Jose M Soler

List of Publications by Year
in descending order

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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	Critical analysis of the response function in low-dimensional materials. Journal of Physics Condensed Matter, 2021, 33, 295701.	1.8	1
2	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
3	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
4	Band unfolding made simple. Journal of Physics Condensed Matter, 2020, 32, 205902.	1.8	16
5	High Electrical Conductivity of Single Metalâ€“Organic Chains. Advanced Materials, 2018, 30, e1705645.	21.0	13
6	Optimization of an exchange-correlation density functional for water. Journal of Chemical Physics, 2016, 144, 224101.	3.0	27
7	Room temperature compressibility and diffusivity of liquid water from first principles. Journal of Chemical Physics, 2013, 139, 194502.	3.0	54
8	Atmospheric contaminants on graphitic surfaces. Carbon, 2013, 61, 33-39.	10.3	72
9	Recovering hidden Bloch character: Unfolding electrons, phonons, and slabs. Physical Review B, 2013, 87, .	3.2	75
10	Intrinsic electrical conductivity of nanostructured metal-organic polymer chains. Nature Communications, 2013, 4, 1709.	12.8	60
11	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
12	Optimal finite-range atomic basis sets for liquid water and ice. Journal of Physics Condensed Matter, 2013, 25, 435504.	1.8	25
13	Anomalous Nuclear Quantum Effects in Ice. Physical Review Letters, 2012, 108, 193003.	7.8	110
14	Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional. Journal of Chemical Physics, 2011, 135, 154505.	3.0	18
15	Density, structure, and dynamics of water: The effect of van der Waals interactions. Journal of Chemical Physics, 2011, 134, 024516.	3.0	242
16	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
17	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
18	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

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19	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
20	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> Scanning tunneling microscopy and first-principles calculations. Physical Review B, 2010, 82, .	3.2	24
21	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>	7.8	83
22	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
23	Anomalous electron-phonon interaction in doped LaFeAsO: First-principles calculations. Physical Review B, 2009, 79, .	3.2	32
24	Optimal Fourier filtering of a function that is strictly confined within a sphere. Computer Physics Communications, 2009, 180, 1134-1136.	7.5	2
25	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
26	Azafullerene-like Nanosized Clusters. ACS Nano, 2009, 3, 3352-3357.	14.6	11
27	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
28	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
29	Formation of Gold Nanowires with Impurities: A First-Principles Molecular Dynamics Simulation. Physical Review Letters, 2007, 98, 096102.	7.8	26
30	Design of molecular wires based on one-dimensional coordination polymers. Applied Physics Letters, 2007, 90, 193107.	3.3	24
31	Order-N and embedded-cluster first-principles DFT calculations using SIESTA/Mosaico. Theoretical Chemistry Accounts, 2007, 118, 541-547.	1.4	10
32	Separating the articles of authors with the same name. Scientometrics, 2007, 72, 281-290.	3.0	36
33	A rational indicator of scientific creativity. Journal of Informetrics, 2007, 1, 123-130.	2.9	48
34	Filtering a distribution simultaneously in real and Fourier space. Physical Review B, 2006, 73, .	3.2	14
35	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
36	Comment on â€œMagnetism in Atomic-Size Palladium Contacts and Nanowiresâ€• Physical Review Letters, 2006, 96, 079701; author reply 079702.	7.8	32

