Risto M Nieminen

List of Publications by Year
in descending order

91 papers	2,784 citations	236833 25 h-index	175177 52 g-index
94 all docs	94 docs citations	94 times ranked	3938 citing authors

#	Article	IF	Citations
1	Migration and Localization of Metal Atoms on Strained Graphene. Physical Review Letters, 2010, 105, 196102.	2.9	304
2	Intrinsic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-Type Behavior in Transparent Conducting Oxides: A Comparative Hybrid-Functional Study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>,<mml:math xmlns:mml	2.9	295
3	Synthesis of Graphene Nanoribbons Encapsulated in Single-Walled Carbon Nanotubes. Nano Letters, 2011, 11, 4352-4356.	4.5	174
4	Electronic structure of boron nitride sheets doped with carbon from first-principles calculations. Physical Review B, 2013, 87, .	1.1	162
5	Linear-scaling self-consistent implementation of the van der Waals density functional. Physical Review B, 2009, 79, .	1.1	151
6	Kohnâ€“Sham Decomposition in Real-Time Time-Dependent Density-Functional Theory: An Efficient Tool for Analyzing Plasmonic Excitations. Journal of Chemical Theory and Computation, 2017, 13, 4779-4790.	2.3	110
7	Energetics of diffusion on the (100) and (111) surfaces of Ag, Au, and Ir from first principles. Physical Review B, 1995, 52, 9078-9085.	1.1	94
8	Mechanisms of Postsynthesis Doping of Boron Nitride Nanostructures with Carbon from First-Principles Simulations. Physical Review Letters, 2011, 107, 035501.	2.9	88
9	Role of tip structure and surface relaxation in atomic resolution dynamic force microscopy:CaF2(111)as a reference surface. Physical Review B, 2002, 66, .	1.1	79
10	l-Alanine in a Droplet of Water:Â A Density-Functional Molecular Dynamics Study. Journal of Physical Chemistry B, 2007, 111, 4227-4234.	1.2	76
11	Issues in first-principles calculations for defects in semiconductors and oxides. Modelling and Simulation in Materials Science and Engineering, 2009, 17, 084001.	0.8	75
12	Influence of van der Waals forces on the adsorption structure of benzene on silicon studied using density functional theory. Physical Review B, 2008, 77, .	1.1	69
13	Charged Point Defects in the Flatland: Accurate Formation Energy Calculations in Two-Dimensional Materials. Physical Review X, 2014, 4, .	2.8	67
14	From atomistic simulation towards multiscale modelling of materials. Journal of Physics Condensed Matter, 2002, 14, 2859-2876.	0.7	57
15	Limits for n-type doping in In2O3 and SnO2: A theoretical approach by first-principles calculations using hybrid-functional methodology. Journal of Applied Physics, 2010, 108, .	1.1	57
16	Quantized Evolution of the Plasmonic Response in a Stretched Nanorod. Physical Review Letters, 2015, 115, 236804.	2.9	52
17	Creation of paired electron states in the gap of semiconducting carbon nanotubes by correlated hydrogen adsorption. New Journal of Physics, 2007, 9, 275-275.	1.2	33
18	Computational study of (111) epitaxially strained ferroelectric perovskites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: Physical Review B, 2008, 78, .	1.1	33

#	Article	IF	Citations
19	Bound and free self-interstitial defects in graphite and bilayer graphene: A computational study. Physical Review B, 2011, 84, .	1.1	32
20	Calculated Positron Annihilation Parameters for Defects in SiC. Materials Science Forum, 2001, 353-356, 533-536.	0.3	31
21	A first-principles study on magnetic coupling between carbon adatoms on graphene. New Journal of Physics, 2010, 12, 113021.	1.2	30
22	Nanoplasmonics simulations at the basis set limit through completeness-optimized, local numerical basis sets. Journal of Chemical Physics, 2015, 142, 094114.	1.2	30
23	Measuring Site-Specific Clusterâ˜Surface Bond Formation. Journal of the American Chemical Society, 2005, 127, 17863-17866.	6.6	29
24	Coronene Encapsulation in Singleâ€Walled Carbon Nanotubes: Stacked Columns, Peapods, and Nanoribbons. ChemPhysChem, 2014, 15, 1660-1665.	1.0	28
25	Photoabsorption in sodium clusters on the basis of time-dependent density-functional theory. Journal of Chemical Physics, 2008, 128, 014707.	1.2	27
26	Density-functional calculations of defect formation energies using the supercell method: Brillouin-zone sampling. Physical Review B, 2005, 71, .	1.1	26
27	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
28	Toward Stronger Alâ€“BN Nanotube Composite Materials: Insights into Bonding at the Al/BN Interface from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 26894-26901.	1.5	24
29	Structure and Dynamics of Dioxygen Bound to Cobalt and Iron Heme. Biophysical Journal, 2006, 91, 2024-2034.	0.2	22
30	Photoabsorption spectra of small fullerenes and Si-heterofullerenes. Journal of Chemical Physics, 2008, 128, 154307.	1.2	22
31	Silicon self-diffusion constants by tight-binding molecular dynamics. Physical Review B, 2001, 64, .	1.1	21
32	Polymer adhesion: First-principles calculations of the adsorption of organic molecules onto Si surfaces. Physical Review B, 2007, 76, .	1.1	21
33	Effect of the surrounding oxide on the photoabsorption spectra of Si nanocrystals. Physical Review B, 2009, 79, .	1.1	21
34	Effect of edge plasmons on the optical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml monolayer flakes. Physical Review B, 2017, 96, .	1.1	21
35	Quantitative modelling in scanning force microscopy on insulators. Applied Surface Science, 2002, 188, 306-318.	3.1	20
36	Influence of high-refractive-index oxide coating on optical properties of metal nanoparticles. Journal of the Optical Society of America B: Optical Physics, 2013, 30, 338.	0.9	20

