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	Interference effects in one-dimensional moirÃ© crystals. Carbon, 2022, 186, 416-422.	5.4	1
2	Unraveling Heat Transport and Dissipation in Suspended MoSe₂ from Bulk to Monolayer. Advanced Materials, 2022, 34, e2108352.	11.1	12
3	Magnetic properties of coordination clusters with {Mn4} and {Co4} antiferromagnetic cores. Physical Chemistry Chemical Physics, 2022, 24, 3780-3787.	1.3	3
4	The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations. Npj Computational Materials, 2022, 8, .	3.5	19
5	Competition between Ta-Ta and Te-Te bonding leading to the commensurate charge density wave in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ta</mml:mi><mml:msub><mml:mi>Te</mml:mi><mml:mi> Physical Review B, 2022, 105, .	1.1	6
6	Atomically Sharp Lateral Superlattice Heterojunctions Builtâ€in Nitrogenâ€Doped Nanoporous Graphene. Advanced Materials, 2022, 34, e2110099.	11.1	14
7	Colossal phonon drag enhanced thermopower in lightly doped diamond. Materials Today Physics, 2022, 27, 100740.	2.9	5
8	Basic aspects of the charge density wave instability of transition metal trichalcogenides NbSe₃ and monoclinic-TaS₃. Journal of Physics Condensed Matter, 2021, 33, 485401.	0.7	2
9	Validity of the on-site spin-orbit coupling approximation. Physical Review B, 2021, 104, .	1.1	9
10	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	1.2	229
11	Fermi surface electronâ€“hole instability of the (TMTSF)₂PF₆ Bechgaard salt revealed by the first-principles Lindhard response function. Journal of Physics Condensed Matter, 2020, 32, 345701.	0.7	4
12	Anion ordering transition and Fermi surface electronâ€“hole instabilities in the (TMTSF)₂ClO₄ and (TMTSF)₂NO₃ Bechgaard salts analyzed through the first-principles Lindhard response function. Journal of Physics Condensed Matter, 2020, 33, 085705.	0.7	4
13	Coexistence of Elastic Modulations in the Charge Density Wave State of 2H-NbSe₂. Nano Letters, 2019, 19, 3027-3032.	4.5	26
14	2 Ã— 2 charge density wave in single-layer TiTe ₂. 2D Materials, 2019, 6, 015027.	2.0	20
15	Evidence for the weak coupling scenario of the Peierls transition in the blue bronze. Physical Review Materials, 2019, 3, .	0.9	15
16	Spin Proximity Effects in Graphene/Topological Insulator Heterostructures. Nano Letters, 2018, 18, 2033-2039.	4.5	86
17	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
18	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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19	Implementation of non-collinear spin-constrained DFT calculations in SIESTA with a fully relativistic Hamiltonian. JPhys Materials, 2018, 1, 015010.	1.8	11
20	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
21	Mechanisms behind the enhancement of thermal properties of graphene nanofluids. Nanoscale, 2018, 10, 15402-15409.	2.8	49
22	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
23	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
24	Growth of Twin-Free and Low-Doped Topological Insulators on BaF₂(111). Crystal Growth and Design, 2017, 17, 4655-4660.	1.4	34
25	Ab initio study of electron-phonon coupling in rubrene. Physical Review B, 2017, 96, .	1.1	23
26	Voltageâ€Induced Coercivity Reduction in Nanoporous Alloy Films: A Boost toward Energyâ€Efficient Magnetic Actuation. Advanced Functional Materials, 2017, 27, 1701904.	7.8	41
27	Thermal and transport properties of pristine single-layer hexagonal boron nitride: A first principles investigation. Physical Review Materials, 2017, 1, .	0.9	11
28	Nanotexturing To Enhance Photoluminescent Response of Atomically Thin Indium Selenide with Highly Tunable Band Gap. Nano Letters, 2016, 16, 3221-3229.	4.5	155
29	Electronic structure of 2 H -NbSe ₂ single-layers in the CDW state. 2D Materials, 2016, 3, 035028.	2.0	50
30	How disorder affects topological surface states in the limit of ultrathin Bi₂Se₃films. 2D Materials, 2016, 3, 045007.	2.0	2
