Daniel Sanchez-Portal

List of Publications by Year
in descending order

182 papers	23,096 citations	28274 55 h-index	7518 151 g-index
183 all docs	183 docs citations	183 times ranked	16799 citing authors

#	Article	IF	Citations
1	Spin-Polarizing Electron Beam Splitter from Crossed Graphene Nanoribbons. Physical Review Letters, 2022, 129, .	7.8	11
2	Magnetic correlations in single-layer NbSe₂. Journal of Physics Condensed Matter, 2021, 33, 295804.	1.8	10
3	Lateral Interactions and Orderâ€“Disorder Phase Transitions of Metal Phthalocyanines on Ag(111). Journal of Physical Chemistry C, 2021, 125, 15623-15635.	3.1	4
4	GW approximation for open-shell molecules: a first-principles study. New Journal of Physics, 2021, 23, 093027.	2.9	5
5	From starphenes to non-benzenoid linear conjugated polymers by substrate templating. Nanoscale Advances, 2021, 3, 2351-2358.	4.6	4
6	Clever substitutions reveal magnetism in zigzag graphene nanoribbons. Nature, 2021, 600, 613-614.	27.8	4
7	Magnetism of Topological Boundary States Induced by Boron Substitution in Graphene Nanoribbons. Physical Review Letters, 2020, 125, 146801.	7.8	73
8	On-Surface Synthesis of Chlorinated Narrow Graphene Nanoribbon Organometallic Hybrids. Journal of Physical Chemistry Letters, 2020, 11, 10290-10297.	4.6	14
9	Catalytic Oxidation of CO on a Curved Pt(111) Surface: Simultaneous Ignition at All Facets through a Transient COâ€Ο Complex**. Angewandte Chemie - International Edition, 2020, 59, 20037-20043.	13.8	13
10	Catalytic Oxidation of CO on a Curved Pt(111) Surface: Simultaneous Ignition at All Facets through a Transient COâ€Ο Complex**. Angewandte Chemie, 2020, 132, 20212-20218.	2.0	1
11	Crossed graphene nanoribbons as beam splitters and mirrors for electron quantum optics. Physical Review B, 2020, 102, .	3.2	10
12	Key Role of the Surface Band Structure in Spin-Dependent Interfacial Electron Transfer: Ar/Fe(110) and Ar/Co(0001). Journal of Physical Chemistry Letters, 2020, 11, 7141-7145.	4.6	3
13	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
14	Probing the Magnetism of Topological End States in 5-Armchair Graphene Nanoribbons. ACS Nano, 2020, 14, 4499-4508.	14.6	75
15	Band Depopulation of Graphene Nanoribbons Induced by Chemical Gating with Amino Groups. ACS Nano, 2020, 14, 1895-1901.	14.6	23
16	PySCF-NAO: An efficient and flexible implementation of linear response time-dependent density functional theory with numerical atomic orbitals. Computer Physics Communications, 2019, 236, 188-204.	7.5	8
17	Directional sub-femtosecond charge transfer dynamics and the dimensionality of 1T-TaS2. Scientific Reports, 2019, 9, 488.	3.3	9
18	Toward Efficient GW Calculations Using Numerical Atomic Orbitals: Benchmarking and Application to Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 4564-4580.	5.3	8