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37	Magnetism of two-dimensional defects in Pd: Stacking faults, twin boundaries, and surfaces. Physical Review B, 2006, 74, .	3.2	43
38	Geometry and electronic structure ofM-DNA (M=Zn2+,Co2+, andFe2+). Physical Review B, 2006, 73, .	3.2	60
39	Planar and cagelike structures of gold clusters: Density-functional pseudopotential calculations. Physical Review B, 2006, 73, .	3.2	108
40	Dislocation formation from a surface step in semiconductors: Anab initiostudy. Physical Review B, 2006, 73, .	3.2	45
41	Electronic Structure Calculations with Localized Orbitals: The Siesta Method. , 2005, , 77-91.		3
42	From Coordination Polymer Macrocrystals to Nanometric Individual Chains. Advanced Materials, 2005, 17, 1761-1765.	21.0	73
43	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
44	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
45	Tip and Surface Determination from Experiments and Simulations of Scanning Tunneling Microscopy and Spectroscopy. Physical Review Letters, 2005, 94, 056103.	7.8	50
46	Strain-Dependence of the Electronic Properties in Periodic Quadruple Helical G4-Wires. Journal of Physical Chemistry B, 2005, 109, 22301-22307.	2.6	28
47	Exchange and correlation as a functional of the local density of states. Physical Review B, 2004, 69, .	3.2	5
48	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
49	Trends in the structure and bonding of noble metal clusters. Physical Review B, 2004, 70, .	3.2	509
50	Density functional simulation of small Fe nanoparticles. European Physical Journal D, 2003, 25, 261-270.	1.3	54
51	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
52	Small Polarons in Dry DNA. Physical Review Letters, 2003, 91, 108105.	7.8	94
53	Electrons in dry DNA from density functional calculations. Molecular Physics, 2003, 101, 1587-1594.	1.7	87
54	Model Hessian for accelerating first-principles structure optimizations. Physical Review B, 2003, 67, .	3.2	19

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55	Efficient mixed-force first-principles molecular dynamics. Physical Review E, 2003, 68, 055701.	2.1	34
56	Molecular Dynamics Simulations of Nanotube Growth. , 2003, , 45-56.		1
57	Systematic generation of finite-range atomic basis sets for linear-scaling calculations. Physical Review B, 2002, 66, .	3.2	251
58	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	1.8	9,150
59	First principles study of the adsorption of C60 on Si(1 1 1). Surface Science, 2001, 482-485, 39-43.	1.9	14
60	Surface layering and local structure in liquid surfaces. Surface Science, 2001, 482-485, 1314-1318.	1.9	10
61	Zigzag equilibrium structure in monatomic wires. Surface Science, 2001, 482-485, 1261-1265.	1.9	42
62	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
63	Variational finite-difference representation of the kinetic energy operator. Physical Review B, 2001, 64, .	3.2	18
64	Structural patterns of unsupported gold clusters. Solid State Communications, 2001, 117, 621-625.	1.9	29
65	First-Principles Simulations of Atomic Structure and Magnetism in Fe Nanoparticles. Materials Research Society Symposia Proceedings, 2001, 704, 891.	0.1	0
66	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
67	Evaluation of exchange-correlation energy, potential, and stress. Physical Review B, 2001, 64, .	3.2	29
68	A computational exploration of cation locations in high- silica Ca-Chabazite. Studies in Surface Science and Catalysis, 2000, 128, 89-98.	1.5	5
69	Seeing molecular orbitals. Chemical Physics Letters, 2000, 321, 78-82.	2.6	117
70	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
71	Metallic bonding and cluster structure. Physical Review B, 2000, 61, 5771-5780.	3.2	163
72	Comment on â€œIdentifying Molecular Orientation of IndividualC60on aSi(111)â˜(7Ã—7)Surfaceâ€• Physical Review Letters, 2000, 85, 2653-2653.	7.8	12

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73	Absence of dc-Conductivity inÎ»-DNA. Physical Review Letters, 2000, 85, 4992-4995.	7.8	602
74	Do Thiols Merely Passivate Gold Nanoclusters?. Physical Review Letters, 2000, 85, 5250-5251.	7.8	158
75	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
76	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. Physical Review Letters, 1999, 83, 3884-3887.	7.8	235
77	Bonding and diffusion of Ba on a Si(001) reconstructed surface. Physical Review B, 1999, 60, 4968-4971.	3.2	36
78	Energetics of the oxidation and opening of a carbon nanotube. Physical Review B, 1999, 60, R2208-R2211.	3.2	69
79	Ab initiostructural, elastic, and vibrational properties of carbon nanotubes. Physical Review B, 1999, 59, 12678-12688.	3.2	854
80	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
81	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. Physical Review Letters, 1999, 82, 3520-3523.	7.8	173
82	Atomic layering at the liquid silicon surface: A first-principles simulation. Physical Review B, 1999, 60, R16283-R16286.	3.2	39
83	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
84	The puzzling stability of monatomic gold wires. Surface Science, 1999, 426, L441-L446.	1.9	120
85	Structure and Stability of an Amorphous Metal. Physical Review Letters, 1998, 81, 3159-3162.	7.8	23
86	Lowest Energy Structures of Gold Nanoclusters. Physical Review Letters, 1998, 81, 1600-1603.	7.8	356
87	Nanocontacts: Probing Electronic Structure under Extreme Uniaxial Strains. Physical Review Letters, 1997, 79, 4198-4201.	7.8	35
88	Electronic Structure Under Extreme Uniaxial Strains: Conductance in Metallic Nanocontacts.. Materials Research Society Symposia Proceedings, 1997, 499, 173.	0.1	0
89	Density-functional method for very large systems with LCAO basis sets. International Journal of Quantum Chemistry, 1997, 65, 453-461.	2.0	1,426
90	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

