JosÃ© LuÃ-s Martins

List of Publications by Year
in descending order

Version: 2024-02-01

92 papers	22,526 citations	66234 42 h-index	51492 86 g-index
93 all docs	93 docs citations	93 times ranked	13264 citing authors

#	Article	IF	Citations
1	Practical Band Interpolation with a Generalized Luttingerâ€“Kohn Method. Physica Status Solidi (B): Basic Research, 2021, 258, 2000260.	0.7	0
2	Practical band interpolation with a modified tight-binding method. Journal of Physics Condensed Matter, 2019, 31, 215501.	0.7	1
3	Relaxation of atomic orbitals in a plane-wave basis. Physical Review B, 2014, 89, .	1.1	1
4	Stability analysis of a bulk material built from silicon cage clusters: A first-principles approach. Physical Review B, 2007, 76, .	1.1	28
5	Study of synthetic ferrimagnet-synthetic antiferromagnet structures for magnetic sensor application. Journal of Applied Physics, 2006, 99, 08B703.	1.1	19
6	An Effective Three-Dimensional Micromagnetic Method and Its Application to Magnetic Tunnel Junctions. Chinese Physics Letters, 2005, 22, 1270-1273.	1.3	1
7	First-principles molecular dynamics of liquid rubidium at low density. Journal of Non-Crystalline Solids, 2004, 347, 100-105.	1.5	7
8	First-principles norm-conserving pseudopotential with explicit incorporation of semicore states. Physical Review B, 2003, 68, .	1.1	25
9	Continuous thin barriers for low-resistance spin-dependent tunnel junctions. Journal of Applied Physics, 2003, 93, 8367-8369.	1.1	23
10	Current-induced switching in low resistance magnetic tunnel junctions. Journal of Applied Physics, 2003, 93, 8385-8387.	1.1	29
11	Density-functional studies of high-pressure properties and molecular dissociations of halogen molecular crystals. Physical Review B, 2003, 68, .	1.1	25
12	Density-functional study of nonmolecular phases of nitrogen: Metastable phase at low pressure. Physical Review B, 2003, 68, .	1.1	98
13	Current-induced magnetization switching in magnetic tunnel junctions. Applied Physics Letters, 2003, 82, 2871-2873.	1.5	78
14	Micromagnetic simulation for tunnel junctions with synthetic antiferromagnetic pinned layers annealed at different external fields. Journal of Applied Physics, 2002, 91, 8296.	1.1	15
15	First-principles study of the possibility of condensed phases of endohedral silicon cage clusters. Physical Review B, 2002, 66, .	1.1	37
16	Ab initio molecular dynamics of liquid Kâ€“Tl. Journal of Non-Crystalline Solids, 2002, 312-314, 69-73.	1.5	1
17	Growth and Formation of Fullerene Clusters. Journal of Cluster Science, 2001, 12, 513-525.	1.7	8
18	Evaluation of exchange-correlation energy, potential, and stress. Physical Review B, 2001, 64, .	1.1	29

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19	Density functional calculations on the structure of crystalline polyethylene under high pressures. Journal of Chemical Physics, 2001, 115, 11317-11324.	1.2	45
20	Parallelization of a Density Functional Program for Monte-Carlo Simulation of Large Molecules. Lecture Notes in Computer Science, 2001, , 230-241.	1.0	0
21	Density functional calculations of the structure of crystalline urea under high pressure. Chemical Physics Letters, 2000, 316, 297-302.	1.2	26
22	Homocoordination preference in NaCs and LiNa liquid alloys by first principles molecular dynamics. Journal of Chemical Physics, 1999, 111, 5067-5072.	1.2	10
23	First principles molecular dynamics of a liquid Liâ€“Na alloy. Computational and Theoretical Chemistry, 1999, 463, 145-149.	1.5	3
24	Electronic structure of silver halides. Solid State Communications, 1998, 105, 377-380.	0.9	23
25	AsNCa3 at high pressure. Computational Materials Science, 1998, 10, 298-301.	1.4	7
26	Ab initiostudies of the structural and electronic properties of solid cubane. Physical Review B, 1998, 58, 15307-15309.	1.1	18
27	Pressure-induced phase transitions in silver halides. Physical Review B, 1998, 57, 5098-5105.	1.1	53
28	Variable-cell-shape-based structural optimization applied to calcium nitrides. Physical Review B, 1998, 57, 7615-7620.	1.1	32
29	Ab initio pseudopotential calculation of the photo-response of metal clusters. Journal of Chemical Physics, 1997, 106, 6039-6044.	1.2	43
30	High-pressure phases of magnesium selenide and magnesium telluride. Physical Review B, 1997, 55, 775-779.	1.1	60
31	Metric tensor as the dynamical variable for variable-cell-shape molecular dynamics. Physical Review B, 1997, 55, 8733-8742.	1.1	167
32	Electronic Structure and Pressure Dependence for Some Ternary Calcium Nitrides. Physica Status Solidi (B): Basic Research, 1996, 198, 87-91.	0.7	7
33	Stability ofNanPb (nâ©½7) clusters: A first-principles molecular-dynamics study. Physical Review B, 1996, 54, 2937-2941.	1.1	22
34	Superconductivity in Alkali Fullerides. Kluwer International Series in Engineering and Computer Science, 1996, , 503-514.	0.2	0
35	High Pressure Properties of the Alkalineâ€Earth Sulphides. Physica Status Solidi (B): Basic Research, 1995, 190, 193-197.	0.7	25
36	First principles molecular dynamics simulation of liquid rubidium. Computational and Theoretical Chemistry, 1995, 330, 273-277.	1.5	0

