Risto M Nieminen

List of Publications by Year in Descending Order

87 papers	2,487 citations	24 h-index	48 g-index
94 ext. papers	2,632 ext. citations	3.8 avg, IF	5 L-index

#	Paper	IF	Citations
87	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	0.7	1
86	Effect of edge plasmons on the optical properties of MoS2 monolayer flakes. *Physical Review B*, **2017**, 96,	3.3	11
85	Kohn-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	5.4	73
84	Effect of Magnetic Ordering on the Stability of NiMnGa(Co,Cu) Alloys Along the Tetragonal Deformation Path. *IEEE Transactions on Magnetics*, **2017**, 53, 1-6	2	3
83	Stability of Tip in Adhesion Process on Atomic Force Microscopy Studied by Coupling Computational Model. *Applied Science and Convergence Technology*, **2017**, 26, 6-10	0.8	1
82	Computational model for noncontact atomic force microscopy: energy dissipation of cantilever. *Journal of Physics Condensed Matter*, **2016**, 28, 375001	1.8	2
81	Grid-Based Projector-Augmented Wave Method **2016**, 191-210		
80	Nanoplasmonics simulations at the basis set limit through completeness-optimized, local numerical basis sets. *Journal of Chemical Physics*, **2015**, 142, 094114	3.9	22
79	Quantized Evolution of the Plasmonic Response in a Stretched Nanorod. *Physical Review Letters*, **2015**, 115, 236804	7.4	46
78	Atomistic approach for simulating plasmons in nanostructures. *Applied Physics A: Materials Science and Processing*, **2014**, 115, 427-431	2.6	6
77	Toward Stronger Al/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	3.8	21
76	Coronene encapsulation in single-walled carbon nanotubes: stacked columns, peapods, and nanoribbons. *ChemPhysChem*, **2014**, 15, 1660-5	3.2	24
75	Dynamical coupling of plasmons and molecular excitations by hybrid quantum/classical calculations: time-domain approach. *Journal of Physics Condensed Matter*, **2014**, 26, 315013	1.8	12
74	Energy Dissipation of AFM Studied by MD/Continuum Coupling Model. *E-Journal of Surface Science and Nanotechnology*, **2014**, 12, 339-342	0.7	3
73	Atomic Force Microscopy Simulation by MD/Continuum Coupling Method. *Integrated Ferroelectrics*, **2014**, 155, 33-38	0.8	1
72	Charged Point Defects in the Flatland: Accurate Formation Energy Calculations in Two-Dimensional Materials. *Physical Review X*, **2014**, 4,	9.1	49
71	Electronic structure of boron nitride sheets doped with carbon from first-principles calculations. *Physical Review B*, **2013**, 87,	3.3	129

70	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	1.7	18
69	Parallel Electronic Structure Calculations Using Multiple Graphics Processing Units (GPUs). *Lecture Notes in Computer Science*, **2013**, 63-76	0.9	12
68	Simulated coating of carbon nanotube networks by a beam of carbon atoms. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 317-323	1.3	
67	Fast convergence to equilibrium for long-chain polymer melts using a MD/continuum hybrid method. *Journal of Chemical Physics*, **2012**, 137, 154115	3.9	4
66	Synthesis of graphene nanoribbons encapsulated in single-walled carbon nanotubes. *Nano Letters*, **2011**, 11, 4352-6	11.5	148
65	Bound and free self-interstitial defects in graphite and bilayer graphene: A computational study. *Physical Review B*, **2011**, 84,	3.3	31
64	A hierarchical dualscale study of bisphenol-A-polycarbonate on a silicon surface: structure, dynamics and impurity diffusion. *Soft Matter*, **2011**, 7, 6457	3.6	11
63	Berseneva, Krasheninnikov, and Nieminen Reply:. *Physical Review Letters*, **2011**, 107,	7.4	5
62	Mechanisms of postsynthesis doping of boron nitride nanostructures with carbon from first-principles simulations. *Physical Review Letters*, **2011**, 107, 035501	7.4	84
61	Boston et al. Reply:. *Physical Review Letters*, **2011**, 106,	7.4	11
60	Ferromagnetism in MgTiO3-Ti2O3 Solid Solutions. *Materials Science Forum*, **2011**, 700, 23-27	0.4	3
59	Mechanical Properties of Silicon Microstructures **2010**, 179-219		1
58	A first-principles study on magnetic coupling between carbon adatoms on graphene. *New Journal of Physics*, **2010**, 12, 113021	2.9	29
57	Dynamics of Biomolecules From First Principles. *Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems*, **2010**, 1, 557-573		1
56	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, 053511	2.5	52
55	Migration and localization of metal atoms on strained graphene. *Physical Review Letters*, **2010**, 105, 196102	7.4	281
54	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
53	Modeling charge-imbalanced NaNbO3/SrTiO3 superlattices: Lattice relaxation and metallicity. *Physical Review B*, **2009**, 80,	3.3	11

