Jose M Soler

List of Publications by Year
in descending order

120 papers	25,323 citations	34105 52 h-index	20358 116 g-index
123 all docs	123 docs citations	123 times ranked	16865 citing authors

#	Article	IF	Citations
1	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	1.8	9,150
2	Self-consistent order-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>density-functional calculations for very large systems. Physical Review B, 1996, 53, R10441-R10444.	3.2	2,422
3	Density-functional method for very large systems with LCAO basis sets. International Journal of Quantum Chemistry, 1997, 65, 453-461.	2.0	1,426
4	Efficient Implementation of a van der Waals Density Functional: Application to Double-Wall Carbon Nanotubes. Physical Review Letters, 2009, 103, 096102.	7.8	1,369
5	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
6	Ab initiostructural, elastic, and vibrational properties of carbon nanotubes. Physical Review B, 1999, 59, 12678-12688.	3.2	854
7	Absence of dc-Conductivity inÎ»-DNA. Physical Review Letters, 2000, 85, 4992-4995.	7.8	602
8	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
9	Trends in the structure and bonding of noble metal clusters. Physical Review B, 2004, 70, .	3.2	509
10	Projection of plane-wave calculations into atomic orbitals. Solid State Communications, 1995, 95, 685-690.	1.9	415
11	Interatomic Forces in Scanning Tunneling Microscopy: Giant Corrugations of the Graphite Surface. Physical Review Letters, 1986, 57, 444-447.	7.8	401
12	Lowest Energy Structures of Gold Nanoclusters. Physical Review Letters, 1998, 81, 1600-1603.	7.8	356
13	Optimal meshes for integrals in real- and reciprocal-space unit cells. Physical Review B, 1992, 45, 13891-13898.	3.2	275
14	Electron-metal-surface interaction potential with vacuum tunneling: Observation of the image force. Physical Review B, 1984, 30, 4816-4818.	3.2	256
15	Systematic generation of finite-range atomic basis sets for linear-scaling calculations. Physical Review B, 2002, 66, .	3.2	251
16	Density, structure, and dynamics of water: The effect of van der Waals interactions. Journal of Chemical Physics, 2011, 134, 024516.	3.0	242
17	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. Physical Review Letters, 1999, 83, 3884-3887.	7.8	235
18	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229

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19	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. Physical Review Letters, 1999, 82, 3520-3523.	7.8	173
20	Metallic bonding and cluster structure. Physical Review B, 2000, 61, 5771-5780.	3.2	163
21	Analysis of atomic orbital basis sets from the projection of plane-wave results. Journal of Physics Condensed Matter, 1996, 8, 3859-3880.	1.8	161
22	Do Thiols Merely Passivate Gold Nanoclusters?. Physical Review Letters, 2000, 85, 5250-5251.	7.8	158
23	Flexibility in a Metalâ€“Organic Framework Material Controlled by Weak Dispersion Forces: The Bistability of MILâ€53(Al). Angewandte Chemie - International Edition, 2010, 49, 7501-7503.	13.8	158
24	Augmented-plane-wave forces. Physical Review B, 1990, 42, 9728-9731.	3.2	153
25	Simple formula for the atomic forces in the augmented-plane-wave method. Physical Review B, 1989, 40, 1560-1564.	3.2	148
26	The puzzling stability of monatomic gold wires. Surface Science, 1999, 426, L441-L446.	1.9	120
27	Seeing molecular orbitals. Chemical Physics Letters, 2000, 321, 78-82.	2.6	117
28	Anomalous Nuclear Quantum Effects in Ice. Physical Review Letters, 2012, 108, 193003.	7.8	110
29	Planar and cagelike structures of gold clusters: Density-functional pseudopotential calculations. Physical Review B, 2006, 73, .	3.2	108
30	Microcluster Growth: Transition from Successive Monomer Addition to Coagulation. Physical Review Letters, 1982, 49, 1857-1860.	7.8	107
31	The effect of ionization on magic numbers of rare-gas clusters. Chemical Physics Letters, 1984, 109, 71-75.	2.6	101
32	Dissociation channels of multiply charged van der Waals clusters. Physical Review A, 1988, 38, 3236-3248.	2.5	101
33	Systematicab initiostudy of the electronic and magnetic properties of different pure and mixed iron systems. Physical Review B, 2000, 61, 13639-13646.	3.2	98
34	Small Polarons in Dry DNA. Physical Review Letters, 2003, 91, 108105.	7.8	94
35	Energetics and Dynamics of<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>Adsorbed in a Nanoporous Material at Low Temperature. Physical Review Letters, 2009, 103, 096103.	7.8	91
36	Self-consistent density-functional calculations of the geometries, electronic structures, and magnetic moments of Ni-Al clusters. Physical Review B, 1999, 60, 2020-2024.	3.2	88

