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	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	1.8	9,150
2	Density-functional method for very large systems with LCAO basis sets. International Journal of Quantum Chemistry, 1997, 65, 453-461.	2.0	1,426
3	Numerical atomic orbitals for linear-scaling calculations. Physical Review B, 2001, 64, .	3.2	992
4	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
5	Ab initiostructural, elastic, and vibrational properties of carbon nanotubes. Physical Review B, 1999, 59, 12678-12688.	3.2	854
6	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
7	Projection of plane-wave calculations into atomic orbitals. Solid State Communications, 1995, 95, 685-690.	1.9	415
8	Lowest Energy Structures of Gold Nanoclusters. Physical Review Letters, 1998, 81, 1600-1603.	7.8	356
9	Direct observation of electron dynamics in the attosecond domain. Nature, 2005, 436, 373-376.	27.8	291
10	Atomistic Near-Field Nanoplasmonics: Reaching Atomic-Scale Resolution in Nanooptics. Nano Letters, 2015, 15, 3410-3419.	9.1	257
11	Ab initiocalculations of the optical properties of 4-Ã…-diameter single-walled nanotubes. Physical Review B, 2002, 66, .	3.2	256
12	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. Physical Review Letters, 1999, 83, 3884-3887.	7.8	235
13	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
14	Electronic Excitations in Metals and at Metal Surfaces. Chemical Reviews, 2006, 106, 4160-4206.	47.7	218
15	First-principles study of substitutional metal impurities in graphene: structural, electronic and magnetic properties. New Journal of Physics, 2010, 12, 053012.	2.9	214
16	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
17	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
18	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. Physical Review Letters, 1999, 82, 3520-3523.	7.8	173

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19	Metallic bonding and cluster structure. Physical Review B, 2000, 61, 5771-5780.	3.2	163
20	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
21	Prediction of New Phases of Nitrogen at High Pressure from First-Principles Simulations. Physical Review Letters, 2004, 93, 125501.	7.8	160
22	Do Thiols Merely Passivate Gold Nanoclusters?. Physical Review Letters, 2000, 85, 5250-5251.	7.8	158
23	Electronic Stopping Power in LiF from First Principles. Physical Review Letters, 2007, 99, 235501.	7.8	157
24	Atomic-Scale Lightning Rod Effect in Plasmonic Picocavities: A Classical View to a Quantum Effect. ACS Nano, 2018, 12, 585-595.	14.6	155
25	Atomic-orbital-based approximate self-interaction correction scheme for molecules and solids. Physical Review B, 2007, 75, .	3.2	150
26	Width-Dependent Band Gap in Armchair Graphene Nanoribbons Reveals Fermi Level Pinning on Au(111). ACS Nano, 2017, 11, 11661-11668.	14.6	149
27	Nonadiabatic Forces in Ion-Solid Interactions: The Initial Stages of Radiation Damage. Physical Review Letters, 2012, 108, 213201.	7.8	138
28	Role of Dispersion Forces in the Structure of Graphene Monolayers on Ru Surfaces. Physical Review Letters, 2011, 106, 186102.	7.8	129
29	Atomic-scale engineering of electrodes for single-molecule contacts. Nature Nanotechnology, 2011, 6, 23-27.	31.5	128
30	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
31	Seeing molecular orbitals. Chemical Physics Letters, 2000, 321, 78-82.	2.6	117
32	Vibrational properties of single-wall nanotubes and monolayers of hexagonal BN. Physical Review B, 2002, 66, .	3.2	114
33	Different origins of the ferromagnetic order in (Ga,Mn)As and (Ga,Mn)N. Physical Review B, 2004, 70, .	3.2	114
34	Computing the Properties of Materials from First Principles with SIESTA. Structure and Bonding, 2004, , 103-170.	1.0	101
35	Tunable Molecular Plasmons in Polycyclic Aromatic Hydrocarbons. ACS Nano, 2013, 7, 3635-3643.	14.6	101
36	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