52	Effect of the surrounding oxide on the photoabsorption spectra of Si nanocrystals. *Physical Review B*, **2009**, 79,	3.3	20
51	Intrinsic n-type behavior in transparent conducting oxides: a comparative hybrid-functional study of In2O3, SnO2, and ZnO. *Physical Review Letters*, **2009**, 103, 245501	7.4	274
50	Linear-scaling self-consistent implementation of the van der Waals density functional. *Physical Review B*, **2009**, 79,	3.3	149
49	Issues in first-principles calculations for defects in semiconductors and oxides. *Modelling and Simulation in Materials Science and Engineering*, **2009**, 17, 084001	2	72
48	Influence of van der Waals forces on the adsorption structure of benzene on silicon studied using density functional theory. *Physical Review B*, **2008**, 77,	3.3	68
47	Electronic energy band structure of the double perovskite Ba2MnWO6. *Journal of Physical Chemistry B*, **2008**, 112, 6742-6	3.4	14
46	Photoabsorption in sodium clusters on the basis of time-dependent density-functional theory. *Journal of Chemical Physics*, **2008**, 128, 014707	3.9	25
45	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	1.8	7
44	Effect of Cu impurities on wet etching of Si(110): formation of trapezoidal hillocks. *New Journal of Physics*, **2008**, 10, 013033	2.9	11
43	Photoabsorption spectra of small fullerenes and Si-heterofullerenes. *Journal of Chemical Physics*, **2008**, 128, 154307	3.9	21
42	Computational study of (111) epitaxially strained ferroelectric perovskites BaTiO3 and PbTiO3. *Physical Review B*, **2008**, 78,	3.3	30
41	Density-functional molecular dynamics studies of biologically relevant iron and cobalt complexes with macrocyclic ligands. *Coordination Chemistry Reviews*, **2008**, 252, 1497-1513	23.2	9
40	The Aqueous and Crystalline Forms of L-Alanine Zwitterion. *Journal of Computational and Theoretical Nanoscience*, **2008**, 5, 277-285	0.3	17
39	L-alanine in a droplet of water: a density-functional molecular dynamics study. *Journal of Physical Chemistry B*, **2007**, 111, 4227-34	3.4	73
38	The effect of interstitial hydrogen on the electronic structure of the B2 FeAl alloy. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 3684-3694	1.3	6
37	Creation of paired electron states in the gap of semiconducting carbon nanotubes by correlated hydrogen adsorption. *New Journal of Physics*, **2007**, 9, 275-275	2.9	31
36	Polymer adhesion: First-principles calculations of the adsorption of organic molecules onto Si surfaces. *Physical Review B*, **2007**, 76,	3.3	21
35	Photoabsorption spectra of boron nitride fullerenelike structures. *Journal of Chemical Physics*, **2007** , 126, 214306	3.9	17

