Pablo Ordejon

List of Publications by Year
in descending order

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221 papers	34,011 citations	14614 66 h-index	3815 178 g-index
222 all docs	222 docs citations	222 times ranked	21619 citing authors

#	Article	IF	Citations
1	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	0.7	9,150
2	Density-functional method for nonequilibrium electron transport. Physical Review B, 2002, 65, .	1.1	4,752
3	Self-consistent order-Ndensity-functional calculations for very large systems. Physical Review B, 1996, 53, R10441-R10444.	1.1	2,422
4	Density-functional method for very large systems with LCAO basis sets. , 1997, 65, 453-461.		1,426
5	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	0.7	922
6	Tight-binding description of graphene. Physical Review B, 2002, 66, .	1.1	904
7	Ab initiostructural, elastic, and vibrational properties of carbon nanotubes. Physical Review B, 1999, 59, 12678-12688.	1.1	854
8	Absence of dc-Conductivity inÎ»-DNA. Physical Review Letters, 2000, 85, 4992-4995.	2.9	602
9	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	0.7	522
10	Theoretical study of the nonlinear conductance of Di-thiol benzene coupled to Au(1 1 1) surfaces via thiol and thiolate bonds. Computational Materials Science, 2003, 27, 151-160.	1.4	463
11	Phonon Dispersion in Graphite. Physical Review Letters, 2004, 92, 075501.	2.9	460
12	Designed Self-Doped Titanium Oxide Thin Films for Efficient Visible-Light Photocatalysis. Advanced Materials, 2002, 14, 1399-1402.	11.1	438
13	Stability and Mobility of Mono- and Di-Interstitials inÎ±-Fe. Physical Review Letters, 2004, 92, 175503.	2.9	403
14	Unconstrained minimization approach for electronic computations that scales linearly with system size. Physical Review B, 1993, 48, 14646-14649.	1.1	377
15	Lowest Energy Structures of Gold Nanoclusters. Physical Review Letters, 1998, 81, 1600-1603.	2.9	356
16	Tight-binding model and direct-gap/indirect-gap transition in single-layer and multilayer MoS<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>. Physical Review B, 2013, 88, .	1.1	351
17	Electronic band structure of isolated and bundled carbon nanotubes. Physical Review B, 2002, 65, .	1.1	327
18	First-principles study of the origin and nature of ferromagnetism inGa1âˆ’xMnxAs. Physical Review B, 2001, 63, .	1.1	288

#	Article	IF	Citations
19	Ab initiocalculations of the optical properties of 4-Ã…-diameter single-walled nanotubes. Physical Review B, 2002, 66, .	1.1	256
20	Linear system-size scaling methods for electronic-structure calculations. Physical Review B, 1995, 51, 1456-1476.	1.1	253
21	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. Physical Review Letters, 1999, 83, 3884-3887.	2.9	235
22	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	1.2	229
23	TranSIESTA: A Spice for Molecular Electronics. Annals of the New York Academy of Sciences, 2003, 1006, 212-226.	1.8	205
24	Density-functional calculations of the structures, binding energies, and magnetic moments of Fe clusters with 2 to 17 atoms. Physical Review B, 2001, 63, .	1.1	189
25	Electronic properties of singleâ€layer and multilayer transition metal dichalcogenides MX₂ (M = Mo, W and X = S, Se). Annalen Der Physik, 2014, 526, 347-357.	0.9	186
26	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. Physical Review Letters, 1999, 82, 3520-3523.	2.9	173
27	Real-Time TD-DFT Simulations in Dye Sensitized Solar Cells: The Electronic Absorption Spectrum of Alizarin Supported on TiO₂ Nanoclusters. Journal of Chemical Theory and Computation, 2010, 6, 2856-2865.	2.3	170