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37	First-principles molecular dynamics of liquid cesium and rubidium. Physical Review B, 1995, 51, 872-877.	1.1	23
38	Ab initiomolecular dynamics with variable cell shape: Application toMgSiO3. Physical Review Letters, 1993, 70, 3947-3950.	2.9	301
39	Electronic properties of K-dopedC60(111): Photoemission and electron correlation. Physical Review B, 1993, 47, 13843-13847.	1.1	78
40	Simulation of Si clusters via Langevin molecular dynamics with quantum forces. Physical Review Letters, 1992, 68, 2956-2959.	2.9	115
41	Electronic structure of neutral and chargedC60clusters. Physical Review B, 1992, 45, 13671-13675.	1.1	81
42	Structural and electronic properties ofKnC60. Physical Review B, 1992, 46, 1766-1772.	1.1	113
43	Electronic structure ofCaxC60fullerides. Physical Review B, 1992, 46, 7961-7964.	1.1	51
44	Metallic and insulating phases ofLixC60,NaxC60, andRbxC60. Physical Review B, 1992, 45, 6348-6351.	1.1	96
45	Energetics of interplanar binding in graphite. Physical Review B, 1992, 46, 7185-7188.	1.1	195
46	Energy versus free-energy conservation in first-principles molecular dynamics. Physical Review B, 1992, 45, 11372-11374.	1.1	171
47	Structural and electronic properties ofC60. Physical Review B, 1992, 46, 1754-1765.	1.1	263
48	Superconductivity in M3C60. , 1992, , 485-491.		1
49	Structural properties ofSiO2in the stishovite structure. Physical Review B, 1991, 44, 4081-4088.	1.1	41
50	Efficient pseudopotentials for plane-wave calculations. II. Operators for fast iterative diagonalization. Physical Review B, 1991, 43, 8861-8869.	1.1	666
51	Pseudopotential plane-wave calculations for ZnS. Physical Review B, 1991, 43, 2213-2217.	1.1	144
52	Band dispersion and empty electronic states in solidC60: Inverse photoemission and theory. Physical Review B, 1991, 44, 1966-1969.	1.1	140
53	Efficient pseudopotentials for plane-wave calculations. Physical Review B, 1991, 43, 1993-2006.	1.1	14,468
54	Electronic States of KxC60: Insulating, Metallic, and Superconducting Character. Science, 1991, 252, 1417-1419.	6.0	277