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91	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
92	Cluster diffusion by evaporation-condensation. Physical Review B, 1996, 53, R10540-R10543.	3.2	49
93	Projection of plane-wave calculations into atomic orbitals. Solid State Communications, 1995, 95, 685-690.	1.9	415
94	Monte Carlo simulation of cluster diffusion in a triangular lattice. Physical Review B, 1994, 50, 5578-5581.	3.2	27
95	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
96	Optimal meshes for integrals in real- and reciprocal-space unit cells. Physical Review B, 1992, 45, 13891-13898.	3.2	275
97	Comment on â€˜â€˜Theory of ideal metalsâ€™â€™. Physical Review Letters, 1991, 67, 3044-3044.	7.8	11
98	Energetics of point and planar defects in aluminium from first-principles calculations. Solid State Communications, 1991, 78, 857-861.	1.9	32
99	Defect energetics in aluminium. Journal of Physics Condensed Matter, 1991, 3, 8777-8792.	1.8	26
100	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
101	Augmented-plane-wave forces. Physical Review B, 1990, 42, 9728-9731.	3.2	153
102	Simple formula for the atomic forces in the augmented-plane-wave method. Physical Review B, 1989, 40, 1560-1564.	3.2	148
103	Work function and image-plane position of metal surfaces. Physical Review B, 1988, 37, 8701-8706.	3.2	57
104	Coulomb fragmentation of doubly ionized molecular clusters. Physical Review A, 1988, 37, 1401-1405.	2.5	31
105	Dissociation channels of multiply charged van der Waals clusters. Physical Review A, 1988, 38, 3236-3248.	2.5	101
106	Work function of metals upon alkali-metal adsorption: Overlayer relaxation. Physical Review B, 1987, 36, 3452-3454.	3.2	34
107	Self-consistent image potential in a metal surface. Physical Review B, 1986, 34, 6767-6769.	3.2	82
108	Interatomic Forces in Scanning Tunneling Microscopy: Giant Corrugations of the Graphite Surface. Physical Review Letters, 1986, 57, 444-447.	7.8	401

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109	Dissociation Channels for Multiply Charged Clusters. Physical Review Letters, 1986, 56, 1551-1554.	7.8	87
110	Magic numbers for positively charged rare-gas clusters. Chemical Physics Letters, 1985, 114, 15-18.	2.6	54
111	Monte Carlo and molecular dynamics studies of microclusters. , 1985, , 143-150.		1
112	Evaporation of small clusters of noble gases by ionization. Surface Science, 1985, 156, 121-125.	1.9	62
113	Electron-metal-surface interaction potential with vacuum tunneling: Observation of the image force. Physical Review B, 1984, 30, 4816-4818.	3.2	256
114	The effect of ionization on magic numbers of rare-gas clusters. Chemical Physics Letters, 1984, 109, 71-75.	2.6	101
115	How much quantitative information may be expected from programmed desorption experiments?. Surface Science, 1983, 124, 563-570.	1.9	33
116	Evaporation of clusters during free flight after homogeneous nucleation in nozzle expansion. Physical Review A, 1983, 27, 3307-3310.	2.5	31
117	Nonequilibrium internal and translational temperature of clusters in homogeneous nucleation. Physical Review A, 1983, 27, 3300-3306.	2.5	22
118	Alternative exact method for random walks on finite and periodic lattices with traps. Physical Review B, 1982, 26, 1067-1070.	3.2	1
119	Microcluster Growth: Transition from Successive Monomer Addition to Coagulation. Physical Review Letters, 1982, 49, 1857-1860.	7.8	107
120	Monte Carlo Calculation of Argon Clusters in Homogeneous Nucleation. Physical Review Letters, 1981, 47, 186-190.	7.8	68