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19	Electronic transport in planar atomic-scale structures measured by two-probe scanning tunneling spectroscopy. Nature Communications, 2019, 10, 1573.	12.8	29
20	San Sebastian, a City of (Nano)Science and Technology. ACS Nano, 2019, 13, 12254-12256.	14.6	2
21	Site-selective reversible Dielsâ€“Alder reaction between a biphenylene-based polyarene and a semiconductor surface. Physical Chemistry Chemical Physics, 2018, 20, 11037-11046.	2.8	11
22	Atomic-Scale Lightning Rod Effect in Plasmonic Picocavities: A Classical View to a Quantum Effect. ACS Nano, 2018, 12, 585-595.	14.6	155
23	Tuning ultrafast electron injection dynamics at organic-graphene/metal interfaces. Nanoscale, 2018, 10, 8014-8022.	5.6	4
24	Effect of Structural Fluctuations on Elastic Lifetimes of Adsorbate States: Isonicotinic Acid on Rutile(110). Journal of Physical Chemistry C, 2018, 122, 7575-7585.	3.1	7
25	Electronic Properties of Substitutionally Boron-Doped Graphene Nanoribbons on a Au(111) Surface. Journal of Physical Chemistry C, 2018, 122, 16092-16099.	3.1	31
26	Orbital-selective spin excitation of a magnetic porphyrin. Communications Physics, 2018, 1, .	5.3	31
27	Building a 22-ring nanographene by combining in-solution and on-surface syntheses. Chemical Communications, 2018, 54, 10256-10259.	4.1	39
28	Atomic-scale forces induced by a hydrogen molecule trapped in a tunneling junction. Surface Science, 2018, 678, 189-193.	1.9	4
29	Structural and Vibrational Properties of the TiOPc Monolayer on Ag(111). Journal of Physical Chemistry C, 2017, 121, 1608-1617.	3.1	20
30	A tunable electronic beam splitter realized with crossed graphene nanoribbons. Journal of Chemical Physics, 2017, 146, 092318.	3.0	18
31	Quantum Dots Embedded in Graphene Nanoribbons by Chemical Substitution. Nano Letters, 2017, 17, 50-56.	9.1	56
32	Doping of Graphene Nanoribbons via Functional Group Edge Modification. ACS Nano, 2017, 11, 7355-7361.	14.6	78
33	Charge-transfer states and optical transitions at the pentacene-TiO₂interface. New Journal of Physics, 2017, 19, 033019.	2.9	13
34	Width-Dependent Band Gap in Armchair Graphene Nanoribbons Reveals Fermi Level Pinning on Au(111). ACS Nano, 2017, 11, 11661-11668.	14.6	149
35	Vicinage effect in the energy loss of H2 dimers: Experiment and calculations based on time-dependent density-functional theory. Physical Review A, 2017, 95, .	2.5	12
36	Publisherâ€™s Note: â€œA tunable electronic beam splitter realized with crossed graphene nanoribbonsâ€•[J. Chem. Phys. 146, 092318 (2017)]. Journal of Chemical Physics, 2017, 146, 199902.	3.0	4

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37	Optical response of silver clusters and their hollow shells from linear-response TDDFT. Journal of Physics Condensed Matter, 2016, 28, 214001.	1.8	20
38	Hybrid cluster-expansion and density-functional-theory approach for optical absorption in TiO_2. Journal of the Optical Society of America B: Optical Physics, 2016, 33, C123.	2.1	4
39	Adsorption geometry and interface states: Relaxed and compressed phases of NTCDA/Ag(111). Physical Review B, 2016, 94, .	3.2	13
40	Search for a Metallic Dangling-Bond Wire on n-Doped H-Passivated Semiconductor Surfaces. Journal of Physical Chemistry C, 2016, 120, 20303-20309.	3.1	11
41	The butterfly â€“ a well-defined constant-current topography pattern on Si(001):H and Ge(001):H resulting from current-induced defect fluctuations. Physical Chemistry Chemical Physics, 2016, 18, 19309-19317.	2.8	16
42	Dielsâ€“Alder attachment of a planar organic molecule to a dangling bond dimer on a hydrogenated semiconductor surface. Physical Chemistry Chemical Physics, 2016, 18, 16757-16765.	2.8	7
43	Interplay between Steps and Oxygen Vacancies on Curved TiO₂(110). Nano Letters, 2016, 16, 2017-2022.	9.1	25
44	Plasmonic Response of Metallic Nanojunctions Driven by Single Atom Motion: Quantum Transport Revealed in Optics. ACS Photonics, 2016, 3, 269-277.	6.6	43
45	Interaction of a conjugated polyaromatic molecule with a single dangling bond quantum dot on a hydrogenated semiconductor. Physical Chemistry Chemical Physics, 2016, 18, 3854-3861.	2.8	14
46	NO adsorption on Cu(110) and O(2 Ã— 1)/Cu(110) surfaces from density functional theory calculations. Physical Chemistry Chemical Physics, 2016, 18, 9476-9483.	2.8	8
47	Electronic stopping power in a narrow band gap semiconductor from first principles. Physical Review B, 2015, 91, .	3.2	57
48	Cubic-scaling iterative solution of the Bethe-Salpeter equation for finite systems. Physical Review B, 2015, 92, .	3.2	37
49	Tunneling spectroscopy of close-spaced dangling-bond pairs in Si(001):H. Scientific Reports, 2015, 5, 14496.	3.3	11
50	Assessment of Density-Functional Tight-Binding Ionization Potentials and Electron Affinities of Molecules of Interest for Organic Solar Cells Against First-Principles GW Calculations. Computation, 2015, 3, 616-656.	2.0	19
51	X-ray photoemission analysis of clean and carbon monoxide-chemisorbed platinum(111) stepped surfaces using a curved crystal. Nature Communications, 2015, 6, 8903.	12.8	48
52	Substrate-Induced Stabilization and Reconstruction of Zigzag Edges in Graphene Nanoislands on Ni(111). Journal of Physical Chemistry C, 2015, 119, 4072-4078.	3.1	15
53	Computation of electron energy loss spectra by an iterative method. Nuclear Instruments & Methods in Physics Research B, 2015, 354, 216-219.	1.4	5
54	Atomistic Near-Field Nanoplasmonics: Reaching Atomic-Scale Resolution in Nanooptics. Nano Letters, 2015, 15, 3410-3419.	9.1	257

