P Ordejon

List of Publications by Year
in descending order

45 papers	6,319 citations	136950 32 h-index	276875 41 g-index
45 all docs	45 docs citations	45 times ranked	7185 citing authors

#	Article	IF	Citations
1	Momentum dependence of spinâ€“orbit interaction effects in single-layer and multi-layer transition metal dichalcogenides. 2D Materials, 2014, 1, 034003.	4.4	85
2	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, .	3.2	351
3	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.	1.5	7
4	Calculation of core level shifts within DFT using pseudopotentials and localized basis sets. European Physical Journal B, 2012, 85, 1.	1.5	44
5	Modulation of Surface Charge Transfer through Competing Long-Range Repulsive versus Short-Range Attractive Interactions. Journal of Physical Chemistry C, 2011, 115, 18640-18648.	3.1	49
6	Quantum transport in chemically modified two-dimensional graphene: From minimal conductivity to Anderson localization. Physical Review B, 2011, 84, .	3.2	84
7	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
8	Simulation of the Growth of Copper Films for Micro and Nano-Electronics. Advances in Science and Technology, 2006, 51, 167-173.	0.2	0
9	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, .	3.2	37
10	Self-doped titanium oxide thin films for efficient visible light photocatalysis. Sensors and Actuators B: Chemical, 2005, 109, 52-56.	7.8	37
11	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.	7.8	68
12	First stages of the oxidation of the Si-rich 3Câ€“SiC(001) surface. Computational Materials Science, 2005, 33, 13-19.	3.0	9
13	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, .	3.2	33
14	First-principles studies of the diffusion of B impurities and vacancies in SiC. Physical Review B, 2004, 69, .	3.2	24
15	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.	1.9	27
16	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
17	Characterization of the unoccupied and partially occupied states of TTF-TCNQ by XANES and first-principles calculations. Physical Review B, 2003, 68, .	3.2	54
18	Theoretical evidence for the kick-out mechanism for B diffusion in SiC. Applied Physics Letters, 2002, 81, 2989-2991.	3.3	26

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19	Angle-resolved photoemission study and first-principles calculation of the electronic structure of GaTe. Physical Review B, 2002, 65, .	3.2	38
20	Electronic band structure of isolated and bundled carbon nanotubes. Physical Review B, 2002, 65, .	3.2	327
21	Tight-binding description of graphene. Physical Review B, 2002, 66, .	3.2	904
22	Ab initiocalculations of the optical properties of 4-Ã…-diameter single-walled nanotubes. Physical Review B, 2002, 66, .	3.2	256
23	Ab initiodetermination of the phonon deformation potentials of graphene. Physical Review B, 2002, 65, .	3.2	72
24	Elastic properties of carbon nanotubes under hydrostatic pressure. Physical Review B, 2002, 65, .	3.2	139
25	Ab initiolocal vibrational modes of light impurities in silicon. Physical Review B, 2002, 65, .	3.2	51
26	Designed Self-Doped Titanium Oxide Thin Films for Efficient Visible-Light Photocatalysis. Advanced Materials, 2002, 14, 1399-1402.	21.0	438
27	Ab-Initio Calculations on the Structural and Electronic Properties of BaO/BatiO3 And SrO/SrTiO3 Interfaces. , 2002, , 561-571.		0
28	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, .	3.2	73
29	Phonon eigenvectors of chiral nanotubes. Physical Review B, 2001, 64, .	3.2	53
30	Linear Scaling DFT Calculations with Numerical Atomic Orbitals. Materials Research Society Symposia Proceedings, 2001, 677, 961.	0.1	77
31	The fascinating dynamics of defects in silicon. Physica B: Condensed Matter, 2001, 308-310, 1-7.	2.7	2
32	Vibrational properties of H-related defects in silicon. Physica B: Condensed Matter, 2001, 308-310, 147-150.	2.7	2
33	The strange behavior of interstitial H2 molecules Si and GaAs. Physica B: Condensed Matter, 2001, 308-310, 202-205.	2.7	10
34	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
35	Unexpected Dynamics for Self-Interstitial Clusters in Silicon. Physical Review Letters, 2001, 86, 1247-1250.	7.8	85
36	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

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37	Absence of dc-Conductivity inÎ»-DNA. Physical Review Letters, 2000, 85, 4992-4995.	7.8	602
38	Do Thiols Merely Passivate Gold Nanoclusters?. Physical Review Letters, 2000, 85, 5250-5251.	7.8	158
39	Energetics of the oxidation and opening of a carbon nanotube. Physical Review B, 1999, 60, R2208-R2211.	3.2	69
40	Structure and thermal stability of gold nanoclusters: The Au38 case. European Physical Journal D, 1999, 9, 211-215.	1.3	52
41	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
42	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
43	Structure and thermal stability of gold nanoclusters: The Au38 case. , 1999, , 211-215.		4
44	Lowest Energy Structures of Gold Nanoclusters. Physical Review Letters, 1998, 81, 1600-1603.	7.8	356
45	The Calculation of Free-Energiesin Semiconductors: Defects, Transitionsand Phase Diagrams. , 0, , 115-140.		1