28	Metallic bonding and cluster structure. Physical Review B, 2000, 61, 5771-5780.	1.1	163
29	Do Thiols Merely Passivate Gold Nanoclusters?. Physical Review Letters, 2000, 85, 5250-5251.	2.9	158
30	Nanotexturing To Enhance Photoluminescent Response of Atomically Thin Indium Selenide with Highly Tunable Band Gap. Nano Letters, 2016, 16, 3221-3229.	4.5	155
31	Damaging Graphene with Ozone Treatment: A Chemically Tunable Metalâ"Insulator Transition. ACS Nano, 2010, 4, 4033-4038.	7.3	149
32	Elastic properties of carbon nanotubes under hydrostatic pressure. Physical Review B, 2002, 65, .	1.1	139
33	Electronic Transport between Graphene Layers Covalently Connected by Carbon Nanotubes. ACS Nano, 2010, 4, 7596-7602.	7.3	133
34	Magnetoresistance and Magnetic Ordering Fingerprints in Hydrogenated Graphene. Physical Review Letters, 2011, 107, 016602.	2.9	132
35	First-principles calculation of the band offset atBaO/BaTiO3andSrO/SrTiO3interfaces. Physical Review B, 2003, 67, .	1.1	121
36	Seeing molecular orbitals. Chemical Physics Letters, 2000, 321, 78-82.	1.2	117

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37	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems:Â Application to Chorismate Mutase. Journal of Physical Chemistry B, 2003, 107, 13728-13736.	1.2	116
38	Orbital Specific Chirality and Homochiral Self-Assembly of Achiral Molecules Induced by Charge Transfer and Spontaneous Symmetry Breaking. Physical Review Letters, 2010, 105, 115702.	2.9	116
39	Structure and energetics of giant fullerenes: An order-Nmolecular-dynamics study. Physical Review B, 1996, 53, 2132-2140.	1.1	115
40	Linear Scaling ab initio Calculations in Nanoscale Materials with SIESTA. Physica Status Solidi (B): Basic Research, 2000, 217, 335-356.	0.7	111
41	Strength of radial breathing mode in single-walled carbon nanotubes. Physical Review B, 2005, 71, .	1.1	109
42	Order-N tight-binding methods for electronic-structure and molecular dynamics. Computational Materials Science, 1998, 12, 157-191.	1.4	105
43	Aggregation of carbon interstitials in silicon carbide: A theoretical study. Physical Review B, 2003, 68, .	1.1	103
44	Computing the Properties of Materials from First Principles with SIESTA. Structure and Bonding, 2004, , 103-170.	1.0	101
45	Optimal strictly localized basis sets for noble metal surfaces. Physical Review B, 2009, 79, .	1.1	100
46	Linear Scaling Method for Phonon Calculations from Electronic Structure. Physical Review Letters, 1995, 75, 1324-1327.	2.9	98
47	Systematicab initiostudy of the electronic and magnetic properties of different pure and mixed iron systems. Physical Review B, 2000, 61, 13639-13646.	1.1	98
48	Origin of current-induced forces in an atomic gold wire:â€,â€A first-principles study. Physical Review B, 2003, 67, .	1.1	98
49	Theoretical study of O2 and CO adsorption on Aun clusters (n=5â€“10). Chemical Physics Letters, 2005, 408, 252-257.	1.2	95
50	Density functional studies of small platinum clusters. Journal of Physics Condensed Matter, 1997, 9, L39-L45.	0.7	89
51	Self-consistent density-functional calculations of the geometries, electronic structures, and magnetic moments of Ni-Al clusters. Physical Review B, 1999, 60, 2020-2024.	1.1	88
52	Electrons in dry DNA from density functional calculations. Molecular Physics, 2003, 101, 1587-1594.	0.8	87
53	Ab initio study of NOx compounds adsorption on SnO2 surface. Sensors and Actuators B: Chemical, 2007, 126, 62-67.	4.0	86
54	Spin Proximity Effects in Graphene/Topological Insulator Heterostructures. Nano Letters, 2018, 18, 2033-2039.	4.5	86