31	Capacitive DNA Detection Driven by Electronic Charge Fluctuations in a Graphene Nanopore. Physical Review Applied, 2015, 3, .	1.5	60
32	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>â’</mml:m Two-band superconductivity and the role of tunneling selectivity. Physical Review B, 2015, 92, .	1.1	66
33	Tunneling and electronic structure of the two-gap superconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MgB</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2015, 92, .	1.1	5
34	Momentum dependence of spinâ€“orbit interaction effects in single-layer and multi-layer transition metal dichalcogenides. 2D Materials, 2014, 1, 034003.	2.0	85
35	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
36	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</m 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></mml:	1.1	7

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37	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
38	Insulating behavior of an amorphous graphene membrane. Physical Review B, 2012, 86, .	1.1	38
39	Carbon nanotubes as substrates for molecular spiropyran-based switches. Journal of Physics Condensed Matter, 2012, 24, 394006.	0.7	19
40	Electroresistance Effect in Ferroelectric Tunnel Junctions with Symmetric Electrodes. ACS Nano, 2012, 6, 1473-1478.	7.3	48
41	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
42	Calculation of core level shifts within DFT using pseudopotentials and localized basis sets. European Physical Journal B, 2012, 85, 1.	0.6	44
43	Dielectric screening in extended systems using the self-consistent Sternheimer equation and localized basis sets. Physical Review B, 2012, 85, .	1.1	12
44	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
45	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
46	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
47	Oxygen Surface Functionalization of Graphene Nanoribbons for Transport Gap Engineering. ACS Nano, 2011, 5, 9271-9277.	7.3	53
48	Magnetoresistance and Magnetic Ordering Fingerprints in Hydrogenated Graphene. Physical Review Letters, 2011, 107, 016602.	2.9	132
49	Magnetism-Dependent Transport Phenomena in Hydrogenated Graphene: From Spin-Splitting to Localization Effects. ACS Nano, 2011, 5, 3987-3992.	7.3	47
50	An efficient implementation of a QMâ€“MM method in SIESTA. Theoretical Chemistry Accounts, 2011, 128, 825-833.	0.5	29
51	Quantum transport in chemically modified two-dimensional graphene: From minimal conductivity to Anderson localization. Physical Review B, 2011, 84, .	1.1	84
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53	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
54	Damaging Graphene with Ozone Treatment: A Chemically Tunable Metalâ^'Insulator Transition. ACS Nano, 2010, 4, 4033-4038.	7.3	149

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55	Electronic Transport between Graphene Layers Covalently Connected by Carbon Nanotubes. ACS Nano, 2010, 4, 7596-7602.	7.3	133
56	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
57	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:mo> Physical Review B, 2010, 82, .	1.1	24
58	Tunneling spectroscopy in core/shell structured Fe/MgO nanospheres. Applied Physics Letters, 2009, 94, 062507.	1.5	11
59	Optimal strictly localized basis sets for noble metal surfaces. Physical Review B, 2009, 79, .	1.1	100
60	Trends in Nanotechnology (TNT2007). Physica Status Solidi (A) Applications and Materials Science, 2008, 205, 1245-1248.	0.8	0
61	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
62	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	0.7	522
63	Resistive and rectifying effects of pulling gold atoms at thiol-gold nanocontacts. Physical Review B, 2007, 75, .	1.1	22
64	Inhomogenities of the CDW vector at the (-201) surface of Quasi-1D blue bronze Rb0.3MoO3. Journal of Physics: Conference Series, 2007, 61, 140-146.	0.3	2
65	Preface: phys. stat. sol. (a) 204/6. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 1607-1610.	0.8	1