#	Article	IF	Citations
37	Defect-induced nucleation and growth of amorphous silicon. Physical Review B, 1996, 54, 1459-1462.	1.1	19
38	The Aqueous and Crystalline Forms of L-Alanine Zwitterion. Journal of Computational and Theoretical Nanoscience, 2008, 5, 277-285.	0.4	19
39	Positron trapping in oxide superconductors. Journal of Physics and Chemistry of Solids, 1991, 52, 1577-1587.	1.9	18
40	Molecular-dynamics study of partial edge dislocations in copper and gold: Interactions, structures, and self-diffusion. Physical Review B, 1996, 53, 8956-8966.	1.1	18
41	Dynamical coupling of plasmons and molecular excitations by hybrid quantum/classical calculations: time-domain approach. Journal of Physics Condensed Matter, 2014, 26, 315013.	0.7	18
42	Photoabsorption spectra of boron nitride fullerenelike structures. Journal of Chemical Physics, 2007, 126, 214306.	1.2	17
43	Electronic Energy Band Structure of the Double Perovskite Ba₂MnWO₆. Journal of Physical Chemistry B, 2008, 112, 6742-6746.	1.2	16
44	A Coupled Finite Element Model for the Sublimation Growth of SiC. Materials Science Forum, 1998, 264-268, 65-68.	0.3	14
45	Parallel Electronic Structure Calculations Using Multiple Graphics Processing Units (GPUs). Lecture Notes in Computer Science, 2013, , 63-76.	1.0	14
46	Modeling charge-imbalanced<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>NaNbO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: Lattice relaxation and metallicity. Physical Review B, 2009, 80, .	1.3	12
47	Hydrogen atoms band together. Nature, 1992, 356, 289-290.	13.7	11
48	Effect of Cu impurities on wet etching of Si(110): formation of trapezoidal hillocks. New Journal of Physics, 2008, 10, 013033.	1.2	11
49	A hierarchical dualscale study of bisphenol-A-polycarbonate on a silicon surface: structure, dynamics and impurity diffusion. Soft Matter, 2011, 7, 6457.	1.2	11
50	ÃgostonetÂal.Reply:. Physical Review Letters, 2011, 106, .	2.9	11
51	Time-dependent simulation of Czochralski silicon crystal growth. Journal of Crystal Growth, 1997, 180, 468-476.	0.7	10
52	Developments in the density-functional theory of electronic structure. Current Opinion in Solid State and Materials Science, 1999, 4, 493-498.	5.6	10
53	Density-functional molecular dynamics studies of biologically relevant iron and cobalt complexes with macrocyclic ligands. Coordination Chemistry Reviews, 2008, 252, 1497-1513.	9.5	10
54	Supercell Methods for Defect Calculations. Topics in Applied Physics, 0, , 29-68.	0.4	10

