Pablo Ordejon

List of Publications by Year in Descending Order

212 papers	29,562 citations	64 h-index	171 g-index
222 ext. papers	31,677 ext. citations	4.3 avg, IF	6.73 L-index

#	Paper	IF	Citations
212	Unraveling Heat Transport and Dissipation in Suspended MoSe from Bulk to Monolayer.. *Advanced Materials*, **2022**, e2108352	24	1
211	The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations. *Npj Computational Materials*, **2022**, 8,	10.9	2
210	Interference effects in one-dimensional moir crystals. *Carbon*, **2022**, 186, 416-422	10.4	0
209	Atomically Sharp Lateral Superlattice Heterojunctions Built-in Nitrogen-doped Nanoporous Graphene.. *Advanced Materials*, **2022**, e2110099	24	1
208	Colossal phonon drag enhanced thermopower in lightly doped diamond. *Materials Today Physics*, **2022**, 100740	8	0
207	Validity of the on-site spin-orbit coupling approximation. *Physical Review B*, **2021**, 104,	3.3	1
206	Siesta: Recent developments and applications. *Journal of Chemical Physics*, **2020**, 152, 204108	3.9	69
205	Fermi surface electron-hole instability of the (TMTSF)PF Bechgaard salt revealed by the first-principles Lindhard response function. *Journal of Physics Condensed Matter*, **2020**, 32, 345701	1.8	1
204	Anion ordering transition and Fermi surface electron-hole instabilities in the (TMTSF)ClO and (TMTSF)NO Bechgaard salts analyzed through the first-principles Lindhard response function. *Journal of Physics Condensed Matter*, **2020**, 33, 085705	1.8	0
203	Coexistence of Elastic Modulations in the Charge Density Wave State of 2 H-NbSe. *Nano Letters*, **2019**, 19, 3027-3032	11.5	8
202	Evidence for the weak coupling scenario of the Peierls transition in the blue bronze. *Physical Review Materials*, **2019**, 3,	3.2	11
201	2 2 charge density wave in single-layer TiTe 2. *2D Materials*, **2019**, 6, 015027	5.9	10
200	Spin Proximity Effects in Graphene/Topological Insulator Heterostructures. *Nano Letters*, **2018**, 18, 2033-2039	11.5	65
199	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	5.9	14
198	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	3.4	14
197	Mechanisms behind the enhancement of thermal properties of graphene nanofluids. *Nanoscale*, **2018**, 10, 15402-15409	7.7	36
196	Optical and electronic properties of 2H MoS2 under pressure: Revealing the spin-polarized nature of bulk electronic bands. *Physical Review Materials*, **2018**, 2,	3.2	14