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55	New Superhard Phases for Three-DimensionalC60-based Fullerites. Physical Review Letters, 2000, 85, 2328-2331.	2.9	85
56	Unexpected Dynamics for Self-Interstitial Clusters in Silicon. Physical Review Letters, 2001, 86, 1247-1250.	2.9	85
57	Momentum dependence of spinâ€“orbit interaction effects in single-layer and multi-layer transition metal dichalcogenides. 2D Materials, 2014, 1, 034003.	2.0	85
58	Quantum transport in chemically modified two-dimensional graphene: From minimal conductivity to Anderson localization. Physical Review B, 2011, 84, .	1.1	84
59	Spectral properties of large fullerenes: From cluster to crystal. Solid State Communications, 1995, 96, 833-838.	0.9	82
60	Sampling the diffusion paths of a neutral vacancy in silicon with quantum mechanical calculations. Physical Review B, 2004, 70, .	1.1	80
61	Linear Scaling DFT Calculations with Numerical Atomic Orbitals. Materials Research Society Symposia Proceedings, 2001, 677, 961.	0.1	77
62	Experimental and theoretical study of band structure of InSe andIn1â^'xGaxSe(x<0.2)under high pressure:â€,Direct to indirect crossovers. Physical Review B, 2001, 63, .	1.1	73
63	Ab initiodetermination of the phonon deformation potentials of graphene. Physical Review B, 2002, 65, .	1.1	72
64	Improved nonorthogonal tight-binding Hamiltonian for molecular-dynamics simulations of silicon clusters. Physical Review B, 1994, 50, 5645-5650.	1.1	69
65	Electronic-structure-based molecular-dynamics method for large biological systems: Application to the 10 basepair poly(dG)â‹…poly(dC) DNA double helix. Physical Review B, 1997, 55, 6880-6887.	1.1	69
66	Energetics of the oxidation and opening of a carbon nanotube. Physical Review B, 1999, 60, R2208-R2211.	1.1	69
67	Comment on â€œMolecular Distortions and Chemical Bonding of a Largeï€-Conjugated Molecule on a Metal Surfaceâ€• Physical Review Letters, 2005, 95, 209601; author reply 209602.	2.9	68
68	Ab initiostudy of silicon-multisubstituted neutral and charged fullerenes. Physical Review B, 2001, 63, .	1.1	67
69	Crystal symmetry and pressure effects on the valence band structure ofÎ³-InSe andÎµ-GaSe: Transport measurements and electronic structure calculations. Physical Review B, 2005, 71, .	1.1	65
70	First principles study of gold adsorption and diffusion on graphite. Surface Science, 2004, 564, 173-178.	0.8	63
71	First-principles study of the neutral molecular metalNi(tmdt)2. Physical Review B, 2002, 65, .	1.1	60
72	Capacitive DNA Detection Driven by Electronic Charge Fluctuations in a Graphene Nanopore. Physical Review Applied, 2015, 3, .	1.5	60

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73	Quasiparticle spectra of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi><mml:mo>&</mml:mo></mml:mrow></mml:math>Two-band superconductivity and the role of tunneling selectivity. Physical Review B, 2015, 92, .	1.1	56
74	Characterization of the unoccupied and partially occupied states of TTF-TCNQ by XANES and first-principles calculations. Physical Review B, 2003, 68, .	1.1	54
75	Fullerene growth and the role of nonclassical isomers. Physical Review B, 2001, 63, .	1.1	53
76	Phonon eigenvectors of chiral nanotubes. Physical Review B, 2001, 64, .	1.1	53
77	Oxygen Surface Functionalization of Graphene Nanoribbons for Transport Gap Engineering. ACS Nano, 2011, 5, 9271-9277.	7.3	53
78	Structure and thermal stability of gold nanoclusters: The Au38 case. European Physical Journal D, 1999, 9, 211-215.	0.6	52