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37	An O(N3) implementation of Hedin's GW approximation for molecules. Journal of Chemical Physics, 2011, 135, 074105.	3.0	98
38	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:n 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:n molecules. Physical Review B, 2014, 89, .	3.2	98
39	Role of Spin-Orbit Splitting and Dynamical Fluctuations in the Si(557)-Au Surface. Physical Review Letters, 2004, 93, 146803.	7.8	89
40	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
41	Electrons in dry DNA from density functional calculations. Molecular Physics, 2003, 101, 1587-1594.	1.7	87
42	Universal magnetic properties of sp³-type defects in covalently functionalized graphene. New Journal of Physics, 2012, 14, 043022.	2.9	87
43	Potential Energy Landscape for Hot Electrons in Periodically Nanostructured Graphene. Physical Review Letters, 2010, 105, 036804.	7.8	85
44	Switching on magnetism in Ni-doped graphene: Density functional calculations. Physical Review B, 2008, 78, .	3.2	83
45	Doping of Graphene Nanoribbons via Functional Group Edge Modification. ACS Nano, 2017, 11, 7355-7361.	14.6	78
46	Probing the Magnetism of Topological End States in 5-Armchair Graphene Nanoribbons. ACS Nano, 2020, 14, 4499-4508.	14.6	75
47	Bonding, moment formation, and magnetic interactions inCa14MnBi11andBa14MnBi11. Physical Review B, 2002, 65, .	3.2	73
48	Magnetism of Topological Boundary States Induced by Boron Substitution in Graphene Nanoribbons. Physical Review Letters, 2020, 125, 146801.	7.8	73
49	Role of Elastic Scattering in Electron Dynamics at Ordered Alkali Overlayers on Cu(111). Physical Review Letters, 2005, 95, 176802.	7.8	71
50	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
51	Electronic potential of a chemisorption interface. Physical Review B, 2008, 78, .	3.2	70
52	Energetics of the oxidation and opening of a carbon nanotube. Physical Review B, 1999, 60, R2208-R2211.	3.2	69
53	Silicate chain formation in the nanostructure of cement-based materials. Journal of Chemical Physics, 2007, 127, 164710.	3.0	59
54	Electronic stopping power in a narrow band gap semiconductor from first principles. Physical Review B, 2015, 91, .	3.2	57

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55	Quantum Dots Embedded in Graphene Nanoribbons by Chemical Substitution. Nano Letters, 2017, 17, 50-56.	9.1	56
56	Exploring the Tilt-Angle Dependence of Electron Tunneling across Molecular Junctions of Self-Assembled Alkanethiols. ACS Nano, 2009, 3, 2073-2080.	14.6	53
57	Structure and thermal stability of gold nanoclusters: The Au38 case. European Physical Journal D, 1999, 9, 211-215.	1.3	52
58	Vibrational spectroscopy on single C60 molecules: The role of molecular orientation. Journal of Chemical Physics, 2002, 117, 9531-9534.	3.0	51
59	Two distinct metallic bands associated with monatomic Au wires on the Si(557)-Au surface. Physical Review B, 2002, 65, .	3.2	48
60	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
61	Characterization of single-molecule pentanedithiol junctions by inelastic electron tunneling spectroscopy and first-principles calculations. Physical Review B, 2010, 81, .	3.2	47
62	Surveying Molecular Vibrations during the Formation of Metalâ^'Molecule Nanocontacts. Nano Letters, 2010, 10, 657-660.	9.1	45
63	Ab initiocalculations of zirconium adsorption and diffusion on graphene. Physical Review B, 2009, 80, .	3.2	44
64	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
65	Plasmonic Response of Metallic Nanojunctions Driven by Single Atom Motion: Quantum Transport Revealed in Optics. ACS Photonics, 2016, 3, 269-277.	6.6	43
66	Zigzag equilibrium structure in monatomic wires. Surface Science, 2001, 482-485, 1261-1265.	1.9	42
67	Magnetism of Single Vacancies in Rippled Graphene. Journal of Physical Chemistry C, 2012, 116, 7602-7606.	3.1	41
68	First principles study of the Si(557)â€“Au surface. Surface Science, 2003, 532-535, 655-660.	1.9	40
69	Atomic layering at the liquid silicon surface: A first-principles simulation. Physical Review B, 1999, 60, R16283-R16286.	3.2	39
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	Building up the screening below the femtosecond scale. Chemical Physics Letters, 2004, 387, 95-100.	2.6	39
72	Mixed-Valency Signature in Vibrational Inelastic Electron Tunneling Spectroscopy. Physical Review Letters, 2010, 104, 136101.	7.8	39