195	Implementation of non-collinear spin-constrained DFT calculations in SIESTA with a fully relativistic Hamiltonian. *JPhys Materials*, **2018**, 1, 015010	4.2	7
194	Spin-Crossover in an Exfoliated 2D Coordination Polymer and Its Implementation in Thermochromic Films. *ACS Applied Nano Materials*, **2018**, 1, 2662-2668	5.6	20
193	Anisotropic features in the electronic structure of the two-dimensional transition metal trichalcogenide TiS 3 : electron doping and plasmons. *2D Materials*, **2017**, 4, 025085	5.9	20
192	Growth of Twin-Free and Low-Doped Topological Insulators on BaF2(111). *Crystal Growth and Design*, **2017**, 17, 4655-4660	3.5	24
191	Ab initio study of electron-phonon coupling in rubrene. *Physical Review B*, **2017**, 96,	3.3	22
190	Voltage-Induced Coercivity Reduction in Nanoporous Alloy Films: A Boost toward Energy-Efficient Magnetic Actuation. *Advanced Functional Materials*, **2017**, 27, 1701904	15.6	31
189	Thermal and transport properties of pristine single-layer hexagonal boron nitride: A first principles investigation. *Physical Review Materials*, **2017**, 1,	3.2	10
188	Electronic structure of 2 H -NbSe 2 single-layers in the CDW state. *2D Materials*, **2016**, 3, 035028	5.9	33
187	How disorder affects topological surface states in the limit of ultrathin Bi 2 Se 3 films. *2D Materials*, **2016**, 3, 045007	5.9	1
186	Nanotexturing To Enhance Photoluminescent Response of Atomically Thin Indium Selenide with Highly Tunable Band Gap. *Nano Letters*, **2016**, 16, 3221-9	11.5	119
185	Capacitive DNA Detection Driven by Electronic Charge Fluctuations in a Graphene Nanopore. *Physical Review Applied*, **2015**, 3,	4.3	54
184	Quasiparticle spectra of 2H□NbSe2: Two-band superconductivity and the role of tunneling selectivity. *Physical Review B*, **2015**, 92,	3.3	32
183	Tunneling and electronic structure of the two-gap superconductor MgB2. *Physical Review B*, **2015**, 92,	3.3	5
182	Electronic properties of single-layer and multilayer transition metal dichalcogenides MX2 (M = Mo, W and X = S, Se). *Annalen Der Physik*, **2014**, 526, 347-357	2.6	143
181	Momentum dependence of spin□orbit interaction effects in single-layer and multi-layer transition metal dichalcogenides. *2D Materials*, **2014**, 1, 034003	5.9	71
180	Manganese 3□ and 3□-R30? structures and structural phase transition on w-GaN(0001□) studied by scanning tunneling microscopy and first-principles theory. *Physical Review B*, **2013**, 87,	3.3	6
179	Tight-binding model and direct-gap/indirect-gap transition in single-layer and multilayer MoS2. *Physical Review B*, **2013**, 88,	3.3	284
178	Insulating behavior of an amorphous graphene membrane. *Physical Review B*, **2012**, 86,	3.3	30

177	Carbon nanotubes as substrates for molecular spiropyran-based switches. *Journal of Physics Condensed Matter*, **2012**, 24, 394006	1.8	14
176	Electroresistance effect in ferroelectric tunnel junctions with symmetric electrodes. *ACS Nano*, **2012**, 6, 1473-8	16.7	42
175	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	1.2	6
174	Calculation of core level shifts within DFT using pseudopotentials and localized basis sets. *European Physical Journal B*, **2012**, 85, 1	1.2	37
173	Dielectric screening in extended systems using the self-consistent Sternheimer equation and localized basis sets. *Physical Review B*, **2012**, 85,	3.3	12
172	Y:BaZrO3 perovskite compounds I: DFT study on the unprotonated and protonated local structures. *Chemistry - an Asian Journal*, **2012**, 7, 1827-37	4.5	10
171	Structural, dynamical, and electronic transport properties of modified DNA duplexes containing size-expanded nucleobases. *Journal of Physical Chemistry A*, **2011**, 115, 11344-54	2.8	15
170	Oxygen surface functionalization of graphene nanoribbons for transport gap engineering. *ACS Nano*, **2011**, 5, 9271-7	16.7	36
169	Magnetoresistance and magnetic ordering fingerprints in hydrogenated graphene. *Physical Review Letters*, **2011**, 107, 016602	7.4	113
168	Magnetism-dependent transport phenomena in hydrogenated graphene: from spin-splitting to localization effects. *ACS Nano*, **2011**, 5, 3987-92	16.7	41
167	An efficient implementation of a QMMM method in SIESTA. *Theoretical Chemistry Accounts*, **2011**, 128, 825-833	1.9	24
166	Modulation of Surface Charge Transfer through Competing Long-Range Repulsive versus Short-Range Attractive Interactions. *Journal of Physical Chemistry C*, **2011**, 115, 18640-18648	3.8	46
165	Quantum transport in chemically modified two-dimensional graphene: From minimal conductivity to Anderson localization. *Physical Review B*, **2011**, 84,	3.3	66
164	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	1.8	11
163	Damaging graphene with ozone treatment: a chemically tunable metal-insulator transition. *ACS Nano*, **2010**, 4, 4033-8	16.7	126
162	Electronic transport between graphene layers covalently connected by carbon nanotubes. *ACS Nano*, **2010**, 4, 7596-602	16.7	109
161	Orbital specific chirality and homochiral self-assembly of achiral molecules induced by charge transfer and spontaneous symmetry breaking. *Physical Review Letters*, **2010**, 105, 115702	7.4	109
160	Density-wave instability in β-BEDT-TTF)2KHg(SCN)4 studied by x-ray diffuse scattering and by first-principles calculations. *Physical Review B*, **2010**, 82,	3.3	22

