Jose M Soler

List of Publications by Year in Descending Order

119 papers	22,307 citations	51 h-index	123 g-index
123 ext. papers	23,731 ext. citations	4.4 avg, IF	6.53 L-index

#	Paper	IF	Citations
119	Siesta: Recent developments and applications. *Journal of Chemical Physics*, **2020**, 152, 204108	3.9	69
118	Band unfolding made simple. *Journal of Physics Condensed Matter*, **2020**, 32, 205902	1.8	4
117	The CECAM electronic structure library and the modular software development paradigm. *Journal of Chemical Physics*, **2020**, 153, 024117	3.9	5
116	High Electrical Conductivity of Single Metal-Organic Chains. *Advanced Materials*, **2018**, 30, e1705645	24	11
115	Optimization of an exchange-correlation density functional for water. *Journal of Chemical Physics*, **2016**, 144, 224101	3.9	23
114	Room temperature compressibility and diffusivity of liquid water from first principles. *Journal of Chemical Physics*, **2013**, 139, 194502	3.9	51
113	Atmospheric contaminants on graphitic surfaces. *Carbon*, **2013**, 61, 33-39	10.4	61
112	Recovering hidden Bloch character: Unfolding electrons, phonons, and slabs. *Physical Review B*, **2013**, 87,	3.3	60
111	Intrinsic electrical conductivity of nanostructured metal-organic polymer chains. *Nature Communications*, **2013**, 4, 1709	17.4	56
110	Coordination chemistry of 6-thioguanine derivatives with cobalt: toward formation of electrical conductive one-dimensional coordination polymers. *Inorganic Chemistry*, **2013**, 52, 5290-9	5.1	26
109	Optimal finite-range atomic basis sets for liquid water and ice. *Journal of Physics Condensed Matter*, **2013**, 25, 435504	1.8	19
108	Anomalous nuclear quantum effects in ice. *Physical Review Letters*, **2012**, 108, 193003	7.4	104
107	Dispersion interactions in room-temperature ionic liquids: results from a non-empirical density functional. *Journal of Chemical Physics*, **2011**, 135, 154505	3.9	18
106	Density, structure, and dynamics of water: the effect of van der Waals interactions. *Journal of Chemical Physics*, **2011**, 134, 024516	3.9	220
105	Ab initio energetics and kinetics study of H2 and CH4 in the SI clathrate hydrate. *Physical Review B*, **2011**, 84,	3.3	29
104	Stability and electronic structure of M-DNA: Role of metal position. *Physical Review B*, **2011**, 84,	3.3	5
103	Adsorption and electronic properties of PTCDA molecules on Si(111)(7×7): Scanning tunneling microscopy and first-principles calculations. *Physical Review B*, **2010**, 82,	3.3	22

102	Stability, adsorption, and diffusion of CH_4, CO_2, and H_2 in clathrate hydrates. *Physical Review Letters*, **2010**, 105, 145901	7.4	75
101	Hollow C3N4 nanoclusters from first principles. *Physical Review B*, **2010**, 82,	3.3	7
100	Flexibility in a Metal–Organic Framework Material Controlled by Weak Dispersion Forces: The Bistability of MIL-53(Al). *Angewandte Chemie*, **2010**, 122, 7663-7665	3.6	30
99	Flexibility in a metal-organic framework material controlled by weak dispersion forces: the bistability of MIL-53(Al). *Angewandte Chemie - International Edition*, **2010**, 49, 7501-3	16.4	141
98	Anomalous electron-phonon interaction in doped LaFeAsO: First-principles calculations. *Physical Review B*, **2009**, 79,	3.3	29
97	Optimal Fourier filtering of a function that is strictly confined within a sphere. *Computer Physics Communications*, **2009**, 180, 1134-1136	4.2	1
96	Efficient implementation of a van der Waals density functional: application to double-wall carbon nanotubes. *Physical Review Letters*, **2009**, 103, 096102	7.4	1208
95	Azafullerene-like nanosized clusters. *ACS Nano*, **2009**, 3, 3352-7	16.7	10
94	Energetics and dynamics of H(2) adsorbed in a nanoporous material at low temperature. *Physical Review Letters*, **2009**, 103, 096103	7.4	88
93	The SIESTA method; developments and applicability. *Journal of Physics Condensed Matter*, **2008**, 20, 064208	2.8	364
92	Order-N and embedded-cluster first-principles DFT calculations using SIESTA/Mosaico. *Theoretical Chemistry Accounts*, **2007**, 118, 541-547	1.9	9
91	Separating the articles of authors with the same name. *Scientometrics*, **2007**, 72, 281-290	3	30
90	A rational indicator of scientific creativity. *Journal of Informetrics*, **2007**, 1, 123-130	3.1	32
89	Formation of gold nanowires with impurities: a first-principles molecular dynamics simulation. *Physical Review Letters*, **2007**, 98, 096102	7.4	25
88	Design of molecular wires based on one-dimensional coordination polymers. *Applied Physics Letters*, **2007**, 90, 193107	3.4	24
87	Magnetism of two-dimensional defects in Pd: Stacking faults, twin boundaries, and surfaces. *Physical Review B*, **2006**, 74,	3.3	39
86	Geometry and electronic structure of M-DNA (M=Zn2+, Co2+, and Fe2+). *Physical Review B*, **2006**, 73,	3.3	56
85	Planar and cagelike structures of gold clusters: Density-functional pseudopotential calculations. *Physical Review B*, **2006**, 73,	3.3	104

