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	Efficient pseudopotentials for plane-wave calculations. Physical Review B, 1991, 43, 1993-2006.	1.1	14,468
2	Efficient pseudopotentials for plane-wave calculations. II. Operators for fast iterative diagonalization. Physical Review B, 1991, 43, 8861-8869.	1.1	666
3	Electronic structure of solidC60: Experiment and theory. Physical Review Letters, 1991, 66, 1741-1744.	2.9	575
4	A straightforward method for generating soft transferable pseudopotentials. Solid State Communications, 1990, 74, 613-616.	0.9	449
5	Bond lengths around isovalent impurities and in semiconductor solid solutions. Physical Review B, 1984, 30, 6217-6220.	1.1	416
6	Atomic structure and ordering in semiconductor alloys. Physical Review B, 1985, 31, 2561-2564.	1.1	360
7	Electronic and structural properties of sodium clusters. Physical Review B, 1985, 31, 1804-1816.	1.1	352
8	Ab initiomolecular dynamics with variable cell shape: Application toMgSiO3. Physical Review Letters, 1993, 70, 3947-3950.	2.9	301
9	Electronic States of KxC60: Insulating, Metallic, and Superconducting Character. Science, 1991, 252, 1417-1419.	6.0	277
10	Structural and electronic properties ofC60. Physical Review B, 1992, 46, 1754-1765.	1.1	263
11	Stability of Ordered Bulk and Epitaxial Semiconductor Alloys. Physical Review Letters, 1986, 56, 1400-1403.	2.9	245
12	Variational spherical model of small metallic particles. Surface Science, 1981, 106, 265-271.	0.8	197
13	Energetics of interplanar binding in graphite. Physical Review B, 1992, 46, 7185-7188.	1.1	195
14	Electronic properties of alkali trimers. Journal of Chemical Physics, 1983, 78, 5646-5655.	1.2	184
15	Diagonalization of large matrices in pseudopotential band-structure calculations: Dual-space formalism. Physical Review B, 1988, 37, 6134-6138.	1.1	175
16	Energy versus free-energy conservation in first-principles molecular dynamics. Physical Review B, 1992, 45, 11372-11374.	1.1	171
17	Metric tensor as the dynamical variable for variable-cell-shape molecular dynamics. Physical Review B, 1997, 55, 8733-8742.	1.1	167
18	Theory of high-pressure phases of hydrogen. Physical Review Letters, 1989, 62, 1150-1153.	2.9	147

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19	Pseudopotential plane-wave calculations for ZnS. Physical Review B, 1991, 43, 2213-2217.	1.1	144
20	Analysis of occupied and empty electronic states of C60. Chemical Physics Letters, 1991, 180, 457-460.	1.2	143
21	Band dispersion and empty electronic states in solidC60: Inverse photoemission and theory. Physical Review B, 1991, 44, 1966-1969.	1.1	140
22	Electronic states of solidC60: Symmetries and photoionization cross sections. Physical Review B, 1991, 44, 1962-1965.	1.1	138
23	First principles molecular dynamics of Li: Test of a new algorithm. Solid State Communications, 1991, 78, 831-834.	0.9	118
24	Simulation of Si clusters via Langevin molecular dynamics with quantum forces. Physical Review Letters, 1992, 68, 2956-2959.	2.9	115
25	Structural and electronic properties ofKnC60. Physical Review B, 1992, 46, 1766-1772.	1.1	113
26	Density-functional study of nonmolecular phases of nitrogen: Metastable phase at low pressure. Physical Review B, 2003, 68, .	1.1	98
27	Metallic and insulating phases ofLixC60,NaxC60, andRbxC60. Physical Review B, 1992, 45, 6348-6351.	1.1	96
28	Structural properties of Î±-quartz near the amorphous transition. Physical Review Letters, 1990, 65, 3309-3312.	2.9	86
29	Electronic properties of Î±-quartz under pressure. Physical Review B, 1991, 44, 4771-4777.	1.1	81
30	Electronic structure of neutral and chargedC60clusters. Physical Review B, 1992, 45, 13671-13675.	1.1	81
31	Electronic properties of K-dopedC60(111): Photoemission and electron correlation. Physical Review B, 1993, 47, 13843-13847.	1.1	78
32	Current-induced magnetization switching in magnetic tunnel junctions. Applied Physics Letters, 2003, 82, 2871-2873.	1.5	78
33	Equilibrium Geometries and Electronic Structures of Small Sodium Clusters. Physical Review Letters, 1984, 53, 655-658.	2.9	76
34	Static electric polarizabilities as evidence for cluster geometries. Physical Review Letters, 1990, 65, 476-479.	2.9	68
35	Pressure dependence of the structural properties of Î±-quartz near the amorphous transition. Physical Review B, 1991, 44, 489-497.	1.1	65
36	High-pressure phases of magnesium selenide and magnesium telluride. Physical Review B, 1997, 55, 775-779.	1.1	60