34	Structure and dynamics of dioxygen bound to cobalt and iron heme. *Biophysical Journal*, **2006**, 91, 2024-34	3.9	20
33	Measuring site-specific cluster-surface bond formation. *Journal of the American Chemical Society*, **2005**, 127, 17863-6	16.4	28
32	Formation of Vacancies and Divacancies in Plane-Stressed Silicon. *Solid State Phenomena*, **2005**, 108-109, 433-438	0.4	2
31	The Effect of Compound Composition and Strain on Vacancies in Si/SiGe Heterostructures. *Solid State Phenomena*, **2005**, 108-109, 457-462	0.4	3
30	Mechanisms of Diffusion and Dissociation of E-Centers in Silicon. *Defect and Diffusion Forum*, **2005**, 237-240, 1129-1134	0.7	
29	Density-functional calculations of defect formation energies using the supercell method: Brillouin-zone sampling. *Physical Review B*, **2005**, 71,	3.3	21
28	Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3. *Solid State Ionics*, **2004**, 168, 291-298	3.3	6
27	Quantitative modelling in scanning force microscopy on insulators. *Applied Surface Science*, **2002**, 188, 306-318	6.7	20
26	Role of tip structure and surface relaxation in atomic resolution dynamic force microscopy: CaF2(111) as a reference surface. *Physical Review B*, **2002**, 66,	3.3	75
25	From atomistic simulation towards multiscale modelling of materials. *Journal of Physics Condensed Matter*, **2002**, 14, 2859-2876	1.8	49
24	Quantum Chemical Study of Effects Produced by Nb- and La-Doping in BaTiO3. *Key Engineering Materials*, **2001**, 206-213, 1325-1328	0.4	4
23	Defects and Diffusion: First- Principles Modeling. *Defect and Diffusion Forum*, **2001**, 194-199, 261-278	0.7	
22	Calculated Positron Annihilation Parameters for Defects in SiC. *Materials Science Forum*, **2001**, 353-356, 533-536	0.4	31
21	Silicon self-diffusion constants by tight-binding molecular dynamics. *Physical Review B*, **2001**, 64,	3.3	18
20	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	2.8	
19	Stability of the maximum-density droplet state in quantum dots: a quantum Monte Carlo study. *Physica B: Condensed Matter*, **2000**, 284-288, 1776-1777	2.8	2
18	Considerations on the Crystal Morphology in the Sublimation Growth of SiC. *Materials Science Forum*, **2000**, 338-342, 95-98	0.4	
17	Developments in the density-functional theory of electronic structure. *Current Opinion in Solid State and Materials Science*, **1999**, 4, 493-498	12	9

16	A Coupled Finite Element Model for the Sublimation Growth of SiC. *Materials Science Forum*, **1998**, 264-268, 65-68	0.4	13
15	AB Initio Studies of Atomic-Scale Defects in GaN and AlN. *Materials Science Forum*, **1997**, 258-263, 1119-1124	0.4	1
14	Metastable Antisite Pair in GaAs. *Materials Science Forum*, **1997**, 258-263, 969-974	0.4	
13	Thermodynamic Considerations of the Role of Hydrogen in Sublimation Growth of Silicon Carbide. *Journal of the Electrochemical Society*, **1997**, 144, 1024-1027	3.9	8
12	Chemical Reactions in Bulk and on Surfaces **1997**, 413-416		
11	Time-dependent simulation of Czochralski silicon crystal growth. *Journal of Crystal Growth*, **1997**, 180, 468-476	1.6	9
10	Molecular-dynamics study of partial edge dislocations in copper and gold: Interactions, structures, and self-diffusion. *Physical Review B*, **1996**, 53, 8956-8966	3.3	13
9	Defect-induced nucleation and growth of amorphous silicon. *Physical Review B*, **1996**, 54, 1459-1462	3.3	18
8	Energetics of diffusion on the (100) and (111) surfaces of Ag, Au, and Ir from first principles. *Physical Review B*, **1995**, 52, 9078-9085	3.3	91
7	Electronic Structure and Positron Trapping in Semiconductors. *Materials Science Forum*, **1994**, 175-178, 279-286	0.4	2
6	Nos□Hoover molecular-dynamics study of self-pipe-diffusion in gold using many-atom interactions. *Physical Review B*, **1994**, 50, 6450-6452	3.3	5
5	First-Principles Simulations of Vacancies and Antisites in InP. *Materials Science Forum*, **1993**, 143-147, 1305-1310	0.4	2
4	Positron trapping in oxide superconductors. *Journal of Physics and Chemistry of Solids*, **1991**, 52, 1577-1587	3.9	17
3	Electronic Properties of Two-Dimensional Systems. *Physica Scripta*, **1988**, T23, 54-58	2.6	2
2	Cluster calculations for H2dissociation on Cu and Ni. *Physica Scripta*, **1988**, 37, 141-144	2.6	4
1	Supercell Methods for Defect Calculations. *Topics in Applied Physics*,29-68	0.5	6