84	Dislocation formation from a surface step in semiconductors: An ab initio study. *Physical Review B*, **2006**, 73,	3.3	41
83	Filtering a distribution simultaneously in real and Fourier space. *Physical Review B*, **2006**, 73,	3.3	9
82	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	1.3	26
81	Comment on "Magnetism in atomic-size palladium contacts and nanowires". *Physical Review Letters* , **2006**, 96, 079701; author reply 079702	7.4	30
80	Strain-dependence of the electronic properties in periodic quadruple helical G4-wires. *Journal of Physical Chemistry B*, **2005**, 109, 22301-7	3.4	28
79	Electronic Structure Calculations with Localized Orbitals: The Siesta Method **2005**, 77-91		3
78	From Coordination Polymer Macrocrystals to Nanometric Individual Chains. *Advanced Materials*, **2005**, 17, 1761-1765	24	70
77	Trends in the structure and bonding of neutral and charged noble metal clusters. *International Journal of Quantum Chemistry*, **2005**, 101, 740-745	2.1	27
76	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	0.4	
75	Tip and surface determination from experiments and simulations of scanning tunneling microscopy and spectroscopy. *Physical Review Letters*, **2005**, 94, 056103	7.4	46
74	Exchange and correlation as a functional of the local density of states. *Physical Review B*, **2004**, 69,	3.3	5
73	Simulations of minerals using density-functional theory based on atomic orbitals for linear scaling. *Physics and Chemistry of Minerals*, **2004**, 31, 12-21	1.6	14
72	Trends in the structure and bonding of noble metal clusters. *Physical Review B*, **2004**, 70,	3.3	472
71	Density functional simulation of small Fe nanoparticles. *European Physical Journal D*, **2003**, 25, 261-270	1.3	54
70	First principles calculation of the geometric and electronic structure of (Al2O3)n(Ox) clusters with n. *Thin Solid Films*, **2003**, 428, 206-210	2.2	8
69	Small polarons in dry DNA. *Physical Review Letters*, **2003**, 91, 108105	7.4	88
68	Electrons in dry DNA from density functional calculations. *Molecular Physics*, **2003**, 101, 1587-1594	1.7	82
67	Model Hessian for accelerating first-principles structure optimizations. *Physical Review B*, **2003**, 67,	3.3	17