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73	Building a 22-ring nanographene by combining in-solution and on-surface syntheses. Chemical Communications, 2018, 54, 10256-10259.	4.1	39
74	Cubic-scaling iterative solution of the Bethe-Salpeter equation for finite systems. Physical Review B, 2015, 92, .	3.2	37
75	Bonding and diffusion of Ba on a Si(001) reconstructed surface. Physical Review B, 1999, 60, 4968-4971.	3.2	36
76	Strain-Tunable Spin Moment in Ni-Doped Graphene. Journal of Physical Chemistry C, 2012, 116, 1174-1178.	3.1	36
77	Nanocontacts: Probing Electronic Structure under Extreme Uniaxial Strains. Physical Review Letters, 1997, 79, 4198-4201.	7.8	35
78	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
79	Lattice-matched versus lattice-mismatched models to describe epitaxial monolayer graphene on Ru(0001). Physical Review B, 2013, 88, .	3.2	35
80	Electron localization in epitaxial graphene on Ru(0001) determined by moirÃ© corrugation. Physical Review B, 2012, 85, .	3.2	34
81	Simulation of inelastic electron tunneling spectroscopy of single molecules with functionalized tips. Physical Review B, 2011, 83, .	3.2	33
82	Resonant and nonresonant processes in attosecond streaking from metals. Physical Review B, 2013, 87, .	3.2	33
83	Spin-Dependent Electron Scattering at Graphene Edges on Ni(111). Physical Review Letters, 2014, 112, 066802.	7.8	33
84	Interplay between electronic and atomic structures in the Si(557)-Au reconstruction from first principles. Physical Review B, 2007, 76, .	3.2	32
85	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
86	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
87	Orbital-selective spin excitation of a magnetic porphyrin. Communications Physics, 2018, 1, .	5.3	31
88	Electronic transport in planar atomic-scale structures measured by two-probe scanning tunneling spectroscopy. Nature Communications, 2019, 10, 1573.	12.8	29
89	Structural models for Si(553)â€“Au atomic chain reconstruction. Nanotechnology, 2005, 16, S218-S223.	2.6	27
90	Systematic investigation of the structure of the Si(553)-Au surface from first principles. Physical Review B, 2008, 77, .	3.2	27