#	Article	IF	Citations
55	Thermodynamic Considerations of the Role of Hydrogen in Sublimation Growth of Silicon Carbide. Journal of the Electrochemical Society, 1997, 144, 1024-1027.	1.3	9
56	Quantum Chemical Study of Effects Produced by Nb- and La-Doping in BaTiO₃. Key Engineering Materials, 2002, 206-213, 1325-1328.	0.4	8
57	The effect of interstitial hydrogen on the electronic structure of the B2 FeAl alloy. Physica Status Solidi (B): Basic Research, 2007, 244, 3684-3694.	0.7	8
58	Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3. Solid State Ionics, 2004, 168, 291-298.	1.3	7
59	Adsorption of metal impurities on H-terminated Si surfaces and their influence on the wet chemical etching of Si. Journal of Physics Condensed Matter, 2008, 20, 485005.	0.7	7
60	NosÃ©-Hoover molecular-dynamics study of self-pipe-diffusion in gold using many-atom interactions. Physical Review B, 1994, 50, 6450-6452.	1.1	6
61	Berseneva, Krasheninnikov, and Nieminen Reply:. Physical Review Letters, 2011, 107, .	2.9	6
62	Atomistic approach for simulating plasmons in nanostructures. Applied Physics A: Materials Science and Processing, 2014, 115, 427-431.	1.1	6
63	Cluster calculations for H2dissociation on Cu and Ni. Physica Scripta, 1988, 37, 141-144.	1.2	5
64	Fast convergence to equilibrium for long-chain polymer melts using a MD/continuum hybrid method. Journal of Chemical Physics, 2012, 137, 154115.	1.2	5
65	Energy Dissipation of AFM Studied by MD/Continuum Coupling Model. E-Journal of Surface Science and Nanotechnology, 2014, 12, 339-342.	0.1	5
66	Formation of Vacancies and Divacancies in Plane-Stressed Silicon. Solid State Phenomena, 2005, 108-109, 433-438.	0.3	3
67	The Effect of Compound Composition and Strain on Vacancies in Si/SiGe Heterostructures. Solid State Phenomena, 2005, 108-109, 457-462.	0.3	3
68	Ferromagnetism in MgTiO₃-Ti₂O₃Solid Solutions. Materials Science Forum, 0, 700, 23-27.	0.3	3
69	Computational model for noncontact atomic force microscopy: energy dissipation of cantilever. Journal of Physics Condensed Matter, 2016, 28, 375001.	0.7	3
70	Effect of Magnetic Ordering on the Stability of Niâ€“Mnâ€“Ga(â€“Coâ€“Cu) Alloys Along the Tetragonal Deformation Path. IEEE Transactions on Magnetics, 2017, 53, 1-6.	1.2	3
71	Electronic Properties of Two-Dimensional Systems. Physica Scripta, 1988, T23, 54-58.	1.2	2
72	First-Principles Simulations of Vacancies and Antisites in InP. Materials Science Forum, 1994, 143-147, 1305-1310.	0.3	2

#	Article	IF	Citations
73	Electronic Structure and Positron Trapping in Semiconductors. Materials Science Forum, 1994, 175-178, 279-286.	0.3	2
74	AB Initio Studies of Atomic-Scale Defects in GaN and AlN. Materials Science Forum, 1997, 258-263, 1119-1124.	0.3	2
75	Stability of the maximum-density droplet state in quantum dots: a quantum Monte Carlo study. Physica B: Condensed Matter, 2000, 284-288, 1776-1777.	1.3	2
76	Dynamics of Biomolecules From First Principles. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, 1, 557-573.	0.6	2
77	Atomic Force Microscopy Simulation by MD/Continuum Coupling Method. Integrated Ferroelectrics, 2014, 155, 33-38.	0.3	2
78	Analysis of Tip Stability in Adhesion Process in AFM Using Potential Energy Surface: Stability Versus Dissipation. E-Journal of Surface Science and Nanotechnology, 2018, 16, 132-136.	0.1	2
79	Mechanical Properties of Silicon Microstructures. , 2010, , 179-219.		1
80	Stability of Tip in Adhesion Process on Atomic Force Microscopy Studied by Coupling Computational Model. Applied Science and Convergence Technology, 2017, 26, 6-10.	0.3	1
81	Military Strategy. Physics Today, 1985, 38, 112-112.	0.3	0
82	The Finnish Effort in Supercomputing. Physica Scripta, 1990, T33, 91-93.	1.2	0
83	Metastable Antisite Pair in GaAs. Materials Science Forum, 1997, 258-263, 969-974.	0.3	0
84	Chemical Reactions in Bulk and on Surfaces. , 1997, , 413-416.		0
85	Ion beams help diamond rise from the ashes. Physics World, 1998, 11, 26-27.	0.0	0
86	Effect of electromagnetic environment on transport of composite fermions in a narrow constriction between compressible quantum Hall liquids. Physica B: Condensed Matter, 2000, 284-288, 1730-1731.	1.3	0
87	Considerations on the Crystal Morphology in the Sublimation Growth of SiC. Materials Science Forum, 2000, 338-342, 95-98.	0.3	0
88	Defects and Diffusion: First- Principles Modeling. Defect and Diffusion Forum, 2001, 194-199, 261-278.	0.4	0
89	Mechanisms of Diffusion and Dissociation of E-Centers in Silicon. Defect and Diffusion Forum, 2005, 237-240, 1129-1134.	0.4	0
90	Simulated coating of carbon nanotube networks by a beam of carbon atoms. Physica Status Solidi (B): Basic Research, 2012, 249, 317-323.	0.7	0

#	Article	IF	Citations
91	An issue dedicated to the Î˙k Volker Heine Young Investigator Award*. European Physical Journal B, 2016, 89, 1.	0.6	0