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55	Role of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>k</mml:mi></mml:math>-point sampling in the supercell approach to inelastic electron tunneling spectroscopy simulations of molecular monolayers. Physical Review B, 2015, 91, .	3.2	11
56	On the mechanical and electronic properties of thiolated gold nanocrystals. Nanoscale, 2015, 7, 1809-1819.	5.6	23
57	Metallic thin films on stepped surfaces: lateral scattering of quantum well states. New Journal of Physics, 2014, 16, 123025.	2.9	6
58	Spin-Dependent Electron Scattering at Graphene Edges on Ni(111). Physical Review Letters, 2014, 112, 066802.	7.8	33
59	Identifying Highly Conducting Auâ€“C Links through Inelastic Electron Tunneling Spectroscopy. Journal of Physical Chemistry C, 2014, 118, 27106-27112.	3.1	10
60	Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles. Journal of Physical Chemistry C, 2014, 118, 8775-8782.	3.1	12
61	Fully self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m quasiparticle self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m molecules. Physical Review B, 2014, 89, .	3.2	98
62	SAM-like arrangement of thiolated graphene nanoribbons: decoupling the edge state from the metal substrate. Physical Chemistry Chemical Physics, 2013, 15, 3233.	2.8	2
63	Interface Dipole Effects as a Function of Molecular Tilt: Mechanical Gating of Electron Tunneling through Self-Assembled Monolayers?. Journal of Physical Chemistry C, 2013, 117, 14272-14280.	3.1	12
64	Lattice-matched versus lattice-mismatched models to describe epitaxial monolayer graphene on Ru(0001). Physical Review B, 2013, 88, .	3.2	35
65	Dynamic screening and energy loss of antiprotons colliding with excited Al clusters. Nuclear Instruments & Methods in Physics Research B, 2013, 317, 56-60.	1.4	9
66	Plane-wave based electron tunneling through field emission resonance states. Physical Review B, 2013, 88, .	3.2	3
67	Electronic stopping power of H and He in Al and LiF from first principles. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 59-61.	1.4	32
68	Tunable Molecular Plasmons in Polycyclic Aromatic Hydrocarbons. ACS Nano, 2013, 7, 3635-3643.	14.6	101
69	Hybridization between Cuâ€“O chain and Cu(110) surface states in the O(2Ã—1)/Cu(110) surface from first principles. Journal of Physics Condensed Matter, 2013, 25, 135003.	1.8	6
70	Resonant and nonresonant processes in attosecond streaking from metals. Physical Review B, 2013, 87, .	3.2	33
71	First-Principles Study of the Electronic and Magnetic Properties of Defects in Carbon Nanostructures. Carbon Materials, 2013, , 41-76.	1.2	1
72	Universal magnetic properties of sp³-type defects in covalently functionalized graphene. New Journal of Physics, 2012, 14, 043022.	2.9	87