66	Transport measurements under pressure in IIIâ€“IV layered semiconductors. Physica Status Solidi (B): Basic Research, 2007, 244, 162-168.	0.7	10
67	GaS and InSe equations of state from single crystal diffraction. Physica Status Solidi (B): Basic Research, 2007, 244, 169-173.	0.7	8
68	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
69	Ab initio study of NOx compounds adsorption on SnO2 surface. Sensors and Actuators B: Chemical, 2007, 126, 62-67.	4.0	86
70	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
71	Electronic Structure and Charge Transfer in the Ternary Intercalated Graphite Î²-KS0.25C3. Inorganic Chemistry, 2006, 45, 9387-9393.	1.9	0
72	Editorial: Trends in Nanotechnology (TNT2005). Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1045-1046.	0.8	0

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73	Scientific Highlights from the Î¨k Network: Towards Atomistic Materials Design. Physica Status Solidi (B): Basic Research, 2006, 243, 2445-2445.	0.7	0
74	Simulation of the Growth of Copper Films for Micro and Nano-Electronics. Advances in Science and Technology, 2006, 51, 167-173.	0.2	0
75	Electron Transport via Local Polarons at Interface Atoms. Physical Review Letters, 2006, 97, 206801.	2.9	50
76	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
77	FIRST PRINCIPLES SLAB RELAXATION STUDY OF THE TiFe(001) SURFACE. Surface Review and Letters, 2006, 13, 495-501.	0.5	1
78	Nanotubes and nanowires: the effect of impurities and defects on their electronic properties. International Journal of Nanotechnology, 2005, 2, 114.	0.1	10
79	Self-doped titanium oxide thin films for efficient visible light photocatalysis. Sensors and Actuators B: Chemical, 2005, 109, 52-56.	4.0	37
80	Theoretical study of O2 and CO adsorption on Aun clusters (n=5â€“10). Chemical Physics Letters, 2005, 408, 252-257.	1.2	95
81	Electronic Structure Calculations with Localized Orbitals: The Siesta Method. , 2005, , 77-91.		3
82	Strength of radial breathing mode in single-walled carbon nanotubes. Physical Review B, 2005, 71, .	1.1	109
83	Composition-dependent structural properties in ScGaN alloy films: A combined experimental and theoretical study. Journal of Applied Physics, 2005, 98, 123501.	1.1	36
84	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
85	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
86	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
87	First stages of the oxidation of the Si-rich 3Câ€“SiC(001) surface. Computational Materials Science, 2005, 33, 13-19.	1.4	9
88	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
89	Phonon dispersion of graphite. AIP Conference Proceedings, 2004, , .	0.3	1
90	Band structure of indium selenide investigated by intrinsic photoluminescence under high pressure. Physical Review B, 2004, 70, .	1.1	35

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91	Systematic study of electron localization in an amorphous semiconductor. Physical Review B, 2004, 69, .	1.1	34
92	Antisites as Possible Origin of Irradiation Induced Photoluminescence Centers in SiC: A Theoretical Study on Clusters of Antisites and Carbon Interstitials in 4H-SiC. Materials Science Forum, 2004, 457-460, 443-448.	0.3	1
93	First-Principles Study of O Adsorption at SiC Surface. Materials Science Forum, 2004, 457-460, 1293-1296.	0.3	3
94	Phonon Dispersion in Graphite. Physical Review Letters, 2004, 92, 075501.	2.9	460
95	Stability and Mobility of Mono- and Di-Interstitials inÎ±-Fe. Physical Review Letters, 2004, 92, 175503.	2.9	403
96	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
97	Self-passivation mechanisms in clusters of N dopants in SiC. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 274-277.	0.8	1
98	Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3. Solid State Ionics, 2004, 168, 291-298.	1.3	7
99	First principles study of gold adsorption and diffusion on graphite. Surface Science, 2004, 564, 173-178.	0.8	63
100	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