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37	Pressure-induced phase transitions in silver halides. Physical Review B, 1998, 57, 5098-5105.	1.1	53
38	Electronic structure ofCaxC60fullerides. Physical Review B, 1992, 46, 7961-7964.	1.1	51
39	Ordering and decomposition in semiconductor alloys. Journal of Materials Research, 1986, 1, 523-526.	1.2	48
40	Electronic and structural properties of TiO2 in the rutile structure. Solid State Communications, 1990, 76, 635-638.	0.9	47
41	Equations of state of alkali hydrides at high pressures. Physical Review B, 1990, 41, 7883-7886.	1.1	45
42	Density functional calculations on the structure of crystalline polyethylene under high pressures. Journal of Chemical Physics, 2001, 115, 11317-11324.	1.2	45
43	Ab initio pseudopotential calculation of the photo-response of metal clusters. Journal of Chemical Physics, 1997, 106, 6039-6044.	1.2	43
44	Static electric polarizabilities of sodium clusters. Physical Review B, 1990, 42, 11598-11609.	1.1	42
45	Structural properties ofSiO2in the stishovite structure. Physical Review B, 1991, 44, 4081-4088.	1.1	41
46	First-principles study of the possibility of condensed phases of endohedral silicon cage clusters. Physical Review B, 2002, 66, .	1.1	37
47	Pseudopotential spin-density-functional calculation of the electronic properties of small lithium and sodium clusters. Surface Science, 1981, 106, 280-286.	0.8	34
48	Variable-cell-shape-based structural optimization applied to calcium nitrides. Physical Review B, 1998, 57, 7615-7620.	1.1	32
49	Ground-state properties of very small silver clusters. Surface Science, 1985, 156, 635-640.	0.8	30
50	Evaluation of exchange-correlation energy, potential, and stress. Physical Review B, 2001, 64, .	1.1	29
51	Current-induced switching in low resistance magnetic tunnel junctions. Journal of Applied Physics, 2003, 93, 8385-8387.	1.1	29
52	Stability analysis of a bulk material built from silicon cage clusters: A first-principles approach. Physical Review B, 2007, 76, .	1.1	28
53	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
54	Structural model for pseudobinary semiconductor alloys. Physical Review B, 1991, 43, 11873-11883.	1.1	27