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55	Electronic structure of solidC60: Experiment and theory. Physical Review Letters, 1991, 66, 1741-1744.	2.9	575
56	Electronic properties of Î±-quartz under pressure. Physical Review B, 1991, 44, 4771-4777.	1.1	81
57	First principles molecular dynamics of Li: Test of a new algorithm. Solid State Communications, 1991, 78, 831-834.	0.9	118
58	Analysis of occupied and empty electronic states of C60. Chemical Physics Letters, 1991, 180, 457-460.	1.2	143
59	Static electric dipole polarizability of small sodium aggregates. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 21, 83-83.	1.0	0
60	The nature of the interactions of poly(methyl methacrylate) oligomers with an aluminum surface. Journal of Chemical Physics, 1991, 95, 8616-8630.	1.2	27
61	Electronic states of solidC60: Symmetries and photoionization cross sections. Physical Review B, 1991, 44, 1962-1965.	1.1	138
62	Structural model for pseudobinary semiconductor alloys. Physical Review B, 1991, 43, 11873-11883.	1.1	27
63	Pressure dependence of the structural properties of Î±-quartz near the amorphous transition. Physical Review B, 1991, 44, 489-497.	1.1	65
64	Electronic and structural properties of TiO2 in the rutile structure. Solid State Communications, 1990, 76, 635-638.	0.9	47
65	A straightforward method for generating soft transferable pseudopotentials. Solid State Communications, 1990, 74, 613-616.	0.9	449
66	Structural properties of Î±-quartz near the amorphous transition. Physical Review Letters, 1990, 65, 3309-3312.	2.9	86
67	Static electric polarizabilities as evidence for cluster geometries. Physical Review Letters, 1990, 65, 476-479.	2.9	68
68	Equations of state of alkali hydrides at high pressures. Physical Review B, 1990, 41, 7883-7886.	1.1	45
69	Static electric polarizabilities of sodium clusters. Physical Review B, 1990, 42, 11598-11609.	1.1	42
70	Comparison of selfâ€consistent calculations of the static polarizability of atoms and molecules. Journal of Chemical Physics, 1990, 92, 527-535.	1.2	26
71	Theory of high-pressure phases of hydrogen. Physical Review Letters, 1989, 62, 1150-1153.	2.9	147
72	New methods for the calculation of the electronic structure of clusters: application for Na13 to Na147. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 347-351.	1.0	9

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73	Static electric dipole polarizability of small sodium aggregates. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 353-356.	1.0	10
74	Static electric dipole polarizability of small sodium aggregates. , 1989, , 353-356.		0
75	Superconductivity in primitive hexagonal germanium. Physical Review B, 1988, 37, 3304-3307.	1.1	19
76	Electronic and structural properties of LiBeH3. Physical Review B, 1988, 38, 12776-12779.	1.1	21
77	Diagonalization of large matrices in pseudopotential band-structure calculations: Dual-space formalism. Physical Review B, 1988, 37, 6134-6138.	1.1	175
78	Reply to â€˜â€˜Comment on â€˜Atomic structure and ordering in semiconductor alloysâ€™ â€™â€™. Physical Review B, 1987, 36, 2902-2905.	1.1	4
79	Stability of Ordered Bulk and Epitaxial Semiconductor Alloys. Physical Review Letters, 1986, 56, 1400-1403.	2.9	245
80	Ordering and decomposition in semiconductor alloys. Journal of Materials Research, 1986, 1, 523-526.	1.2	48
81	Electronic and structural properties of sodium clusters. Physical Review B, 1985, 31, 1804-1816.	1.1	352
82	Structural and chemical changes in binary versus ternary tetrahedral semiconductors. Physical Review B, 1985, 32, 2689-2692.	1.1	19
83	Ground-state properties of very small silver clusters. Surface Science, 1985, 156, 635-640.	0.8	30
84	Atomic structure and ordering in semiconductor alloys. Physical Review B, 1985, 31, 2561-2564.	1.1	360
85	Forces in pseudopotential molecular calculations. Journal of Chemical Physics, 1984, 80, 1525-1528.	1.2	8
86	Equilibrium Geometries and Electronic Structures of Small Sodium Clusters. Physical Review Letters, 1984, 53, 655-658.	2.9	76
87	Bond lengths around isovalent impurities and in semiconductor solid solutions. Physical Review B, 1984, 30, 6217-6220.	1.1	416
88	Calculation of Cluster Geometries with the Help of Hellmannâ€Feynman Forces. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1984, 88, 239-240.	0.9	13
89	Electronic properties of alkali trimers. Journal of Chemical Physics, 1983, 78, 5646-5655.	1.2	184
90	Ground-state properties ofAg2: A local-density pseudopotential approach. Physical Review A, 1983, 28, 3637-3639.	1.0	17

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91	Variational spherical model of small metallic particles. Surface Science, 1981, 106, 265-271.	0.8	197
92	Pseudopotential spin-density-functional calculation of the electronic properties of small lithium and sodium clusters. Surface Science, 1981, 106, 280-286.	0.8	34