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91	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
92	Interplay between Steps and Oxygen Vacancies on Curved TiO₂(110). Nano Letters, 2016, 16, 2017-2022.	9.1	25
93	Water Adsorption and Diffusion on NaCl(100). Journal of Physical Chemistry B, 2006, 110, 24559-24564.	2.6	24
94	Orthogonal Interactions of CO Molecules on a One-Dimensional Substrate. ACS Nano, 2011, 5, 8877-8883.	14.6	24
95	Metalâ€“insulator transition in the In/Si(111) surface. Surface Science, 2006, 600, 3821-3824.	1.9	23
96	Optical detection of plasmonic and interband excitations in 1-nm-wide indium atomic wires. Applied Physics Letters, 2010, 96, 243101.	3.3	23
97	On the mechanical and electronic properties of thiolated gold nanocrystals. Nanoscale, 2015, 7, 1809-1819.	5.6	23
98	Band Depopulation of Graphene Nanoribbons Induced by Chemical Gating with Amino Groups. ACS Nano, 2020, 14, 1895-1901.	14.6	23
99	Water adsorption onO(2Ã—2)âˆ•Ru(0001): STM experiments and first-principles calculations. Physical Review B, 2007, 76, .	3.2	22
100	Dynamics of surface-localised electronic excitations studied with the scanning tunnelling microscope. Progress in Surface Science, 2007, 82, 293-312.	8.3	22
101	Optical response of silver clusters and their hollow shells from linear-response TDDFT. Journal of Physics Condensed Matter, 2016, 28, 214001.	1.8	20
102	Structural and Vibrational Properties of the TiOPc Monolayer on Ag(111). Journal of Physical Chemistry C, 2017, 121, 1608-1617.	3.1	20
103	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
104	A tunable electronic beam splitter realized with crossed graphene nanoribbons. Journal of Chemical Physics, 2017, 146, 092318.	3.0	18
105	Ultrafast charge transfer and atomic orbital polarization. Journal of Chemical Physics, 2007, 127, 174708.	3.0	17
106	Spontaneous Emergence of Cl-Anions from NaCl(100) at Low Relative Humidity. Journal of Physical Chemistry C, 2007, 111, 8000-8004.	3.1	17
107	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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109	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
110	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
111	Ab initio study of the double row model of the Si(553)â€“Au reconstruction. Surface Science, 2006, 600, 1201-1206.	1.9	15
112	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
113	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
114	First principles study of the adsorption of C60 on Si(1 1 1). Surface Science, 2001, 482-485, 39-43.	1.9	14
115	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
116	Transport properties of armchair graphene nanoribbon junctions between graphene electrodes. Physical Chemistry Chemical Physics, 2012, 14, 10683.	2.8	14
117	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
118	On-Surface Synthesis of Chlorinated Narrow Graphene Nanoribbon Organometallic Hybrids. Journal of Physical Chemistry Letters, 2020, 11, 10290-10297.	4.6	14
119	Application of local-spin-density approximation toaâˆ'Siand tetrahedralaâˆ'C. Physical Review B, 1999, 60, 10594-10597.	3.2	13
120	Slab calculations and Greenâ€™s function recursive methods combined to study the electronic structure of surfaces: application to Cu(111)â€“(4Ã—4)-Na. Progress in Surface Science, 2007, 82, 313-335.	8.3	13
121	Adsorption geometry and interface states: Relaxed and compressed phases of NTCDA/Ag(111). Physical Review B, 2016, 94, .	3.2	13
122	Charge-transfer states and optical transitions at the pentacene-TiO₂interface. New Journal of Physics, 2017, 19, 033019.	2.9	13
123	Catalytic Oxidation of CO on a Curved Pt(111) Surface: Simultaneous Ignition at All Facets through a Transient COâ€O Complex**. Angewandte Chemie - International Edition, 2020, 59, 20037-20043.	13.8	13
124	Surface electronic structure of metastable FeSi(CsCl)(111) epitaxially grown on Si(111). Physical Review B, 1997, 55, R16065-R16068.	3.2	12
125	Comment on â€œIdentifying Molecular Orientation of IndividualC60on aSi(111)âˆ'(7Ã—7)Surfaceâ€• Physical Review Letters, 2000, 85, 2653-2653.	7.8	12
126	Dimensionality effects in time-dependent screening. Chemical Physics Letters, 2004, 393, 132-137.	2.6	12

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127	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
128	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:mi>Ru(0001). Physical Review B, 2010, 82, .	3.2	12
129	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
130	Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles. Journal of Physical Chemistry C, 2014, 118, 8775-8782.	3.1	12
131	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
132	Tunneling spectroscopy of close-spaced dangling-bond pairs in Si(001):H. Scientific Reports, 2015, 5, 14496.	3.3	11
133	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
134	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
135	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
136	Spin-Polarizing Electron Beam Splitter from Crossed Graphene Nanoribbons. Physical Review Letters, 2022, 129, .	7.8	11
137	Zr-metal adhesion on graphenic nanostructures. Applied Physics Letters, 2008, 93, 053101.	3.3	10
138	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
139	Identifying Highly Conducting Auâ€“C Links through Inelastic Electron Tunneling Spectroscopy. Journal of Physical Chemistry C, 2014, 118, 27106-27112.	3.1	10
140	Crossed graphene nanoribbons as beam splitters and mirrors for electron quantum optics. Physical Review B, 2020, 102, .	3.2	10
141	Magnetic correlations in single-layer NbSe₂. Journal of Physics Condensed Matter, 2021, 33, 295804.	1.8	10
142	Magnetism of covalently functionalized carbon nanotubes. Applied Physics Letters, 2011, 99, .	3.3	9
143	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
144	Directional sub-femtosecond charge transfer dynamics and the dimensionality of 1T-TaS2. Scientific Reports, 2019, 9, 488.	3.3	9

