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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	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
2	Tight-binding description of graphene. Physical Review B, 2002, 66, .	3.2	904
3	Absence of dc-Conductivity inÎ»-DNA. Physical Review Letters, 2000, 85, 4992-4995.	7.8	602
4	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
5	Designed Self-Doped Titanium Oxide Thin Films for Efficient Visible-Light Photocatalysis. Advanced Materials, 2002, 14, 1399-1402.	21.0	438
6	Lowest Energy Structures of Gold Nanoclusters. Physical Review Letters, 1998, 81, 1600-1603.	7.8	356
7	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
8	Electronic band structure of isolated and bundled carbon nanotubes. Physical Review B, 2002, 65, .	3.2	327
9	Ab initiocalculations of the optical properties of 4-Ã…-diameter single-walled nanotubes. Physical Review B, 2002, 66, .	3.2	256
10	Do Thiols Merely Passivate Gold Nanoclusters?. Physical Review Letters, 2000, 85, 5250-5251.	7.8	158
11	Elastic properties of carbon nanotubes under hydrostatic pressure. Physical Review B, 2002, 65, .	3.2	139
12	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
13	Unexpected Dynamics for Self-Interstitial Clusters in Silicon. Physical Review Letters, 2001, 86, 1247-1250.	7.8	85
14	Momentum dependence of spinâ€“orbit interaction effects in single-layer and multi-layer transition metal dichalcogenides. 2D Materials, 2014, 1, 034003.	4.4	85
15	Quantum transport in chemically modified two-dimensional graphene: From minimal conductivity to Anderson localization. Physical Review B, 2011, 84, .	3.2	84
16	Linear Scaling DFT Calculations with Numerical Atomic Orbitals. Materials Research Society Symposia Proceedings, 2001, 677, 961.	0.1	77
17	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
18	Ab initiodetermination of the phonon deformation potentials of graphene. Physical Review B, 2002, 65, .	3.2	72

#	Article	IF	Citations
19	Energetics of the oxidation and opening of a carbon nanotube. Physical Review B, 1999, 60, R2208-R2211.	3.2	69
20	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
21	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
22	Phonon eigenvectors of chiral nanotubes. Physical Review B, 2001, 64, .	3.2	53
23	Structure and thermal stability of gold nanoclusters: The Au38 case. European Physical Journal D, 1999, 9, 211-215.	1.3	52
24	Ab initiolocal vibrational modes of light impurities in silicon. Physical Review B, 2002, 65, .	3.2	51
25	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
26	Calculation of core level shifts within DFT using pseudopotentials and localized basis sets. European Physical Journal B, 2012, 85, 1.	1.5	44
27	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
28	Angle-resolved photoemission study and first-principles calculation of the electronic structure of GaTe. Physical Review B, 2002, 65, .	3.2	38
29	Self-doped titanium oxide thin films for efficient visible light photocatalysis. Sensors and Actuators B: Chemical, 2005, 109, 52-56.	7.8	37
30	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
31	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
32	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
33	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
34	Theoretical evidence for the kick-out mechanism for B diffusion in SiC. Applied Physics Letters, 2002, 81, 2989-2991.	3.3	26
35	First-principles studies of the diffusion of B impurities and vacancies in SiC. Physical Review B, 2004, 69, .	3.2	24
36	The strange behavior of interstitial H2 molecules Si and GaAs. Physica B: Condensed Matter, 2001, 308-310, 202-205.	2.7	10

#	Article	IF	Citations
37	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
38	First stages of the oxidation of the Si-rich 3Câ€“SiC(001) surface. Computational Materials Science, 2005, 33, 13-19.	3.0	9
39	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
40	Structure and thermal stability of gold nanoclusters: The Au38 case. , 1999, , 211-215.		4
41	The fascinating dynamics of defects in silicon. Physica B: Condensed Matter, 2001, 308-310, 1-7.	2.7	2
42	Vibrational properties of H-related defects in silicon. Physica B: Condensed Matter, 2001, 308-310, 147-150.	2.7	2
43	The Calculation of Free-Energiesin Semiconductors: Defects, Transitionsand Phase Diagrams. , 0, , 115-140.		1
44	Simulation of the Growth of Copper Films for Micro and Nano-Electronics. Advances in Science and Technology, 2006, 51, 167-173.	0.2	0
45	Ab-Initio Calculations on the Structural and Electronic Properties of BaO/BatiO3 And SrO/SrTiO3 Interfaces. , 2002, , 561-571.		0