79	Ab initiolocal vibrational modes of light impurities in silicon. Physical Review B, 2002, 65, .	1.1	51
80	Electron Transport via Local Polarons at Interface Atoms. Physical Review Letters, 2006, 97, 206801.	2.9	50
81	Electronic structure of 2 H -NbSe ₂ single-layers in the CDW state. 2D Materials, 2016, 3, 035028.	2.0	50
82	Modulation of Surface Charge Transfer through Competing Long-Range Repulsive versus Short-Range Attractive Interactions. Journal of Physical Chemistry C, 2011, 115, 18640-18648.	1.5	49
83	Mechanisms behind the enhancement of thermal properties of graphene nanofluids. Nanoscale, 2018, 10, 15402-15409.	2.8	49
84	Electroresistance Effect in Ferroelectric Tunnel Junctions with Symmetric Electrodes. ACS Nano, 2012, 6, 1473-1478.	7.3	48
85	Magnetism-Dependent Transport Phenomena in Hydrogenated Graphene: From Spin-Splitting to Localization Effects. ACS Nano, 2011, 5, 3987-3992.	7.3	47
86	Elastic properties and pressure-induced phase transitions of single-walled carbon nanotubes. Physica Status Solidi (B): Basic Research, 2003, 235, 354-359.	0.7	44
87	Calculation of core level shifts within DFT using pseudopotentials and localized basis sets. European Physical Journal B, 2012, 85, 1.	0.6	44
88	Voltageâ€Induced Coercivity Reduction in Nanoporous Alloy Films: A Boost toward Energyâ€Efficient Magnetic Actuation. Advanced Functional Materials, 2017, 27, 1701904.	7.8	41
89	Atomic layering at the liquid silicon surface: A first-principles simulation. Physical Review B, 1999, 60, R16283-R16286.	1.1	39
90	The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods. Chemical Physics, 2000, 261, 189-203.	0.9	39

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91	First-principles study of the blue bronzeK0.3MoO3. Physical Review B, 2002, 65, .	1.1	39
92	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. Nanotechnology, 2002, 13, 346-351.	1.3	39
93	Modulation of the NO trans effect in heme proteins: implications for the activation of soluble guanylate cyclase. Journal of Biological Inorganic Chemistry, 2003, 8, 595-600.	1.1	39
94	Dynamics of interstitial hydrogen molecules in crystalline silicon. Journal of Physics Condensed Matter, 2001, 13, 6271-6283.	0.7	38
95	Angle-resolved photoemission study and first-principles calculation of the electronic structure of GaTe. Physical Review B, 2002, 65, .	1.1	38
96	Insulating behavior of an amorphous graphene membrane. Physical Review B, 2012, 86, .	1.1	38
97	Tight binding molecular dynamics studies of boron assisted nanotube growth. Journal of Chemical Physics, 2000, 113, 3814-3821.	1.2	37
98	Self-doped titanium oxide thin films for efficient visible light photocatalysis. Sensors and Actuators B: Chemical, 2005, 109, 52-56.	4.0	37
99	High-pressure, high-temperature phase diagram of InSe: A comprehensive study of the electronic and structural properties of the monoclinic phase of InSe under high pressure. Physical Review B, 2006, 73, .	1.1	37
100	Bonding and diffusion of Ba on a Si(001) reconstructed surface. Physical Review B, 1999, 60, 4968-4971.	1.1	36
101	Composition-dependent structural properties in ScGaN alloy films: A combined experimental and theoretical study. Journal of Applied Physics, 2005, 98, 123501.	1.1	36
102	Optical absorption in plasmaâ€deposited silicon oxynitride films. Applied Physics Letters, 1992, 60, 1399-1401.	1.5	35
103	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	1.3	35
104	Band structure of indium selenide investigated by intrinsic photoluminescence under high pressure. Physical Review B, 2004, 70, .	1.1	35