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145	Ab initio predictions of ferroelectric ternary fluorides with the LiNbO3structure. Chemical Communications, 2003, , 2440-2441.	4.1	8
146	Quantum-size effects in the energy loss of charged particles interacting with a confined two-dimensional electron gas. Physical Review A, 2006, 73, .	2.5	8
147	Dynamic screening and electron dynamics in low-dimensional metal systems. Nuclear Instruments & Methods in Physics Research B, 2007, 258, 72-78.	1.4	8
148	BorcaetÂal.Reply:. Physical Review Letters, 2010, 105, .	7.8	8
149	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
150	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
151	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
152	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
153	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
154	Substrate-induced cooperative effects in water adsorption from density functional calculations. Physical Review B, 2010, 82, .	3.2	6
155	Theory of orthogonal interactions of CO molecules on a one-dimensional substrate. Physical Review B, 2012, 85, .	3.2	6
156	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
157	Metallic thin films on stepped surfaces: lateral scattering of quantum well states. New Journal of Physics, 2014, 16, 123025.	2.9	6
158	Computation of electron energy loss spectra by an iterative method. Nuclear Instruments & Methods in Physics Research B, 2015, 354, 216-219.	1.4	5
159	GW approximation for open-shell molecules: a first-principles study. New Journal of Physics, 2021, 23, 093027.	2.9	5
160	LCAO calculation of dynamical charges and ferroelectricity. AIP Conference Proceedings, 2000, , .	0.4	4
161	Heating electrons with ion irradiation: A first-principles approach. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 590-593.	1.4	4
162	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

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163	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
164	Tuning ultrafast electron injection dynamics at organic-graphene/metal interfaces. Nanoscale, 2018, 10, 8014-8022.	5.6	4
165	Atomic-scale forces induced by a hydrogen molecule trapped in a tunneling junction. Surface Science, 2018, 678, 189-193.	1.9	4
166	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
167	From starphenes to non-benzenoid linear conjugated polymers by substrate templating. Nanoscale Advances, 2021, 3, 2351-2358.	4.6	4
168	Clever substitutions reveal magnetism in zigzag graphene nanoribbons. Nature, 2021, 600, 613-614.	27.8	4
169	Electronic Structure Calculations with Localized Orbitals: The Siesta Method. , 2005, , 77-91.		3
170	Plane-wave based electron tunneling through field emission resonance states. Physical Review B, 2013, 88, .	3.2	3
171	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
172	Lattice dynamics of the h-BN monolayer and single-walled BN nanotubes using a tight-binding model. , 2003, , .		2
173	Dynamic screening of a localized hole during photoemission from a metal cluster. Nanoscale Research Letters, 2012, 7, 447.	5.7	2
174	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
175	San Sebastian, a City of (Nano)Science and Technology. ACS Nano, 2019, 13, 12254-12256.	14.6	2
176	Band structure and optical properties of isolated and bundled nanotubes. AIP Conference Proceedings, 2002, , .	0.4	1
177	Van der Waals contribution to the inelastic atom-surface scattering. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 213-218.	1.7	1
178	Catalytic Oxidation of CO on a Curved Pt(111) Surface: Simultaneous Ignition at All Facets through a Transient COâ€Ō Complex**. Angewandte Chemie, 2020, 132, 20212-20218.	2.0	1
179	First-Principles Study of the Electronic and Magnetic Properties of Defects in Carbon Nanostructures. Carbon Materials, 2013, , 41-76.	1.2	1
180	Electronic Structure Under Extreme Uniaxial Strains: Conductance in Metallic Nanocontacts.. Materials Research Society Symposia Proceedings, 1997, 499, 173.	0.1	0

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181	Ab initio Predictions of Ferroelectric Ternary Fluorides with the LiNbO3 Structure.. ChemInform, 2003, 34, no.	0.0	0
182	Quantum mechanics calculations on the diastereomeric salts of cyclic phosphoric acids with ephedrine. Computational and Theoretical Chemistry, 2005, 717, 205-214.	1.5	0