101	First-principles studies of the diffusion of B impurities and vacancies in SiC. Physical Review B, 2004, 69, .	1.1	24
102	Computing the Properties of Materials from First Principles with SIESTA. Structure and Bonding, 2004, , 103-170.	1.0	101
103	Sampling the diffusion paths of a neutral vacancy in silicon with quantum mechanical calculations. Physical Review B, 2004, 70, .	1.1	80
104	The strength of the radial-breathing mode in single-walled carbon nanotubes. AIP Conference Proceedings, 2004, , .	0.3	2
105	TranSIESTA: A Spice for Molecular Electronics. Annals of the New York Academy of Sciences, 2003, 1006, 212-226.	1.8	205
106	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
107	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
108	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

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109	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
110	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
111	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
112	First principles studies of neutral vacancies diffusion in SiC. Computational Materials Science, 2003, 27, 36-42.	1.4	18
113	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
114	Hexagonal diamond from single-walled carbon nanotubes. AIP Conference Proceedings, 2003, , .	0.3	1
115	Electrons in dry DNA from density functional calculations. Molecular Physics, 2003, 101, 1587-1594.	0.8	87
116	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
117	First-Principles Studies of N and P Dopant Interactions in SiC: Implications for Co-Doping. Materials Science Forum, 2003, 433-436, 649-652.	0.3	2
118	First-principles calculation of the band offset atBaO/BaTiO3andSrO/SrTiO3interfaces. Physical Review B, 2003, 67, .	1.1	121
119	Origin of current-induced forces in an atomic gold wire:â€,â€,A first-principles study. Physical Review B, 2003, 67, .	1.1	98
120	Aggregation of carbon interstitials in silicon carbide: A theoretical study. Physical Review B, 2003, 68, .	1.1	103
121	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
122	First-principles characterization of the electronic structure of the molecular superconductorÎ²â€²(BEDTâ€“TTF)2IBr2. Physical Review B, 2003, 67, .	1.1	18
123	First-principles study of n-type dopants and their clustering in SiC. Applied Physics Letters, 2003, 82, 4298-4300.	1.5	24
124	Density functional theory calculations of quantum electron transport: carbon nanotubes-gold contacts. Advances in Quantum Chemistry, 2003, , 299-314.	0.4	8
125	Vibrational properties of double-walled carbon nanotubes. AIP Conference Proceedings, 2003, , .	0.3	5
126	Ab initio studies of electron-phonon coupling in single-walled nanotubes. AIP Conference Proceedings, 2003, , .	0.3	0

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127	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
128	Molecular Dynamics Simulations of Nanotube Growth. , 2003, , 45-56.		1
129	Theoretical evidence for the kick-out mechanism for B diffusion in SiC. Applied Physics Letters, 2002, 81, 2989-2991.	1.5	26
130	First-principles study of the blue bronzeK0.3MoO3. Physical Review B, 2002, 65, .	1.1	39
131	First-principles study of the neutral molecular metalNi(tmdt)2. Physical Review B, 2002, 65, .	1.1	60
132	SnO 2 : Bulk and Surface Simulations by an Ab Initio Numerical Local Orbitals Method. Phase Transitions, 2002, 75, 143-149.	0.6	13
133	Ab Initio Calculations of B Diffusion in SiC. Materials Science Forum, 2002, 389-393, 553-556.	0.3	1
134	Angle-resolved photoemission study and first-principles calculation of the electronic structure of GaTe. Physical Review B, 2002, 65, .	1.1	38
135	Electronic band structure of isolated and bundled carbon nanotubes. Physical Review B, 2002, 65, .	1.1	327
136	Tight-binding description of graphene. Physical Review B, 2002, 66, .	1.1	904
137	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. Nanotechnology, 2002, 13, 346-351.	1.3	39