159	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, 2856-65	6.4	142
158	Tunneling spectroscopy in core/shell structured Fe/MgO nanospheres. *Applied Physics Letters*, **2009**, 94, 062507	3.4	10
157	Optimal strictly localized basis sets for noble metal surfaces. *Physical Review B*, **2009**, 79,	3.3	90
156	The SIESTA method; developments and applicability. *Journal of Physics Condensed Matter*, **2008**, 20, 064208	2.8	364
155	Trends in Nanotechnology (TNT2007). *Physica Status Solidi (A) Applications and Materials Science*, **2008**, 205, 1245-1248	1.6	
154	Band bending and quasi-2DEG in the metallized □SiC(001) surface. *Physica Status Solidi - Rapid Research Letters*, **2008**, 2, 218-220	2.5	9
153	Preface: phys. stat. sol. (a) 204/6. *Physica Status Solidi (A) Applications and Materials Science*, **2007**, 204, 1607-1610	1.6	1
152	Transport measurements under pressure in III□V layered semiconductors. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 162-168	1.3	10
151	GaS and InSe equations of state from single crystal diffraction. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 169-173	1.3	7
150	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, 861-4	2	10
149	Ab initio study of NOx compounds adsorption on SnO2 surface. *Sensors and Actuators B: Chemical*, **2007**, 126, 62-67	8.5	82
148	Resistive and rectifying effects of pulling gold atoms at thiol-gold nanocontacts. *Physical Review B*, **2007**, 75,	3.3	17
147	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
146	Simulation of the Growth of Copper Films for Micro and Nano-Electronics. *Advances in Science and Technology*, **2006**, 51, 167-173	0.1	
145	Electron transport via local polarons at interface atoms. *Physical Review Letters*, **2006**, 97, 206801	7.4	46
144	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,	3.3	32
143	FIRST PRINCIPLES SLAB RELAXATION STUDY OF THE TiFe(001) SURFACE. *Surface Review and Letters*, **2006**, 13, 495-501	1.1	1
142	Analysis of scanning tunneling microscopy images of the charge-density-wave phase in quasi-one-dimensional Rb0.3MoO3. *Physical Review B*, **2006**, 74,	3.3	6