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73	Electron localization in epitaxial graphene on Ru(0001) determined by moirÃ© corrugation. Physical Review B, 2012, 85, .	3.2	34
74	Theory of orthogonal interactions of CO molecules on a one-dimensional substrate. Physical Review B, 2012, 85, .	3.2	6
75	Strain-Tunable Spin Moment in Ni-Doped Graphene. Journal of Physical Chemistry C, 2012, 116, 1174-1178.	3.1	36
76	Magnetism of Single Vacancies in Rippled Graphene. Journal of Physical Chemistry C, 2012, 116, 7602-7606.	3.1	41
77	Dynamic screening of a localized hole during photoemission from a metal cluster. Nanoscale Research Letters, 2012, 7, 447.	5.7	2
78	Transport properties of armchair graphene nanoribbon junctions between graphene electrodes. Physical Chemistry Chemical Physics, 2012, 14, 10683.	2.8	14
79	Nonadiabatic Forces in Ion-Solid Interactions: The Initial Stages of Radiation Damage. Physical Review Letters, 2012, 108, 213201.	7.8	138
80	Electronic Stopping Power in Gold: The Role of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>Electrons and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="bold">H</mml:mi><mml:mo>/</mml:mo><mml:mi>He</mml:mi></mml:math>Anomaly. Physical Review Letters, 2012, 108, 225504.	7.8	125
81	Orthogonal Interactions of CO Molecules on a One-Dimensional Substrate. ACS Nano, 2011, 5, 8877-8883.	14.6	24
82	An O(N3) implementation of Hedin's GW approximation for molecules. Journal of Chemical Physics, 2011, 135, 074105.	3.0	98
83	Atomic-scale engineering of electrodes for single-molecule contacts. Nature Nanotechnology, 2011, 6, 23-27.	31.5	128
84	Role of Dispersion Forces in the Structure of Graphene Monolayers on Ru Surfaces. Physical Review Letters, 2011, 106, 186102.	7.8	129
85	Time-dependent electron phenomena at surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 971-976.	7.1	71
86	Simulation of inelastic electron tunneling spectroscopy of single molecules with functionalized tips. Physical Review B, 2011, 83, .	3.2	33
87	Magnetism of covalently functionalized carbon nanotubes. Applied Physics Letters, 2011, 99, .	3.3	9
88	Mixed-Valency Signature in Vibrational Inelastic Electron Tunneling Spectroscopy. Physical Review Letters, 2010, 104, 136101.	7.8	39
89	Potential Energy Landscape for Hot Electrons in Periodically Nanostructured Graphene. Physical Review Letters, 2010, 105, 036804.	7.8	85
90	First-principles study of substitutional metal impurities in graphene: structural, electronic and magnetic properties. New Journal of Physics, 2010, 12, 053012.	2.9	214

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91	Characterization of single-molecule pentanedithiol junctions by inelastic electron tunneling spectroscopy and first-principles calculations. Physical Review B, 2010, 81, .	3.2	47
92	Substrate-induced cooperative effects in water adsorption from density functional calculations. Physical Review B, 2010, 82, .	3.2	6
93	BorcaetÂal.Reply:. Physical Review Letters, 2010, 105, .	7.8	8
94	Water-induced surface reconstruction of oxygen<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>2</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>2</mml:mn></mml:mrow><mml:mo>)</mml:mo></mml:mrow><mml:mo>−</mml:mo><mml:mi>O</mml:mi></mml:mrow></mml:math>/Ru(0001). Physical Review B, 2010, 82, .	3.2	12
95	Magnetism of substitutional Co impurities in graphene: Realization of single<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math>vacancies. Physical Review B, 2010, 81, .	3.2	178
96	Surveying Molecular Vibrations during the Formation of Metalâ'Molecule Nanocontacts. Nano Letters, 2010, 10, 657-660.	9.1	45
97	Optical detection of plasmonic and interband excitations in 1-nm-wide indium atomic wires. Applied Physics Letters, 2010, 96, 243101.	3.3	23
98	First-principles investigation of electron-induced cross-linking of aromatic self-assembled monolayers on Au(111). Physical Chemistry Chemical Physics, 2010, 12, 1578.	2.8	10
99	Heating electrons with ion irradiation: A first-principles approach. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 590-593.	1.4	4
100	Exploring the Tilt-Angle Dependence of Electron Tunneling across Molecular Junctions of Self-Assembled Alkanethiols. ACS Nano, 2009, 3, 2073-2080.	14.6	53
101	Ab initiocalculations of zirconium adsorption and diffusion on graphene. Physical Review B, 2009, 80, .	3.2	44
102	Systematic investigation of the structure of the Si(553)-Au surface from first principles. Physical Review B, 2008, 77, .	3.2	27
103	Electronic potential of a chemisorption interface. Physical Review B, 2008, 78, .	3.2	70
104	Switching on magnetism in Ni-doped graphene: Density functional calculations. Physical Review B, 2008, 78, .	3.2	83
105	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
106	Adsorption of Water on O(2 Ã— 2)/Ru(0001): Thermal Stability and Inhibition of Dissociation. Journal of Physical Chemistry C, 2008, 112, 14052-14057.	3.1	12
107	Decisive role of the energetics of dissociation products in the adsorption of water on O/Ru(0001). Physical Review B, 2008, 78, .	3.2	15
108	Zr-metal adhesion on graphenic nanostructures. Applied Physics Letters, 2008, 93, 053101.	3.3	10