138	Ab initiocalculations of the optical properties of 4-Ã…-diameter single-walled nanotubes. Physical Review B, 2002, 66, .	1.1	256
139	Density-functional method for nonequilibrium electron transport. Physical Review B, 2002, 65, .	1.1	4,752
140	Ab initiodetermination of the phonon deformation potentials of graphene. Physical Review B, 2002, 65, .	1.1	72
141	Elastic properties of carbon nanotubes under hydrostatic pressure. Physical Review B, 2002, 65, .	1.1	139
142	Solid phosphorus carbide?. Chemical Communications, 2002, , 2494-2495.	2.2	16
143	Ab initiolocal vibrational modes of light impurities in silicon. Physical Review B, 2002, 65, .	1.1	51
144	Band structure and optical properties of isolated and bundled nanotubes. AIP Conference Proceedings, 2002, , .	0.3	1

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145	Designed Self-Doped Titanium Oxide Thin Films for Efficient Visible-Light Photocatalysis. Advanced Materials, 2002, 14, 1399-1402.	11.1	438
146	Environment effects on chemical reactivity of heme proteins. International Journal of Quantum Chemistry, 2002, 90, 1505-1514.	1.0	23
147	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	0.7	9,150
148	Ab-Initio Calculations on the Structural and Electronic Properties of BaO/BatiO3 And SrO/SrTiO3 Interfaces. , 2002, , 561-571.		0
149	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
150	Ab initiostudy of silicon-multisubstituted neutral and charged fullerenes. Physical Review B, 2001, 63, .	1.1	67
151	Fullerene growth and the role of nonclassical isomers. Physical Review B, 2001, 63, .	1.1	53
152	Experimental and theoretical study of band structure of InSe andIn1âˆ'xGaxSe(x<0.2)under high pressure:â€,Direct to indirect crossovers. Physical Review B, 2001, 63, .	1.1	73
153	Phonon eigenvectors of chiral nanotubes. Physical Review B, 2001, 64, .	1.1	53
154	Ring closure in dioxin formation process: An ab initio molecular dynamics study. Journal of Chemical Physics, 2001, 115, 6401-6405.	1.2	12
155	Surface electronic structure of metastable FeSi(CsCl)(1 1 1). Surface Science, 2001, 482-485, 625-631.	0.8	7
156	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
157	Structural and vibrational properties of single walled nanotubes under hydrostatic pressure. AIP Conference Proceedings, 2001, , .	0.3	1
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159	The fascinating dynamics of defects in silicon. Physica B: Condensed Matter, 2001, 308-310, 1-7.	1.3	2
160	Vibrational properties of H-related defects in silicon. Physica B: Condensed Matter, 2001, 308-310, 147-150.	1.3	2
161	The strange behavior of interstitial H2 molecules Si and GaAs. Physica B: Condensed Matter, 2001, 308-310, 202-205.	1.3	10
162	Copper-Defect and Copper-Impurity Interactions in Silicon. Solid State Phenomena, 2001, 82-84, 341-348.	0.3	10

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164	Dynamics of interstitial hydrogen molecules in crystalline silicon. Journal of Physics Condensed Matter, 2001, 13, 6271-6283.	0.7	38
165	Self-interstitialâ€“hydrogen complexes in Si. Physical Review B, 2001, 64, .	1.1	11
166	First-principles study of the origin and nature of ferromagnetism inGa1âˆ’xMnxAs. Physical Review B, 2001, 63, .	1.1	288
167	Unexpected Dynamics for Self-Interstitial Clusters in Silicon. Physical Review Letters, 2001, 86, 1247-1250.	2.9	85
168	First Principles Electronic Structure Methods. , 2001, , 189-220.		0
169	Linear Scaling ab initio Calculations in Nanoscale Materials with SIESTA. Physica Status Solidi (B): Basic Research, 2000, 217, 335-356.	0.7	111
170	Seeing molecular orbitals. Chemical Physics Letters, 2000, 321, 78-82.	1.2	117
171	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
172	Metallic bonding and cluster structure. Physical Review B, 2000, 61, 5771-5780.	1.1	163
173	New Method For First Principles Modeling of Electron Transport through Nanoelectronic Devices.. Materials Research Society Symposia Proceedings, 2000, 636, 9251.	0.1	5
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