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37	Dissociation Channels for Multiply Charged Clusters. Physical Review Letters, 1986, 56, 1551-1554.	7.8	87
38	Electrons in dry DNA from density functional calculations. Molecular Physics, 2003, 101, 1587-1594.	1.7	87
39	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
40	Self-consistent image potential in a metal surface. Physical Review B, 1986, 34, 6767-6769.	3.2	82
41	Recovering hidden Bloch character: Unfolding electrons, phonons, and slabs. Physical Review B, 2013, 87, .	3.2	75
42	From Coordination Polymer Macrocrystals to Nanometric Individual Chains. Advanced Materials, 2005, 17, 1761-1765.	21.0	73
43	Atmospheric contaminants on graphitic surfaces. Carbon, 2013, 61, 33-39.	10.3	72
44	Energetics of the oxidation and opening of a carbon nanotube. Physical Review B, 1999, 60, R2208-R2211.	3.2	69
45	Monte Carlo Calculation of Argon Clusters in Homogeneous Nucleation. Physical Review Letters, 1981, 47, 186-190.	7.8	68
46	Evaporation of small clusters of noble gases by ionization. Surface Science, 1985, 156, 121-125.	1.9	62
47	Geometry and electronic structure ofM-DNA (M=Zn2+,Co2+, andFe2+). Physical Review B, 2006, 73, .	3.2	60
48	Intrinsic electrical conductivity of nanostructured metal-organic polymer chains. Nature Communications, 2013, 4, 1709.	12.8	60
49	Work function and image-plane position of metal surfaces. Physical Review B, 1988, 37, 8701-8706.	3.2	57
50	Magic numbers for positively charged rare-gas clusters. Chemical Physics Letters, 1985, 114, 15-18.	2.6	54
51	Density functional simulation of small Fe nanoparticles. European Physical Journal D, 2003, 25, 261-270.	1.3	54
52	Room temperature compressibility and diffusivity of liquid water from first principles. Journal of Chemical Physics, 2013, 139, 194502.	3.0	54
53	Tip and Surface Determination from Experiments and Simulations of Scanning Tunneling Microscopy and Spectroscopy. Physical Review Letters, 2005, 94, 056103.	7.8	50
54	Cluster diffusion by evaporation-condensation. Physical Review B, 1996, 53, R10540-R10543.	3.2	49