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55	Comparison of selfâ€consistent calculations of the static polarizability of atoms and molecules. Journal of Chemical Physics, 1990, 92, 527-535.	1.2	26
56	Density functional calculations of the structure of crystalline urea under high pressure. Chemical Physics Letters, 2000, 316, 297-302.	1.2	26
57	High Pressure Properties of the Alkalineâ€Earth Sulphides. Physica Status Solidi (B): Basic Research, 1995, 190, 193-197.	0.7	25
58	First-principles norm-conserving pseudopotential with explicit incorporation of semicore states. Physical Review B, 2003, 68, .	1.1	25
59	Density-functional studies of high-pressure properties and molecular dissociations of halogen molecular crystals. Physical Review B, 2003, 68, .	1.1	25
60	First-principles molecular dynamics of liquid cesium and rubidium. Physical Review B, 1995, 51, 872-877.	1.1	23
61	Electronic structure of silver halides. Solid State Communications, 1998, 105, 377-380.	0.9	23
62	Continuous thin barriers for low-resistance spin-dependent tunnel junctions. Journal of Applied Physics, 2003, 93, 8367-8369.	1.1	23
63	Stability ofNanPb (nâ©½7) clusters: A first-principles molecular-dynamics study. Physical Review B, 1996, 54, 2937-2941.	1.1	22
64	Electronic and structural properties of LiBeH3. Physical Review B, 1988, 38, 12776-12779.	1.1	21
65	Structural and chemical changes in binary versus ternary tetrahedral semiconductors. Physical Review B, 1985, 32, 2689-2692.	1.1	19
66	Superconductivity in primitive hexagonal germanium. Physical Review B, 1988, 37, 3304-3307.	1.1	19
67	Study of synthetic ferrimagnet-synthetic antiferromagnet structures for magnetic sensor application. Journal of Applied Physics, 2006, 99, 08B703.	1.1	19
68	Ab initiostudies of the structural and electronic properties of solid cubane. Physical Review B, 1998, 58, 15307-15309.	1.1	18
69	Ground-state properties ofAg2: A local-density pseudopotential approach. Physical Review A, 1983, 28, 3637-3639.	1.0	17
70	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
71	Calculation of Cluster Geometries with the Help of Hellmannâ€Feynman Forces. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1984, 88, 239-240.	0.9	13
72	Static electric dipole polarizability of small sodium aggregates. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 353-356.	1.0	10

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73	Homocoordination preference in NaCs and LiNa liquid alloys by first principles molecular dynamics. Journal of Chemical Physics, 1999, 111, 5067-5072.	1.2	10
74	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
75	Forces in pseudopotential molecular calculations. Journal of Chemical Physics, 1984, 80, 1525-1528.	1.2	8
76	Growth and Formation of Fullerene Clusters. Journal of Cluster Science, 2001, 12, 513-525.	1.7	8
77	Electronic Structure and Pressure Dependence for Some Ternary Calcium Nitrides. Physica Status Solidi (B): Basic Research, 1996, 198, 87-91.	0.7	7
78	AsNCa3 at high pressure. Computational Materials Science, 1998, 10, 298-301.	1.4	7
79	First-principles molecular dynamics of liquid rubidium at low density. Journal of Non-Crystalline Solids, 2004, 347, 100-105.	1.5	7
80	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
81	First principles molecular dynamics of a liquid Liâ€“Na alloy. Computational and Theoretical Chemistry, 1999, 463, 145-149.	1.5	3
82	Ab initio molecular dynamics of liquid Kâ€“Tl. Journal of Non-Crystalline Solids, 2002, 312-314, 69-73.	1.5	1
83	An Effective Three-Dimensional Micromagnetic Method and Its Application to Magnetic Tunnel Junctions. Chinese Physics Letters, 2005, 22, 1270-1273.	1.3	1
84	Relaxation of atomic orbitals in a plane-wave basis. Physical Review B, 2014, 89, .	1.1	1
85	Practical band interpolation with a modified tight-binding method. Journal of Physics Condensed Matter, 2019, 31, 215501.	0.7	1
86	Superconductivity in M3C60. , 1992, , 485-491.		1
87	Static electric dipole polarizability of small sodium aggregates. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 21, 83-83.	1.0	0
88	First principles molecular dynamics simulation of liquid rubidium. Computational and Theoretical Chemistry, 1995, 330, 273-277.	1.5	0
89	Practical Band Interpolation with a Generalized Luttingerâ€“Kohn Method. Physica Status Solidi (B): Basic Research, 2021, 258, 2000260.	0.7	0
90	Parallelization of a Density Functional Program for Monte-Carlo Simulation of Large Molecules. Lecture Notes in Computer Science, 2001, , 230-241.	1.0	0

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91	Static electric dipole polarizability of small sodium aggregates. , 1989, , 353-356.		0
92	Superconductivity in Alkali Fullerides. Kluwer International Series in Engineering and Computer Science, 1996, , 503-514.	0.2	0