141	Electronic structure and charge transfer in the ternary intercalated graphite beta-KS0.25C3. *Inorganic Chemistry*, **2006**, 45, 9387-93	5.1	
140	Scientific Highlights from the Network: Towards Atomistic Materials Design. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2445-2445	1.3	
139	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, 7608-14	4	31
138	First stages of the oxidation of the Si-rich 3C SiC(0 0 1) surface. *Computational Materials Science*, **2005**, 33, 13-19	3.2	9
137	Crystal symmetry and pressure effects on the valence band structure of InSe and GaSe: Transport measurements and electronic structure calculations. *Physical Review B*, **2005**, 71,	3.3	54
136	Nanotubes and nanowires: the effect of impurities and defects on their electronic properties. *International Journal of Nanotechnology*, **2005**, 2, 114	1.5	10
135	Self-doped titanium oxide thin films for efficient visible light photocatalysis: An example: Nonylphenol photodegradation. *Sensors and Actuators B: Chemical*, **2005**, 109, 52-56	8.5	31
134	Theoretical study of O2 and CO adsorption on Aun clusters (n=5 10). *Chemical Physics Letters*, **2005** , 408, 252-257	2.5	92
133	Electronic Structure Calculations with Localized Orbitals: The Siesta Method **2005**, 77-91		3
132	Strength of radial breathing mode in single-walled carbon nanotubes. *Physical Review B*, **2005**, 71,	3.3	104
131	Composition-dependent structural properties in ScGaN alloy films: A combined experimental and theoretical study. *Journal of Applied Physics*, **2005**, 98, 123501	2.5	33
130	Comment on "Molecular distortions and chemical bonding of a large pi-conjugated molecule on a metal surface". *Physical Review Letters*, **2005**, 95, 209601; author reply 209602	7.4	66
129	Scanning tunneling microscopy and surface simulation of zinc-blende GaN(001) intrinsic 4x reconstruction: linear gallium tetramers?. *Physical Review Letters*, **2005**, 95, 146102	7.4	12
128	Band structure of indium selenide investigated by intrinsic photoluminescence under high pressure. *Physical Review B*, **2004**, 70,	3.3	28
127	Systematic study of electron localization in an amorphous semiconductor. *Physical Review B*, **2004**, 69,	3.3	31
126	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	0.4	1
125	First-Principles Study of O Adsorption at SiC Surface. *Materials Science Forum*, **2004**, 457-460, 1293-1296	0.4	2
124	Phonon dispersion in graphite. *Physical Review Letters*, **2004**, 92, 075501	7.4	410

123	Stability and mobility of mono- and di-interstitials in alpha-Fe. *Physical Review Letters*, **2004**, 92, 175503	7.4	369
122	Simulations of minerals using density-functional theory based on atomic orbitals for linear scaling. *Physics and Chemistry of Minerals*, **2004**, 31, 12-21	1.6	14
121	Self-passivation mechanisms in clusters of N dopants in SiC. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2004**, 1, 274-277		1
120	Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3. *Solid State Ionics*, **2004**, 168, 291-298	3.3	6
119	First principles study of gold adsorption and diffusion on graphite. *Surface Science*, **2004**, 564, 173-178	1.8	58
118	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,	3.3	33
117	First-principles studies of the diffusion of B impurities and vacancies in SiC. *Physical Review B*, **2004**, 69,	3.3	23
116	Computing the Properties of Materials from First Principles with SIESTA. *Structure and Bonding*, **2004**, 103-170	0.9	96
115	Sampling the diffusion paths of a neutral vacancy in silicon with quantum mechanical calculations. *Physical Review B*, **2004**, 70,	3.3	70
114	Density functional theory calculations of quantum electron transport: carbon nanotubes-gold contacts. *Advances in Quantum Chemistry*, **2003**, 299-314	1.4	5
113	Vibrational properties of double-walled carbon nanotubes. *AIP Conference Proceedings*, **2003**,	0	4
112	First-principles molecular dynamics study of the stretching frequencies of hydrogen molecules in carbon nanotubes. *New Journal of Physics*, **2003**, 5, 124-124	2.9	12
111	TranSIESTA: a spice for molecular electronics. *Annals of the New York Academy of Sciences*, **2003**, 1006, 212-26	6.5	175
110	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	3.7	39
109	Defects of the SiC/SiO2 interface: energetics of the elementary steps of the oxidation reaction. *Physica B: Condensed Matter*, **2003**, 340-342, 1069-1073	2.8	16
108	Compressibility of CO adsorbed on Ni from 10⁻⁸ mbar to 1.2 bar ambient CO pressures investigated with X-ray diffraction. *Surface Science*, **2003**, 522, 161-166	1.8	26
107	Specific features of the electronic structure of III^{IV}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	1.3	17
106	Elastic properties and pressure-induced phase transitions of single-walled carbon nanotubes. *Physica Status Solidi (B): Basic Research*, **2003**, 235, 354-359	1.3	41