105	Linear-Scaling ab-initio Calculations for Large and Complex Systems. , 1999, 215, 809.		35
106	Systematic study of electron localization in an amorphous semiconductor. Physical Review B, 2004, 69, .	1.1	34
107	Growth of Twin-Free and Low-Doped Topological Insulators on BaF₂(111). Crystal Growth and Design, 2017, 17, 4655-4660.	1.4	34
108	Dynamical screening and absorption within a strictly localized basis implementation of time-dependent LDA: From small clusters and molecules to aza-fullerenes. Physical Review B, 2004, 69, .	1.1	33

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109	Quantum phase transitions involving a change in polarization. Physical Review B, 1996, 54, 13515-13528.	1.1	32
110	Order-N tight-binding molecular dynamics on parallel computers. Computer Physics Communications, 1995, 88, 173-185.	3.0	31
111	First-Principles Analyses and Predictions on the Reactivity of Barrier Layers of Ta and TaN toward Organometallic Precursors for Deposition of Copper Films. Langmuir, 2005, 21, 7608-7614.	1.6	31
112	An efficient implementation of a QMâ€“MM method in SIESTA. Theoretical Chemistry Accounts, 2011, 128, 825-833.	0.5	29
113	Compressibility of CO adsorbed on Ni from 10â^'6 mbar to 1.2 bar ambient CO pressures investigated with X-ray diffraction. Surface Science, 2003, 522, 161-166.	0.8	27
114	Theoretical evidence for the kick-out mechanism for B diffusion in SiC. Applied Physics Letters, 2002, 81, 2989-2991.	1.5	26
115	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.	0.7	26
116	Coexistence of Elastic Modulations in the Charge Density Wave State of 2H-NbSe₂. Nano Letters, 2019, 19, 3027-3032.	4.5	26
117	Nonparametrized calculation of the electronic and vibrational structure of amorphousSiOx. Physical Review B, 1991, 43, 4552-4555.	1.1	24
118	First-principles study of n-type dopants and their clustering in SiC. Applied Physics Letters, 2003, 82, 4298-4300.	1.5	24
119	First-principles studies of the diffusion of B impurities and vacancies in SiC. Physical Review B, 2004, 69, .	1.1	24
120	Density-wave instability in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><mml:mrow><mml:mo>(Physical Review B, 2010, 82, .	1.1	24
121	Anisotropic features in the electronic structure of the two-dimensional transition metal trichalcogenide TiS ₃ : electron doping and plasmons. 2D Materials, 2017, 4, 025085.	2.0	24
122	Environment effects on chemical reactivity of heme proteins. International Journal of Quantum Chemistry, 2002, 90, 1505-1514.	1.0	23
123	Ab initio study of electron-phonon coupling in rubrene. Physical Review B, 2017, 96, .	1.1	23
124	Resistive and rectifying effects of pulling gold atoms at thiol-gold nanocontacts. Physical Review B, 2007, 75, .	1.1	22
125	Spin-Crossover in an Exfoliated 2D Coordination Polymer and Its Implementation in Thermochromic Films. ACS Applied Nano Materials, 2018, 1, 2662-2668.	2.4	22
126	Addressing the Environment Electrostatic Effect on Ballistic Electron Transport in Large Systems: A QM/MM-NEGF Approach. Journal of Physical Chemistry B, 2018, 122, 485-492.	1.2	21

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127	First principles analysis of the CDW instability of single-layer 1 T -TiSe ₂ and its evolution with charge carrier density. 2D Materials, 2018, 5, 025024.	2.0	20
128	2 Ã— 2 charge density wave in single-layer TiTe ₂. 2D Materials, 2019, 6, 015027.	2.0	20
129	Carbon nanotubes as substrates for molecular spiropyran-based switches. Journal of Physics Condensed Matter, 2012, 24, 394006.	0.7	19
