Jos Lus Martins

List of Publications by Year in Descending Order

92 papers	20,618 citations	42 h-index	93 g-index
93 ext. papers	21,531 ext. citations	3.7 avg, IF	6.7 L-index

#	Paper	IF	Citations
92	Practical Band Interpolation with a Generalized Luttinger–Kohn Method. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2000260	1.3	
91	Practical band interpolation with a modified tight-binding method. *Journal of Physics Condensed Matter*, **2019**, 31, 215501	1.8	1
90	Relaxation of atomic orbitals in a plane-wave basis. *Physical Review B*, **2014**, 89,	3.3	1
89	Stability analysis of a bulk material built from silicon cage clusters: A first-principles approach. *Physical Review B*, **2007**, 76,	3.3	25
88	Study of synthetic ferrimagnet-synthetic antiferromagnet structures for magnetic sensor application. *Journal of Applied Physics*, **2006**, 99, 08B703	2.5	15
87	An Effective Three-Dimensional Micromagnetic Method and Its Application to Magnetic Tunnel Junctions. *Chinese Physics Letters*, **2005**, 22, 1270-1273	1.8	1
86	First-principles molecular dynamics of liquid rubidium at low density. *Journal of Non-Crystalline Solids*, **2004**, 347, 100-105	3.9	7
85	First-principles norm-conserving pseudopotential with explicit incorporation of semicore states. *Physical Review B*, **2003**, 68,	3.3	23
84	Continuous thin barriers for low-resistance spin-dependent tunnel junctions. *Journal of Applied Physics*, **2003**, 93, 8367-8369	2.5	22
83	Current-induced switching in low resistance magnetic tunnel junctions. *Journal of Applied Physics*, **2003**, 93, 8385-8387	2.5	28
82	Density-functional studies of high-pressure properties and molecular dissociations of halogen molecular crystals. *Physical Review B*, **2003**, 68,	3.3	23
81	Density-functional study of nonmolecular phases of nitrogen: Metastable phase at low pressure. *Physical Review B*, **2003**, 68,	3.3	79
80	Current-induced magnetization switching in magnetic tunnel junctions. *Applied Physics Letters*, **2003**, 82, 2871-2873	3.4	70
79	Micromagnetic simulation for tunnel junctions with synthetic antiferromagnetic pinned layers annealed at different external fields. *Journal of Applied Physics*, **2002**, 91, 8296	2.5	13
78	First-principles study of the possibility of condensed phases of endohedral silicon cage clusters. *Physical Review B*, **2002**, 66,	3.3	28
77	Ab initio molecular dynamics of liquid KCl. *Journal of Non-Crystalline Solids*, **2002**, 312-314, 69-73	3.9	1
76	Growth and Formation of Fullerene Clusters. *Journal of Cluster Science*, **2001**, 12, 513-525	3	8

75	Evaluation of exchange-correlation energy, potential, and stress. *Physical Review B*, **2001**, 64,	3.3	26
74	Density functional calculations on the structure of crystalline polyethylene under high pressures. *Journal of Chemical Physics*, **2001**, 115, 11317-11324	3.9	34
73	Parallelization of a Density Functional Program for Monte-Carlo Simulation of Large Molecules. *Lecture Notes in Computer Science*, **2001**, 230-241	0.9	
72	Density functional calculations of the structure of crystalline urea under high pressure. *Chemical Physics Letters*, **2000**, 316, 297-302	2.5	22
71	Homocoordination preference in NaCs and LiNa liquid alloys by first principles molecular dynamics. *Journal of Chemical Physics*, **1999**, 111, 5067-5072	3.9	10
70	First principles molecular dynamics of a liquid LiNa alloy. *Computational and Theoretical Chemistry*, **1999**, 463, 145-149		2
69	Electronic structure of silver halides. *Solid State Communications*, **1998**, 105, 377-380	1.6	18
68	AsNCa3 at high pressure. *Computational Materials Science*, **1998**, 10, 298-301	3.2	7
67	Ab initio studies of the structural and electronic properties of solid cubane. *Physical Review B*, **1998**, 58, 15307-15309	3.3	16
66	Pressure-induced phase transitions in silver halides. *Physical Review B*, **1998**, 57, 5098-5105	3.3	45
65	Variable-cell-shape-based structural optimization applied to calcium nitrides. *Physical Review B*, **1998**, 57, 7615-7620	3.3	29
64	Ab initio pseudopotential calculation of the photo-response of metal clusters. *Journal of Chemical Physics*, **1997**, 106, 6039-6044	3.9	39
63	High-pressure phases of magnesium selenide and magnesium telluride. *Physical Review B*, **1997**, 55, 775-779	3.3	51
62	Metric tensor as the dynamical variable for variable-cell-shape molecular dynamics. *Physical Review B*, **1997**, 55, 8733-8742	3.3	128
61	Electronic Structure and Pressure Dependence for Some Ternary Calcium Nitrides. *Physica Status Solidi (B): Basic Research*, **1996**, 198, 87-91	1.3	7
60	Stability of NanPb (n . *Physical Review B*, **1996**, 54, 2937-2941	3.3	22
59	Superconductivity in Alkali Fullerides. *Kluwer International Series in Engineering and Computer Science*, **1996**, 503-514		
58	High Pressure Properties of the Alkaline-Earth Sulphides. *Physica Status Solidi (B): Basic Research*, **1995**, 190, 193-197	1.3	23