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109	On the structure of the first hydration layer on NaCl(100): Role of hydrogen bonding. Journal of Chemical Physics, 2007, 126, 214707.	3.0	14
110	Ultrafast charge transfer and atomic orbital polarization. Journal of Chemical Physics, 2007, 127, 174708.	3.0	17
111	Interplay between electronic and atomic structures in the Si(557)-Au reconstruction from first principles. Physical Review B, 2007, 76, .	3.2	32
112	Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids. Physical Review B, 2007, 75, .	3.2	150
113	Water adsorption onO(2Ã—2)âˆ•Ru(0001): STM experiments and first-principles calculations. Physical Review B, 2007, 76, .	3.2	22
114	First-principles calculation of charge transfer at surfaces: The case of core-excited<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi		

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127	Electronic Structure Calculations with Localized Orbitals: The Siesta Method. , 2005, , 77-91.		3
128	Direct observation of electron dynamics in the attosecond domain. Nature, 2005, 436, 373-376.	27.8	291
129	Structural models for Si(553)â€“Au atomic chain reconstruction. Nanotechnology, 2005, 16, S218-S223.	2.6	27
130	Role of Elastic Scattering in Electron Dynamics at Ordered Alkali Overlayers on Cu(111). Physical Review Letters, 2005, 95, 176802.	7.8	71
131	First-principles study of the atomic and electronic structure of theSi(111)â˜(5Ã—2)â˜Ausurface reconstruction. Physical Review B, 2005, 71, .	3.2	43
132	Prediction of New Phases of Nitrogen at High Pressure from First-Principles Simulations. Physical Review Letters, 2004, 93, 125501.	7.8	160
133	Role of Spin-Orbit Splitting and Dynamical Fluctuations in the Si(557)-Au Surface. Physical Review Letters, 2004, 93, 146803.	7.8	89
134	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
135	Building up the screening below the femtosecond scale. Chemical Physics Letters, 2004, 387, 95-100.	2.6	39
136	Dimensionality effects in time-dependent screening. Chemical Physics Letters, 2004, 393, 132-137.	2.6	12
137	Different origins of the ferromagnetic order in (Ga,Mn)As and (Ga,Mn)N. Physical Review B, 2004, 70, .	3.2	114
138	Computing the Properties of Materials from First Principles with SIESTA. Structure and Bonding, 2004, , 103-170.	1.0	101
139	Ab initio Predictions of Ferroelectric Ternary Fluorides with the LiNbO3 Structure.. ChemInform, 2003, 34, no.	0.0	0
140	First principles study of the Si(557)â€“Au surface. Surface Science, 2003, 532-535, 655-660.	1.9	40
141	Van der Waals contribution to the inelastic atom-surface scattering. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 213-218.	1.7	1
142	Specific features of the electronic structure of IIIâ€“VI layered semiconductors: recent results on structural and optical measurements under pressure and electronic structure calculations. Physica Status Solidi (B): Basic Research, 2003, 235, 267-276.	1.5	26
143	Electrons in dry DNA from density functional calculations. Molecular Physics, 2003, 101, 1587-1594.	1.7	87
144	Ab initio predictions of ferroelectric ternary fluorides with the LiNbO3structure. Chemical Communications, 2003, , 2440-2441.	4.1	8