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55	A rational indicator of scientific creativity. Journal of Informetrics, 2007, 1, 123-130.	2.9	48
56	Dislocation formation from a surface step in semiconductors: Anab initiostudy. Physical Review B, 2006, 73, .	3.2	45
57	Magnetism of two-dimensional defects in Pd: Stacking faults, twin boundaries, and surfaces. Physical Review B, 2006, 74, .	3.2	43
58	Zigzag equilibrium structure in monatomic wires. Surface Science, 2001, 482-485, 1261-1265.	1.9	42
59	Atomic layering at the liquid silicon surface: A first-principles simulation. Physical Review B, 1999, 60, R16283-R16286.	3.2	39
60	The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods. Chemical Physics, 2000, 261, 189-203.	1.9	39
61	Bonding and diffusion of Ba on a Si(001) reconstructed surface. Physical Review B, 1999, 60, 4968-4971.	3.2	36
62	Separating the articles of authors with the same name. Scientometrics, 2007, 72, 281-290.	3.0	36
63	Nanocontacts: Probing Electronic Structure under Extreme Uniaxial Strains. Physical Review Letters, 1997, 79, 4198-4201.	7.8	35
64	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
65	Flexibility in a Metalâ€“Organic Framework Material Controlled by Weak Dispersion Forces: The Bistability of MILâ€53(Al). Angewandte Chemie, 2010, 122, 7663-7665.	2.0	35
66	Work function of metals upon alkali-metal adsorption: Overlayer relaxation. Physical Review B, 1987, 36, 3452-3454.	3.2	34
67	Efficient mixed-force first-principles molecular dynamics. Physical Review E, 2003, 68, 055701.	2.1	34
68	How much quantitative information may be expected from programmed desorption experiments?. Surface Science, 1983, 124, 563-570.	1.9	33
69	Energetics of point and planar defects in aluminium from first-principles calculations. Solid State Communications, 1991, 78, 857-861.	1.9	32
70	Onset and evolution of â€˜â€˜magic numbersâ€™â€™ in mass spectra of molecular clusters. Journal of Chemical Physics, 1991, 95, 2927-2935.	3.0	32
71	Comment on â€œMagnetism in Atomic-Size Palladium Contacts and Nanowiresâ€• Physical Review Letters, 2006, 96, 079701; author reply 079702.	7.8	32
72	Anomalous electron-phonon interaction in doped LaFeAsO: First-principles calculations. Physical Review B, 2009, 79, .	3.2	32

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73	Evaporation of clusters during free flight after homogeneous nucleation in nozzle expansion. Physical Review A, 1983, 27, 3307-3310.	2.5	31
74	Coulomb fragmentation of doubly ionized molecular clusters. Physical Review A, 1988, 37, 1401-1405.	2.5	31
75	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
76	Structural patterns of unsupported gold clusters. Solid State Communications, 2001, 117, 621-625.	1.9	29
77	Evaluation of exchange-correlation energy, potential, and stress. Physical Review B, 2001, 64, .	3.2	29
78	Efficient and reliable method for the simulation of scanning tunneling images and spectra with local basis sets. Physica Status Solidi (B): Basic Research, 2006, 243, 1080-1094.	1.5	29
79	Trends in the structure and bonding of neutral and charged noble metal clusters. International Journal of Quantum Chemistry, 2005, 101, 740-745.	2.0	28
80	Strain-Dependence of the Electronic Properties in Periodic Quadruple Helical G4-Wires. Journal of Physical Chemistry B, 2005, 109, 22301-22307.	2.6	28
81	Monte Carlo simulation of cluster diffusion in a triangular lattice. Physical Review B, 1994, 50, 5578-5581.	3.2	27
82	Coordination Chemistry of 6-Thioguanine Derivatives with Cobalt: Toward Formation of Electrical Conductive One-Dimensional Coordination Polymers. Inorganic Chemistry, 2013, 52, 5290-5299.	4.0	27
83	Optimization of an exchange-correlation density functional for water. Journal of Chemical Physics, 2016, 144, 224101.	3.0	27
84	Defect energetics in aluminium. Journal of Physics Condensed Matter, 1991, 3, 8777-8792.	1.8	26
85	Formation of Gold Nanowires with Impurities: A First-Principles Molecular Dynamics Simulation. Physical Review Letters, 2007, 98, 096102.	7.8	26
86	Optimal finite-range atomic basis sets for liquid water and ice. Journal of Physics Condensed Matter, 2013, 25, 435504.	1.8	25
87	Design of molecular wires based on one-dimensional coordination polymers. Applied Physics Letters, 2007, 90, 193107.	3.3	24
88	Adsorption and electronic properties of PTCDA molecules on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>111</mml:mn></mml:mrow> Scanning tunneling microscopy and first-principles calculations. Physical Review B, 2010, 82, .	3.2	24
89	Comment on â€˜â€˜All-electron and pseudopotential force calculations using the linearized-augmented-plane-wave methodâ€™â€™. Physical Review B, 1993, 47, 6784-6786.	3.2	23
90	Structure and Stability of an Amorphous Metal. Physical Review Letters, 1998, 81, 3159-3162.	7.8	23