105	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems: Application to Chorismate Mutase. *Journal of Physical Chemistry B*, **2003**, 107, 13728-13736	3.4	110
104	First principles studies of neutral vacancies diffusion in SiC. *Computational Materials Science*, **2003**, 27, 36-42	3.2	18
103	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	3.2	425
102	Hexagonal diamond from single-walled carbon nanotubes. *AIP Conference Proceedings*, **2003**,	0	1
101	Electrons in dry DNA from density functional calculations. *Molecular Physics*, **2003**, 101, 1587-1594	1.7	82
100	A Cause for SiC/SiO2 Interface States: the Site Selection of Oxygen in SiC. *Materials Science Forum*, **2003**, 433-436, 535-538	0.4	9
99	First-Principles Studies of N and P Dopant Interactions in SiC: Implications for Co-Doping. *Materials Science Forum*, **2003**, 433-436, 649-652	0.4	2
98	First-principles calculation of the band offset at BaO/BaTiO3 and SrO/SrTiO3 interfaces. *Physical Review B*, **2003**, 67,	3.3	111
97	Origin of current-induced forces in an atomic gold wire: A first-principles study. *Physical Review B*, **2003**, 67,	3.3	87
96	Aggregation of carbon interstitials in silicon carbide: A theoretical study. *Physical Review B*, **2003**, 68,	3.3	94
95	Characterization of the unoccupied and partially occupied states of TTF-TCNQ by XANES and first-principles calculations. *Physical Review B*, **2003**, 68,	3.3	50
94	First-principles characterization of the electronic structure of the molecular superconductor (BEDT‐TTF)2IBr2. *Physical Review B*, **2003**, 67,	3.3	17
93	First-principles study of n-type dopants and their clustering in SiC. *Applied Physics Letters*, **2003**, 82, 4298-4300	3.4	21
92	Molecular Dynamics Simulations of Nanotube Growth **2003**, 45-56		
91	Designed Self-Doped Titanium Oxide Thin Films for Efficient Visible-Light Photocatalysis. *Advanced Materials*, **2002**, 14, 1399-1402	24	412
90	Environment effects on chemical reactivity of heme proteins. *International Journal of Quantum Chemistry*, **2002**, 90, 1505-1514	2.1	23
89	The SIESTA method forab initioorder-Nmaterials simulation. *Journal of Physics Condensed Matter*, **2002**, 14, 2745-2779	1.8	7828
88	Theoretical evidence for the kick-out mechanism for B diffusion in SiC. *Applied Physics Letters*, **2002**, 81, 2989-2991	3.4	22

87	First-principles study of the blue bronze K0.3MoO3. *Physical Review B*, **2002**, 65,	3.3	36
86	First-principles study of the neutral molecular metal Ni(tmdt)2. *Physical Review B*, **2002**, 65,	3.3	55
85	SnO 2 : Bulk and Surface Simulations by an Ab Initio Numerical Local Orbitals Method. *Phase Transitions*, **2002**, 75, 143-149	1.3	12
84	Ab Initio Calculations of B Diffusion in SiC. *Materials Science Forum*, **2002**, 389-393, 553-556	0.4	1
83	Angle-resolved photoemission study and first-principles calculation of the electronic structure of GaTe. *Physical Review B*, **2002**, 65,	3.3	34
82	Electronic band structure of isolated and bundled carbon nanotubes. *Physical Review B*, **2002**, 65,	3.3	297
81	Tight-binding description of graphene. *Physical Review B*, **2002**, 66,	3.3	761
80	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. *Nanotechnology*, **2002**, 13, 346-351	3.4	34
79	Ab initio calculations of the optical properties of 4-□diameter single-walled nanotubes. *Physical Review B*, **2002**, 66,	3.3	219
78	Density-functional method for nonequilibrium electron transport. *Physical Review B*, **2002**, 65,	3.3	4039
77	Ab initio determination of the phonon deformation potentials of graphene. *Physical Review B*, **2002** , 65,	3.3	58
76	Elastic properties of carbon nanotubes under hydrostatic pressure. *Physical Review B*, **2002**, 65,	3.3	133
75	Solid phosphorus carbide?. *Chemical Communications*, **2002**, 2494-2495	5.8	15
74	Ab initio local vibrational modes of light impurities in silicon. *Physical Review B*, **2002**, 65,	3.3	50
73	Ab-Initio Calculations on the Structural and Electronic Properties of BaO/BatiO3 And SrO/SrTiO3 Interfaces **2002**, 561-571		
72	The fascinating dynamics of defects in silicon. *Physica B: Condensed Matter*, **2001**, 308-310, 1-7	2.8	2
71	Vibrational properties of H-related defects in silicon. *Physica B: Condensed Matter*, **2001**, 308-310, 147-150	2.8	2
70	The strange behavior of interstitial H2 molecules Si and GaAs. *Physica B: Condensed Matter*, **2001**, 308-310, 202-205	2.8	10