66	Efficient mixed-force first-principles molecular dynamics. *Physical Review E*, **2003**, 68, 055701	2.4	29
65	Molecular Dynamics Simulations of Nanotube Growth **2003**, 45-56		
64	The SIESTA method forab initioorder-Nmaterials simulation. *Journal of Physics Condensed Matter*, **2002**, 14, 2745-2779	1.8	7828
63	Systematic generation of finite-range atomic basis sets for linear-scaling calculations. *Physical Review B*, **2002**, 66,	3.3	228
62	Structural patterns of unsupported gold clusters. *Solid State Communications*, **2001**, 117, 621-625	1.6	28
61	First-Principles Simulations of Atomic Structure and Magnetism in Fe Nanoparticles. *Materials Research Society Symposia Proceedings*, **2001**, 704, 891		
60	Hybrid DNA-gold nanostructured materials: anab initioapproach. *Nanotechnology*, **2001**, 12, 126-131	3.4	33
59	Evaluation of exchange-correlation energy, potential, and stress. *Physical Review B*, **2001**, 64,	3.3	26
58	First principles study of the adsorption of C60 on Si(1 1 1). *Surface Science*, **2001**, 482-485, 39-43	1.8	13
57	Surface layering and local structure in liquid surfaces. *Surface Science*, **2001**, 482-485, 1314-1318	1.8	9
56	Zigzag equilibrium structure in monatomic wires. *Surface Science*, **2001**, 482-485, 1261-1265	1.8	41
55	Interplay between theory and experiment insolid state inorganic chemistry. *Journal of Materials Chemistry*, **2001**, 11, 1-10		14
54	Variational finite-difference representation of the kinetic energy operator. *Physical Review B*, **2001**, 64,	3.3	14
53	A computational exploration of cation locations in high- silica Ca-Chabazite. *Studies in Surface Science and Catalysis*, **2000**, 128, 89-98	1.8	5
52	Seeing molecular orbitals. *Chemical Physics Letters*, **2000**, 321, 78-82	2.5	111
51	The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods. *Chemical Physics*, **2000**, 261, 189-203	2.3	37
50	Metallic bonding and cluster structure. *Physical Review B*, **2000**, 61, 5771-5780	3.3	157
49	Comment on "Identifying molecular orientation of individual C60 on a Si(111)-(7x7) Surface". *Physical Review Letters*, **2000**, 85, 2653	7.4	11

48	Absence of dc-conductivity in lambda-DNA. *Physical Review Letters*, **2000**, 85, 4992-5	7.4	531
47	Do thiols merely passivate gold nanoclusters?. *Physical Review Letters*, **2000**, 85, 5250-1	7.4	142
46	Systematic ab initio study of the electronic and magnetic properties of different pure and mixed iron systems. *Physical Review B*, **2000**, 61, 13639-13646	3.3	93
45	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. *Physical Review Letters*, **1999**, 83, 3884-3887	7.4	227
44	Bonding and diffusion of Ba on a Si(001) reconstructed surface. *Physical Review B*, **1999**, 60, 4968-4971	3.3	34
43	Energetics of the oxidation and opening of a carbon nanotube. *Physical Review B*, **1999**, 60, R2208-R2211	3.3	68
42	Ab initio structural, elastic, and vibrational properties of carbon nanotubes. *Physical Review B*, **1999** , 59, 12678-12688	3.3	779
41	Linear-Scaling ab-initio Calculations for Large and Complex Systems. *Physica Status Solidi (B): Basic Research*, **1999**, 215, 809-817	1.3	839
40	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. *Physical Review Letters*, **1999**, 82, 3520-3523	7.4	165
39	Atomic layering at the liquid silicon surface: A first-principles simulation. *Physical Review B*, **1999**, 60, R16283-R16286	3.3	37
38	Self-consistent density-functional calculations of the geometries, electronic structures, and magnetic moments of Ni-Al clusters. *Physical Review B*, **1999**, 60, 2020-2024	3.3	85
37	The puzzling stability of monatomic gold wires. *Surface Science*, **1999**, 426, L441-L446	1.8	109
36	Structure and Stability of an Amorphous Metal. *Physical Review Letters*, **1998**, 81, 3159-3162	7.4	22
35	Lowest Energy Structures of Gold Nanoclusters. *Physical Review Letters*, **1998**, 81, 1600-1603	7.4	334
34	Nanocontacts: Probing Electronic Structure under Extreme Uniaxial Strains. *Physical Review Letters*, **1997**, 79, 4198-4201	7.4	33
33	Electronic Structure Under Extreme Uniaxial Strains: Conductance in Metallic Nanocontacts. *Materials Research Society Symposia Proceedings*, **1997**, 499, 173		
32	Density-functional method for very large systems with LCAO basis sets **1997**, 65, 453-461		1360
31	Self-consistent order-N density-functional calculations for very large systems. *Physical Review B*, **1996**, 53, R10441-R10444	3.3	2229