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91	Nonequilibrium internal and translational temperature of clusters in homogeneous nucleation. Physical Review A, 1983, 27, 3300-3306.	2.5	22
92	Model Hessian for accelerating first-principles structure optimizations. Physical Review B, 2003, 67, .	3.2	19
93	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
94	Variational finite-difference representation of the kinetic energy operator. Physical Review B, 2001, 64, .	3.2	18
95	Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional. Journal of Chemical Physics, 2011, 135, 154505.	3.0	18
96	Band unfolding made simple. Journal of Physics Condensed Matter, 2020, 32, 205902.	1.8	16
97	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
98	Simulations of minerals using density-functional theory based on atomic orbitals for linear scaling. Physics and Chemistry of Minerals, 2004, 31, 12-21.	0.8	15
99	First principles study of the adsorption of C60 on Si(1 1 1). Surface Science, 2001, 482-485, 39-43.	1.9	14
100	Filtering a distribution simultaneously in real and Fourier space. Physical Review B, 2006, 73, .	3.2	14
101	High Electrical Conductivity of Single Metalâ€“Organic Chains. Advanced Materials, 2018, 30, e1705645.	21.0	13
102	Comment on â€œIdentifying Molecular Orientation of IndividualC60on aSi(111)â^'(7Ã—7)Surfaceâ€• Physical Review Letters, 2000, 85, 2653-2653.	7.8	12
103	Comment on â€˜â€˜Theory of ideal metalsâ€™â€™. Physical Review Letters, 1991, 67, 3044-3044.	7.8	11
104	Azafullerene-like Nanosized Clusters. ACS Nano, 2009, 3, 3352-3357.	14.6	11
105	Surface layering and local structure in liquid surfaces. Surface Science, 2001, 482-485, 1314-1318.	1.9	10
106	Order-N and embedded-cluster first-principles DFT calculations using SIESTA/Mosaico. Theoretical Chemistry Accounts, 2007, 118, 541-547.	1.4	10
107	First principles calculation of the geometric and electronic structure of (Al2O3)n(Ox) clusters with n<15 and x=0, 1, 2. Thin Solid Films, 2003, 428, 206-210.	1.8	9
108	Hollow<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>C</mml:mtext><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mtext> from first principles. Physical Review B, 2010, 82, .	3.2	8

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109	Stability and electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>M</mml:mi></mml:mrow></mml:math>-DNA: Role of metal position. Physical Review B, 2011, 84, .	3.2	6
110	A computational exploration of cation locations in high- silica Ca-Chabazite. Studies in Surface Science and Catalysis, 2000, 128, 89-98.	1.5	5
111	Exchange and correlation as a functional of the local density of states. Physical Review B, 2004, 69, .	3.2	5
112	Electronic Structure Calculations with Localized Orbitals: The Siesta Method. , 2005, , 77-91.		3
113	Optimal Fourier filtering of a function that is strictly confined within a sphere. Computer Physics Communications, 2009, 180, 1134-1136.	7.5	2
114	Alternative exact method for random walks on finite and periodic lattices with traps. Physical Review B, 1982, 26, 1067-1070.	3.2	1
115	Monte Carlo and molecular dynamics studies of microclusters. , 1985, , 143-150.		1
116	Critical analysis of the response function in low-dimensional materials. Journal of Physics Condensed Matter, 2021, 33, 295701.	1.8	1
117	Molecular Dynamics Simulations of Nanotube Growth. , 2003, , 45-56.		1
118	Electronic Structure Under Extreme Uniaxial Strains: Conductance in Metallic Nanocontacts.. Materials Research Society Symposia Proceedings, 1997, 499, 173.	0.1	0
119	First-Principles Simulations of Atomic Structure and Magnetism in Fe Nanoparticles. Materials Research Society Symposia Proceedings, 2001, 704, 891.	0.1	0
120	A Theoretical Study of Dislocation Formation at Surfaces in Covalent Materials: Effect of Step Geometry and Reactivity. Solid State Phenomena, 2005, 108-109, 193-198.	0.3	0