation of photoemission spectra of Cu in terms of surface density of states. Solid State Communications, 1979, 29, 635-640.	1.9	9
89	Lattice vibrations at (111) surfaces and stacking faults in transition metals: Ni. Surface Science, 1979, 85, 107-124.	1.9	16
90	Electronic structure of H chemisorbed on Si(111) surfaces. Solid State Communications, 1978, 25, 439-441.	1.9	13

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91	New interpretation of the electronic structure of SiO2. Solid State Communications, 1978, 27, 75-80.	1.9	17
92	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
93	Effects of overlap and next-nearest-neighbor interactions in tight-binding calculations. Physical Review B, 1978, 17, 3063-3069.	3.2	8
94	Vibrational properties of alloys: Study ofSixGe1â^'x. Physical Review B, 1978, 18, 2876-2883.	3.2	14
95	Effects of topology versus disorder on the vibrational properties of amorphous semiconductors. Physical Review B, 1977, 15, 5076-5077.	3.2	8
96	Electron states at planar and stepped semiconductor surfaces. Physical Review B, 1977, 16, 1542-1551.	3.2	32
97	Electron states at steps in semiconductor surfaces. Solid State Communications, 1977, 22, 147-151.	1.9	12
98	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
99	Electronic surface properties of group V semimetals. Surface Science, 1976, 57, 375-384.	1.9	11
100	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
101	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
102	Theory of Vibrational Properties of Amorphous Alloys: Application toSixGe1â^'x. Physical Review Letters, 1976, 37, 1062-1065.	7.8	33
103	Electronic Structure of Stacking Faults in Transition Metals: Nickel. Physical Review Letters, 1976, 37, 928-930.	7.8	21
104	Metal-semiconductor junction for (110) surfaces of zinc-blende compounds. Physical Review B, 1976, 13, 4408-4418.	3.2	85
105	Effects of the local configuration on the lattice dynamics of group-IV semiconductors. Physical Review B, 1976, 14, 531-537.	3.2	50
106	New approach to the study of binary alloys. Physical Review B, 1976, 13, 4387-4395.	3.2	30
107	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
108	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

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109	New theory of binary alloys with short-range order properties. Solid State Communications, 1975, 17, 1545-1548.	1.9	22
110	"Clusterâ€"Bethe-lattice" method: The electronic density of states of heteropolar systems. Physical Review B, 1975, 11, 2957-2964.	3.2	53
111	Theory of binary alloys including short-range order properties. Physical Review B, 1975, 12, 5664-5675.	3.2	90
112	Density of states of tight-binding disordered systems. Journal of Physics C: Solid State Physics, 1975, 8, 434-444.	1.5	12
113	Electronic surface structure of a tetrahedrally coordinated binary compound. Journal of Physics C: Solid State Physics, 1975, 8, 1571-1580.	1.5	19
114	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
115	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
116	"Cluster-Bethe-lattice" method: Electronic density of states of amorphous and crystalline homopolar solids. Physical Review B, 1974, 10, 5164-5174.	3.2	166
117	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
118	Exact results for the density of states of a cluster. Journal of Physics C: Solid State Physics, 1974, 7, 61-64.	1.5	9
119	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
120	A rigorous proof of the existence of band tails in disordered magnetic insulators. Solid State Communications, 1974, 14, 1065-1068.	1.9	1
121	New theoretical method to study densities of states of tetrahedrally coordinated solids. Solid State Communications, 1974, 15, 617-620.	1.9	68
122	Surface states and ionicity. Physica Status Solidi (B): Basic Research, 1973, 57, 175-186.	1.5	16
123	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
124	Electronic surface states in Ge. Journal of Physics C: Solid State Physics, 1972, 5, L146-L150.	1.5	14
125	Surface states calculation for the (100), (110) and (111) faces of Si. Surface Science, 1972, 29, 540-554.	1.9	33
126	Density of states and barrier height of metal-Si contacts. Journal of Physics C: Solid State Physics, 1971, 4, 2849-2858.	1.5	47

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127	Absence of Surface States in Oxidized Si. Physical Review Letters, 1971, 26, 138-140.	7.8	25