57	First principles molecular dynamics simulation of liquid rubidium. *Computational and Theoretical Chemistry*, **1995**, 330, 273-277		
56	First-principles molecular dynamics of liquid cesium and rubidium. *Physical Review B*, **1995**, 51, 872-877	3.3	21
55	Ab initio molecular dynamics with variable cell shape: Application to MgSiO3. *Physical Review Letters*, **1993**, 70, 3947-3950	7.4	247
54	Electronic properties of K-doped C60(111): Photoemission and electron correlation. *Physical Review B*, **1993**, 47, 13843-13847	3.3	75
53	Simulation of Si clusters via Langevin molecular dynamics with quantum forces. *Physical Review Letters*, **1992**, 68, 2956-2959	7.4	110
52	Electronic structure of neutral and charged C60 clusters. *Physical Review B*, **1992**, 45, 13671-13675	3.3	78
51	Structural and electronic properties of KnC60. *Physical Review B*, **1992**, 46, 1766-1772	3.3	102
50	Electronic structure of CaxC60 fullerides. *Physical Review B*, **1992**, 46, 7961-7964	3.3	47
49	Metallic and insulating phases of LixC60, NaxC60, and RbxC60. *Physical Review B*, **1992**, 45, 6348-6351	3.3	91
48	Energetics of interplanar binding in graphite. *Physical Review B*, **1992**, 46, 7185-7188	3.3	181
47	Energy versus free-energy conservation in first-principles molecular dynamics. *Physical Review B*, **1992**, 45, 11372-11374	3.3	151
46	Structural and electronic properties of C60. *Physical Review B*, **1992**, 46, 1754-1765	3.3	253
45	Superconductivity in M3C60 **1992**, 485-491		1
44	First principles molecular dynamics of Li: Test of a new algorithm. *Solid State Communications*, **1991**, 78, 831-834	1.6	101
43	Analysis of occupied and empty electronic states of C60. *Chemical Physics Letters*, **1991**, 180, 457-460	2.5	137
42	Static electric dipole polarizability of small sodium aggregates. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1991**, 21, 83-83		
41	The nature of the interactions of poly(methyl methacrylate) oligomers with an aluminum surface. *Journal of Chemical Physics*, **1991**, 95, 8616-8630	3.9	26
40	Electronic states of solid C60: Symmetries and photoionization cross sections. *Physical Review B*, **1991**, 44, 1962-1965	3.3	135