69	Copper-Defect and Copper-Impurity Interactions in Silicon. *Solid State Phenomena*, **2001**, 82-84, 341-348	0.4	10
68	Hybrid DNA-gold nanostructured materials: anab initioapproach. *Nanotechnology*, **2001**, 12, 126-131	3.4	33
67	Dynamics of interstitial hydrogen molecules in crystalline silicon. *Journal of Physics Condensed Matter*, **2001**, 13, 6271-6283	1.8	33
66	Self-interstitial–hydrogen complexes in Si. *Physical Review B*, **2001**, 64,	3.3	11
65	First-principles study of the origin and nature of ferromagnetism in Ga1−xMnxAs. *Physical Review B*, **2001**, 63,	3.3	258
64	Unexpected dynamics for self-interstitial clusters in silicon. *Physical Review Letters*, **2001**, 86, 1247-50	7.4	82
63	Density-functional calculations of the structures, binding energies, and magnetic moments of Fe clusters with 2 to 17 atoms. *Physical Review B*, **2001**, 63,	3.3	175
62	Ab initio study of silicon-multisubstituted neutral and charged fullerenes. *Physical Review B*, **2001**, 63,	3.3	61
61	Fullerene growth and the role of nonclassical isomers. *Physical Review B*, **2001**, 63,	3.3	52
60	Experimental and theoretical study of band structure of InSe and In1−xGaxSe (x. *Physical Review B*, **2001**, 63,	3.3	64
59	Phonon eigenvectors of chiral nanotubes. *Physical Review B*, **2001**, 64,	3.3	48
58	Ring closure in dioxin formation process: An ab initio molecular dynamics study. *Journal of Chemical Physics*, **2001**, 115, 6401-6405	3.9	10
57	Surface electronic structure of metastable FeSi(CsCl)(1 1 1). *Surface Science*, **2001**, 482-485, 625-631	1.8	7
56	Interplay between theory and experiment insolid state inorganic chemistry. *Journal of Materials Chemistry*, **2001**, 11, 1-10		14
55	Linear Scaling DFT Calculations with Numerical Atomic Orbitals. *Materials Research Society Symposia Proceedings*, **2001**, 677, 961		53
54	First Principles Electronic Structure Methods **2001**, 189-220		
53	Linear Scaling ab initio Calculations in Nanoscale Materials with SIESTA. *Physica Status Solidi (B): Basic Research*, **2000**, 217, 335-356	1.3	106
52	Seeing molecular orbitals. *Chemical Physics Letters*, **2000**, 321, 78-82	2.5	111