130	Optical and electronic properties of 2Hâˆ’MoS2 under pressure: Revealing the spin-polarized nature of bulk electronic bands. Physical Review Materials, 2018, 2, .	0.9	19
131	The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations. Npj Computational Materials, 2022, 8, .	3.5	19
132	First principles studies of neutral vacancies diffusion in SiC. Computational Materials Science, 2003, 27, 36-42.	1.4	18
133	First-principles characterization of the electronic structure of the molecular superconductorÎ²â€²(BEDTâ€“TTF)2IBr2. Physical Review B, 2003, 67, .	1.1	18
134	Defects of the SiC/SiO2 interface: energetics of the elementary steps of the oxidation reaction. Physica B: Condensed Matter, 2003, 340-342, 1069-1073.	1.3	17
135	Correlation between electronic structure and local ordering in hydrogenated amorphous silicon. Physical Review B, 1989, 40, 12416-12422.	1.1	16
136	Solid phosphorus carbide?. Chemical Communications, 2002, , 2494-2495.	2.2	16
137	Structural, Dynamical, and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases. Journal of Physical Chemistry A, 2011, 115, 11344-11354.	1.1	16
138	Manipulation of spin transport in graphene/transition metal dichalcogenide heterobilayers upon twisting. 2D Materials, 0, , .	2.0	16
139	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
140	Simulations of minerals using density-functional theory based on atomic orbitals for linear scaling. Physics and Chemistry of Minerals, 2004, 31, 12-21.	0.3	15
141	Scanning Tunneling Microscopy and Surface Simulation of Zinc-Blende GaN(001) Intrinsic4Ã—Reconstruction: Linear Gallium Tetramers?. Physical Review Letters, 2005, 95, 146102.	2.9	15
142	Evidence for the weak coupling scenario of the Peierls transition in the blue bronze. Physical Review Materials, 2019, 3, .	0.9	15
143	Theoretical study of a-SiNxHy alloys. Journal of Non-Crystalline Solids, 1991, 137-138, 891-894.	1.5	14
144	Y:BaZrO₃ Perovskite Compounds I: DFT Study on the Unprotonated and Protonated Local Structures. Chemistry - an Asian Journal, 2012, 7, 1827-1837.	1.7	14

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145	Atomically Sharp Lateral Superlattice Heterojunctions Builtâ€in Nitrogenâ€Doped Nanoporous Graphene. Advanced Materials, 2022, 34, e2110099.	11.1	14
146	Application of local-spin-density approximation toaâ^'Siand tetrahedralaâ^'C. Physical Review B, 1999, 60, 10594-10597.	1.1	13
147	Electronic structure of the superconducting layered ternary nitridesCaTaN2andCaNbN2. Physical Review B, 2000, 62, 1512-1515.	1.1	13
148	SnO 2 : Bulk and Surface Simulations by an Ab Initio Numerical Local Orbitals Method. Phase Transitions, 2002, 75, 143-149.	0.6	13
149	Surface electronic structure of metastable FeSi(CsCl)(111) epitaxially grown on Si(111). Physical Review B, 1997, 55, R16065-R16068.	1.1	12
150	Comment on â€œIdentifying Molecular Orientation of IndividualC60on aSi(111)â^'(7Ã—7)Surfaceâ€• Physical Review Letters, 2000, 85, 2653-2653.	2.9	12
151	Ring closure in dioxin formation process: An ab initio molecular dynamics study. Journal of Chemical Physics, 2001, 115, 6401-6405.	1.2	12
152	First-principles molecular dynamics study of the stretching frequencies of hydrogen molecules in carbon nanotubes. New Journal of Physics, 2003, 5, 124-124.	1.2	12
153	Dielectric screening in extended systems using the self-consistent Sternheimer equation and localized basis sets. Physical Review B, 2012, 85, .	1.1	12
154	Unraveling Heat Transport and Dissipation in Suspended MoSe₂ from Bulk to Monolayer. Advanced Materials, 2022, 34, e2108352.	11.1	12