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145	Lattice dynamics of the h-BN monolayer and single-walled BN nanotubes using a tight-binding model. , 2003, , .		2
146	Bonding, moment formation, and magnetic interactions inCa14MnBi11andBa14MnBi11. Physical Review B, 2002, 65, .	3.2	73
147	Vibrational properties of single-wall nanotubes and monolayers of hexagonal BN. Physical Review B, 2002, 66, .	3.2	114
148	Vibrational spectroscopy on single C60 molecules: The role of molecular orientation. Journal of Chemical Physics, 2002, 117, 9531-9534.	3.0	51
149	Two distinct metallic bands associated with monatomic Au wires on the Si(557)-Au surface. Physical Review B, 2002, 65, .	3.2	48
150	Calculation of the optical response of atomic clusters using time-dependent density functional theory and local orbitals. Physical Review B, 2002, 66, .	3.2	197
151	Ab initiocalculations of the optical properties of 4-Ã…-diameter single-walled nanotubes. Physical Review B, 2002, 66, .	3.2	256
152	Band structure and optical properties of isolated and bundled nanotubes. AIP Conference Proceedings, 2002, , .	0.4	1
153	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	1.8	9,150
154	Numerical atomic orbitals for linear-scaling calculations. Physical Review B, 2001, 64, .	3.2	992
155	First principles study of the adsorption of C60 on Si(1 1 1). Surface Science, 2001, 482-485, 39-43.	1.9	14
156	Zigzag equilibrium structure in monatomic wires. Surface Science, 2001, 482-485, 1261-1265.	1.9	42
157	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
158	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
159	Seeing molecular orbitals. Chemical Physics Letters, 2000, 321, 78-82.	2.6	117
160	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
161	Metallic bonding and cluster structure. Physical Review B, 2000, 61, 5771-5780.	3.2	163
162	LCAO calculation of dynamical charges and ferroelectricity. AIP Conference Proceedings, 2000, , .	0.4	4

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163	Comment on â€œIdentifying Molecular Orientation of IndividualC60on aSi(111)â^'(7Ã—7)Surfaceâ€• Physical Review Letters, 2000, 85, 2653-2653.	7.8	12
164	Do Thiols Merely Passivate Gold Nanoclusters?. Physical Review Letters, 2000, 85, 5250-5251.	7.8	158
165	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
166	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. Physical Review Letters, 1999, 83, 3884-3887.	7.8	235
167	Bonding and diffusion of Ba on a Si(001) reconstructed surface. Physical Review B, 1999, 60, 4968-4971.	3.2	36
168	Application of local-spin-density approximation toaâ^'Siand tetrahedralaâ^'C. Physical Review B, 1999, 60, 10594-10597.	3.2	13
169	Energetics of the oxidation and opening of a carbon nanotube. Physical Review B, 1999, 60, R2208-R2211.	3.2	69
170	Structure and thermal stability of gold nanoclusters: The Au38 case. European Physical Journal D, 1999, 9, 211-215.	1.3	52
171	Ab initiostructural, elastic, and vibrational properties of carbon nanotubes. Physical Review B, 1999, 59, 12678-12688.	3.2	854
172	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
173	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. Physical Review Letters, 1999, 82, 3520-3523.	7.8	173
174	Atomic layering at the liquid silicon surface: A first-principles simulation. Physical Review B, 1999, 60, R16283-R16286.	3.2	39
175	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
176	Lowest Energy Structures of Gold Nanoclusters. Physical Review Letters, 1998, 81, 1600-1603.	7.8	356
177	Nanocontacts: Probing Electronic Structure under Extreme Uniaxial Strains. Physical Review Letters, 1997, 79, 4198-4201.	7.8	35
178	Surface electronic structure of metastable FeSi(CsCl)(111) epitaxially grown on Si(111). Physical Review B, 1997, 55, R16065-R16068.	3.2	12
179	Electronic Structure Under Extreme Uniaxial Strains: Conductance in Metallic Nanocontacts.. Materials Research Society Symposia Proceedings, 1997, 499, 173.	0.1	0
180	Density-functional method for very large systems with LCAO basis sets. International Journal of Quantum Chemistry, 1997, 65, 453-461.	2.0	1,426

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181	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
182	Projection of plane-wave calculations into atomic orbitals. Solid State Communications, 1995, 95, 685-690.	1.9	415