39	Structural model for pseudobinary semiconductor alloys. *Physical Review B*, **1991**, 43, 11873-11883	3.3	26
38	Pressure dependence of the structural properties of alpha -quartz near the amorphous transition. *Physical Review B*, **1991**, 44, 489-497	3.3	55
37	Structural properties of SiO2 in the stishovite structure. *Physical Review B*, **1991**, 44, 4081-4088	3.3	34
36	Efficient pseudopotentials for plane-wave calculations. II. Operators for fast iterative diagonalization. *Physical Review B*, **1991**, 43, 8861-8869	3.3	584
35	Pseudopotential plane-wave calculations for ZnS. *Physical Review B*, **1991**, 43, 2213-2217	3.3	134
34	Band dispersion and empty electronic states in solid C60: Inverse photoemission and theory. *Physical Review B*, **1991**, 44, 1966-1969	3.3	134
33	Efficient pseudopotentials for plane-wave calculations. *Physical Review B*, **1991**, 43, 1993-2006	3.3	13225
32	Electronic States of KxC60: Insulating, Metallic, and Superconducting Character. *Science*, **1991**, 252, 1417-9	3.3	266
31	Electronic structure of solid C60: Experiment and theory. *Physical Review Letters*, **1991**, 66, 1741-1744	7.4	548
30	Electronic properties of alpha -quartz under pressure. *Physical Review B*, **1991**, 44, 4771-4777	3.3	73
29	Electronic and structural properties of TiO2 in the rutile structure. *Solid State Communications*, **1990**, 76, 635-638	1.6	46
28	A straightforward method for generating soft transferable pseudopotentials. *Solid State Communications*, **1990**, 74, 613-616	1.6	403
27	Structural properties of alpha -quartz near the amorphous transition. *Physical Review Letters*, **1990**, 65, 3309-3312	7.4	73
26	Static electric polarizabilities as evidence for cluster geometries. *Physical Review Letters*, **1990**, 65, 476-479	7.4	65
25	Equations of state of alkali hydrides at high pressures. *Physical Review B*, **1990**, 41, 7883-7886	3.3	42
24	Static electric polarizabilities of sodium clusters. *Physical Review B*, **1990**, 42, 11598-11609	3.3	42
23	Comparison of self-consistent calculations of the static polarizability of atoms and molecules. *Journal of Chemical Physics*, **1990**, 92, 527-535	3.9	24
22	Theory of high-pressure phases of hydrogen. *Physical Review Letters*, **1989**, 62, 1150-1153	7.4	137

21	New methods for the calculation of the electronic structure of clusters: application for Na13 to Na147. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1989**, 12, 347-351		8
20	Static electric dipole polarizability of small sodium aggregates. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1989**, 12, 353-356		10
19	Static electric dipole polarizability of small sodium aggregates **1989**, 353-356		
18	Superconductivity in primitive hexagonal germanium. *Physical Review B*, **1988**, 37, 3304-3307	3.3	18
17	Electronic and structural properties of LiBeH3. *Physical Review B*, **1988**, 38, 12776-12779	3.3	21
16	Diagonalization of large matrices in pseudopotential band-structure calculations: Dual-space formalism. *Physical Review B*, **1988**, 37, 6134-6138	3.3	147
15	Reply to "Comment on \Atomic structure and ordering in semiconductor alloysV". *Physical Review B*, **1987**, 36, 2902-2905	3.3	4
14	Stability of ordered bulk and epitaxial semiconductor alloys. *Physical Review Letters*, **1986**, 56, 1400-1403	7.4	224
13	Ordering and decomposition in semiconductor alloys. *Journal of Materials Research*, **1986**, 1, 523-526	2.5	47
12	Electronic and structural properties of sodium clusters. *Physical Review B*, **1985**, 31, 1804-1816	3.3	347
11	Structural and chemical changes in binary versus ternary tetrahedral semiconductors. *Physical Review B*, **1985**, 32, 2689-2692	3.3	16
10	Ground-state properties of very small silver clusters. *Surface Science*, **1985**, 156, 635-640	1.8	29
9	Atomic structure and ordering in semiconductor alloys. *Physical Review B*, **1985**, 31, 2561-2564	3.3	347
8	Forces in pseudopotential molecular calculations. *Journal of Chemical Physics*, **1984**, 80, 1525-1528	3.9	8
7	Equilibrium Geometries and Electronic Structures of Small Sodium Clusters. *Physical Review Letters*, **1984**, 53, 655-658	7.4	75
6	Bond lengths around isovalent impurities and in semiconductor solid solutions. *Physical Review B*, **1984**, 30, 6217-6220	3.3	395
5	Calculation of Cluster Geometries with the Help of Hellmann-Feynman Forces. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1984**, 88, 239-240		13
4	Electronic properties of alkali trimers. *Journal of Chemical Physics*, **1983**, 78, 5646-5655	3.9	172

3	Ground-state properties of Ag2: A local-density pseudopotential approach. *Physical Review A*, **1983**, 28, 3637-3639	2.6	17
2	Variational spherical model of small metallic particles. *Surface Science*, **1981**, 106, 265-271	1.8	183
1	Pseudopotential spin-density-functional calculation of the electronic properties of small lithium and sodium clusters. *Surface Science*, **1981**, 106, 280-286	1.8	32