155	Self-interstitialâ€“hydrogen complexes in Si. Physical Review B, 2001, 64, .	1.1	11
156	Tunneling spectroscopy in core/shell structured Fe/MgO nanospheres. Applied Physics Letters, 2009, 94, 062507.	1.5	11
157	Band selection and disentanglement using maximally localized Wannier functions: the cases of Co impurities in bulk copper and the Cu(111) surface. Journal of Physics Condensed Matter, 2010, 22, 385601.	0.7	11
158	Implementation of non-collinear spin-constrained DFT calculations in SIESTA with a fully relativistic Hamiltonian. JPhys Materials, 2018, 1, 015010.	1.8	11
159	Thermal and transport properties of pristine single-layer hexagonal boron nitride: A first principles investigation. Physical Review Materials, 2017, 1, .	0.9	11
160	The strange behavior of interstitial H2 molecules Si and GaAs. Physica B: Condensed Matter, 2001, 308-310, 202-205.	1.3	10
161	Copper-Defect and Copper-Impurity Interactions in Silicon. Solid State Phenomena, 2001, 82-84, 341-348.	0.3	10
162	Nanotubes and nanowires: the effect of impurities and defects on their electronic properties. International Journal of Nanotechnology, 2005, 2, 114.	0.1	10

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163	Transport measurements under pressure in IIIâ€"IV layered semiconductors. Physica Status Solidi (B): Basic Research, 2007, 244, 162-168.	0.7	10
164	Interaction of copper organometallic precursors with barrier layers of Ti, Ta and W and their nitrides: a first-principles molecular dynamics study. Journal of Molecular Modeling, 2007, 13, 861-864.	0.8	10
165	Mixed Approach to Incorporate Self-Consistency into Order-N LCAO Methods. Materials Research Society Symposia Proceedings, 1995, 408, 85.	0.1	9
166	A Cause for SiC/SiO₂ Interface States: the Site Selection of Oxygen in SiC. Materials Science Forum, 2003, 433-436, 535-538.	0.3	9
167	First stages of the oxidation of the Si-rich 3Câ€"SiC(001) surface. Computational Materials Science, 2005, 33, 13-19.	1.4	9
168	Band bending and quasiâ€2DEG in the metallized Î²â€SiC(001) surface. Physica Status Solidi - Rapid Research Letters, 2008, 2, 218-220.	1.2	9
169	Validity of the on-site spin-orbit coupling approximation. Physical Review B, 2021, 104, .	1.1	9
170	Density functional theory calculations of quantum electron transport: carbon nanotubes-gold contacts. Advances in Quantum Chemistry, 2003, , 299-314.	0.4	8
171	GaS and InSe equations of state from single crystal diffraction. Physica Status Solidi (B): Basic Research, 2007, 244, 169-173.	0.7	8
172	Localization in the interacting-random-dimer model. Physical Review B, 1994, 50, 14682-14685.	1.1	7
173	Surface electronic structure of metastable FeSi(CsCl)(1 1 1). Surface Science, 2001, 482-485, 625-631.	0.8	7
174	Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3. Solid State Ionics, 2004, 168, 291-298.	1.3	7
175	Analysis of scanning tunneling microscopy images of the charge-density-wave phase in quasi-one-dimensionalRb0.3MoO3. Physical Review B, 2006, 74, .	1.1	7
176	Performance of local orbital basis sets in the self-consistent Sternheimer method for dielectric matrices of extended systems. European Physical Journal B, 2012, 85, 1.	0.6	7
177	Manganese 3<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>Ã—</mml:mo></mml:math>3 and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msqrt><mml:mn>3</mml:mn></mml:msqrt><mml:mo>Ã—</mml:mo><mml:msqrt><mml:mn>3 xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>R</mml:mi><mml:msup><mml:mn>30</mml:mn><mml:mo>â˜</mml:mo></mml:msup>	1.1	7
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