51	The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods. *Chemical Physics*, **2000**, 261, 189-203	2.3	37
50	Metallic bonding and cluster structure. *Physical Review B*, **2000**, 61, 5771-5780	3.3	157
49	New Method For First Principles Modeling of Electron Transport through Nanoelectronic Devices. *Materials Research Society Symposia Proceedings*, **2000**, 636, 9251		1
48	Tight binding molecular dynamics studies of boron assisted nanotube growth. *Journal of Chemical Physics*, **2000**, 113, 3814-3821	3.9	34
47	Electronic structure of the superconducting layered ternary nitrides CaTaN2 and CaNbN2. *Physical Review B*, **2000**, 62, 1512-1515	3.3	11
46	Comment on "Identifying molecular orientation of individual C60 on a Si(111)-(7x7) Surface". *Physical Review Letters*, **2000**, 85, 2653	7.4	11
45	New superhard phases for three-dimensional C60-based fullerites. *Physical Review Letters*, **2000**, 85, 2328-31	7.4	82
44	Absence of dc-conductivity in lambda-DNA. *Physical Review Letters*, **2000**, 85, 4992-5	7.4	531
43	Do thiols merely passivate gold nanoclusters?. *Physical Review Letters*, **2000**, 85, 5250-1	7.4	142
42	Electronic structure of monoclinic TeMo5O16: Prediction of semiconducting behavior. *Physical Review B*, **2000**, 62, 16430-16434	3.3	5
41	Systematic ab initio study of the electronic and magnetic properties of different pure and mixed iron systems. *Physical Review B*, **2000**, 61, 13639-13646	3.3	93
40	Linear Scaling ab initio Calculations in Nanoscale Materials with SIESTA **2000**, 217, 335		3
39	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. *Physical Review Letters*, **1999**, 83, 3884-3887	7.4	227
38	Bonding and diffusion of Ba on a Si(001) reconstructed surface. *Physical Review B*, **1999**, 60, 4968-4971	3.3	34
37	Application of local-spin-density approximation to a Si and tetrahedral a C. *Physical Review B*, **1999**, 60, 10594-10597	3.3	13
36	Energetics of the oxidation and opening of a carbon nanotube. *Physical Review B*, **1999**, 60, R2208-R2211	3.3	68
35	Structure and thermal stability of gold nanoclusters: The Au38 case. *European Physical Journal D*, **1999**, 9, 211-215	1.3	47
34	Ab initio structural, elastic, and vibrational properties of carbon nanotubes. *Physical Review B*, **1999**, 59, 12678-12688	3.3	779

33	Linear-Scaling ab-initio Calculations for Large and Complex Systems. *Physica Status Solidi (B): Basic Research*, **1999**, 215, 809-817	1.3	839
32	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. *Physical Review Letters*, **1999**, 82, 3520-3523	7.4	165
31	Atomic layering at the liquid silicon surface: A first-principles simulation. *Physical Review B*, **1999**, 60, R16283-R16286	3.3	37
30	Self-consistent density-functional calculations of the geometries, electronic structures, and magnetic moments of Ni-Al clusters. *Physical Review B*, **1999**, 60, 2020-2024	3.3	85
29	Structure and thermal stability of gold nanoclusters: The Au38 case **1999**, 211-215		4
28	Linear-Scaling ab-initio Calculations for Large and Complex Systems **1999**, 215, 809		24
27	Order-N tight-binding methods for electronic-structure and molecular dynamics. *Computational Materials Science*, **1998**, 12, 157-191	3.2	94
26	Lowest Energy Structures of Gold Nanoclusters. *Physical Review Letters*, **1998**, 81, 1600-1603	7.4	334
25	Electronic-structure-based molecular-dynamics method for large biological systems: Application to the 10 basepair poly(dG)?poly(dC) DNA double helix. *Physical Review B*, **1997**, 55, 6880-6887	3.3	66
24	Surface electronic structure of metastable FeSi(CsCl)(111) epitaxially grown on Si(111). *Physical Review B*, **1997**, 55, R16065-R16068	3.3	12
23	Density functional studies of small platinum clusters. *Journal of Physics Condensed Matter*, **1997**, 9, L39-L48		81
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