30	Analysis of atomic orbital basis sets from the projection of plane-wave results. *Journal of Physics Condensed Matter*, **1996**, 8, 3859-3880	1.8	146
29	Cluster diffusion by evaporation-condensation. *Physical Review B*, **1996**, 53, R10540-R10543	3.3	49
28	Projection of plane-wave calculations into atomic orbitals. *Solid State Communications*, **1995**, 95, 685-690	1.6	359
27	Monte Carlo simulation of cluster diffusion in a triangular lattice. *Physical Review B*, **1994**, 50, 5578-5581	3.3	26
26	Comment on "All-electron and pseudopotential force calculations using the linearized-augmented-plane-wave method". *Physical Review B*, **1993**, 47, 6784-6786	3.3	23
25	Optimal meshes for integrals in real- and reciprocal-space unit cells. *Physical Review B*, **1992**, 45, 13891-13898	3.3	228
24	Energetics of point and planar defects in aluminium from first-principles calculations. *Solid State Communications*, **1991**, 78, 857-861	1.6	26
23	Defect energetics in aluminium. *Journal of Physics Condensed Matter*, **1991**, 3, 8777-8792	1.8	24
22	Onset and evolution of magic numbers in mass spectra of molecular clusters. *Journal of Chemical Physics*, **1991**, 95, 2927-2935	3.9	32
21	Comment on "Theory of ideal metals". *Physical Review Letters*, **1991**, 67, 3044	7.4	11
20	Augmented-plane-wave forces. *Physical Review B*, **1990**, 42, 9728-9731	3.3	122
19	Simple formula for the atomic forces in the augmented-plane-wave method. *Physical Review B*, **1989**, 40, 1560-1564	3.3	140
18	Work function and image-plane position of metal surfaces. *Physical Review B*, **1988**, 37, 8701-8706	3.3	54
17	Coulomb fragmentation of doubly ionized molecular clusters. *Physical Review A*, **1988**, 37, 1401-1405	2.6	30
16	Dissociation channels of multiply charged van der Waals clusters. *Physical Review A*, **1988**, 38, 3236-3248	2.6	94
15	Work function of metals upon alkali-metal adsorption: Overlayer relaxation. *Physical Review B*, **1987**, 36, 3452-3454	3.3	30
14	Dissociation channels for multiply charged clusters. *Physical Review Letters*, **1986**, 56, 1551-1554	7.4	86
13	Self-consistent image potential in a metal surface. *Physical Review B*, **1986**, 34, 6767-6769	3.3	75

12	Interatomic forces in scanning tunneling microscopy: Giant corrugations of the graphite surface. *Physical Review Letters*, **1986**, 57, 444-447	7.4	335
11	Magic numbers for positively charged rare-gas clusters. *Chemical Physics Letters*, **1985**, 114, 15-18	2.5	54
10	Monte Carlo and molecular dynamics studies of microclusters **1985**, 143-150		1
9	Evaporation of small clusters of noble gases by ionization. *Surface Science*, **1985**, 156, 121-125	1.8	61
8	Electron-metal-surface interaction potential with vacuum tunneling: Observation of the image force. *Physical Review B*, **1984**, 30, 4816-4818	3.3	204
7	The effect of ionization on magic numbers of rare-gas clusters. *Chemical Physics Letters*, **1984**, 109, 71-75	2.5	96
6	How much quantitative information may be expected from programmed desorption experiments?. *Surface Science*, **1983**, 124, 563-570	1.8	31
5	Evaporation of clusters during free flight after homogeneous nucleation in nozzle expansion. *Physical Review A*, **1983**, 27, 3307-3310	2.6	28
4	Nonequilibrium internal and translational temperature of clusters in homogeneous nucleation. *Physical Review A*, **1983**, 27, 3300-3306	2.6	21
3	Alternative exact method for random walks on finite and periodic lattices with traps. *Physical Review B*, **1982**, 26, 1067-1070	3.3	1
2	Microcluster Growth: Transition from Successive Monomer Addition to Coagulation. *Physical Review Letters*, **1982**, 49, 1857-1860	7.4	98
1	Monte Carlo Calculation of Argon Clusters in Homogeneous Nucleation. *Physical Review Letters*, **1981**, 47, 186-190	7.4	67