

# Risto M Nieminen

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Migration and localization of metal atoms on strained graphene. <i>Physical Review Letters</i> , <b>2010</b> , 105, 1961-1964	10.2	281
86	Intrinsic n-type behavior in transparent conducting oxides: a comparative hybrid-functional study of In <sub>2</sub> O <sub>3</sub> , SnO <sub>2</sub> , and ZnO. <i>Physical Review Letters</i> , <b>2009</b> , 103, 245501	7.4	274
85	Linear-scaling self-consistent implementation of the van der Waals density functional. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	149
84	Synthesis of graphene nanoribbons encapsulated in single-walled carbon nanotubes. <i>Nano Letters</i> , <b>2011</b> , 11, 4352-6	11.5	148
83	Electronic structure of boron nitride sheets doped with carbon from first-principles calculations. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	129
82	Energetics of diffusion on the (100) and (111) surfaces of Ag, Au, and Ir from first principles. <i>Physical Review B</i> , <b>1995</b> , 52, 9078-9085	3.3	91
81	Mechanisms of postsynthesis doping of boron nitride nanostructures with carbon from first-principles simulations. <i>Physical Review Letters</i> , <b>2011</b> , 107, 035501	7.4	84
80	Role of tip structure and surface relaxation in atomic resolution dynamic force microscopy: CaF <sub>2</sub> (111) as a reference surface. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	75
79	Kohn-Sham Decomposition in Real-Time Time-Dependent Density-Functional Theory: An Efficient Tool for Analyzing Plasmonic Excitations. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 4779-4790	6.1	73
78	L-alanine in a droplet of water: a density-functional molecular dynamics study. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 4227-34	3.4	73
77	Issues in first-principles calculations for defects in semiconductors and oxides. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2009</b> , 17, 084001	2	72
76	Influence of van der Waals forces on the adsorption structure of benzene on silicon studied using density functional theory. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	68
75	Limits for n-type doping in In <sub>2</sub> O <sub>3</sub> and SnO <sub>2</sub> : A theoretical approach by first-principles calculations using hybrid-functional methodology. <i>Journal of Applied Physics</i> , <b>2010</b> , 108, 053511	2.5	52
74	Charged Point Defects in the Flatland: Accurate Formation Energy Calculations in Two-Dimensional Materials. <i>Physical Review X</i> , <b>2014</b> , 4,	9.1	49
73	From atomistic simulation towards multiscale modelling of materials. <i>Journal of Physics Condensed Matter</i> , <b>2002</b> , 14, 2859-2876	1.8	49
72	Quantized Evolution of the Plasmonic Response in a Stretched Nanorod. <i>Physical Review Letters</i> , <b>2015</b> , 115, 236804	7.4	46
71	Bound and free self-interstitial defects in graphite and bilayer graphene: A computational study. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	31

70	Creation of paired electron states in the gap of semiconducting carbon nanotubes by correlated hydrogen adsorption. <i>New Journal of Physics</i> , <b>2007</b> , 9, 275-275	2.9	31
69	Calculated Positron Annihilation Parameters for Defects in SiC. <i>Materials Science Forum</i> , <b>2001</b> , 353-356, 533-536	0.4	31
68	Computational study of (111) epitaxially strained ferroelectric perovskites BaTiO <sub>3</sub> and PbTiO <sub>3</sub> . <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	30
67	A first-principles study on magnetic coupling between carbon adatoms on graphene. <i>New Journal of Physics</i> , <b>2010</b> , 12, 113021	2.9	29
66	Measuring site-specific cluster-surface bond formation. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 17863-6	16.4	28
65	Photoabsorption in sodium clusters on the basis of time-dependent density-functional theory. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 014707	3.9	25
64	Coronene encapsulation in single-walled carbon nanotubes: stacked columns, peapods, and nanoribbons. <i>ChemPhysChem</i> , <b>2014</b> , 15, 1660-5	3.2	24
63	Nanoplasmonics simulations at the basis set limit through completeness-optimized, local numerical basis sets. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 094114	3.9	22
62	Density-wave instability in $\text{K}(\text{BEDT-TTF})_2\text{KHg}(\text{SCN})_4$ studied by x-ray diffuse scattering and by first-principles calculations. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	22
61	Toward Stronger AlBN Nanotube Composite Materials: Insights into Bonding at the Al/BN Interface From First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 26894-26901	3.8	21
60	Photoabsorption spectra of small fullerenes and Si-heterofullerenes. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 154307	3.9	21
59	Polymer adhesion: First-principles calculations of the adsorption of organic molecules onto Si surfaces. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	21
58	Density-functional calculations of defect formation energies using the supercell method: Brillouin-zone sampling. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	21
57	Effect of the surrounding oxide on the photoabsorption spectra of Si nanocrystals. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	20
56	Structure and dynamics of dioxygen bound to cobalt and iron heme. <i>Biophysical Journal</i> , <b>2006</b> , 91, 2024-2034	3.4	20
55	Quantitative modelling in scanning force microscopy on insulators. <i>Applied Surface Science</i> , <b>2002</b> , 188, 306-318	6.7	20
54	Influence of high-refractive-index oxide coating on optical properties of metal nanoparticles. <i>Journal of the Optical Society of America B: Optical Physics</i> , <b>2013</b> , 30, 338	1.7	18
53	Silicon self-diffusion constants by tight-binding molecular dynamics. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	18

52	Defect-induced nucleation and growth of amorphous silicon. <i>Physical Review B</i> , <b>1996</b> , 54, 1459-1462	3.3	18
51	Photoabsorption spectra of boron nitride fullerenelike structures. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 214306	3.9	17
50	Positron trapping in oxide superconductors. <i>Journal of Physics and Chemistry of Solids</i> , <b>1991</b> , 52, 1577-1587	3.9	17
49	The Aqueous and Crystalline Forms of L-Alanine Zwitterion. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2008</b> , 5, 277-285	0.3	17
48	Electronic energy band structure of the double perovskite Ba <sub>2</sub> MnWO <sub>6</sub> . <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 6742-6	3.4	14
47	A Coupled Finite Element Model for the Sublimation Growth of SiC. <i>Materials Science Forum</i> , <b>1998</b> , 264-268, 65-68	0.4	13
46	Molecular-dynamics study of partial edge dislocations in copper and gold: Interactions, structures, and self-diffusion. <i>Physical Review B</i> , <b>1996</b> , 53, 8956-8966	3.3	13
45	Dynamical coupling of plasmons and molecular excitations by hybrid quantum/classical calculations: time-domain approach. <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 315013	1.8	12
44	Parallel Electronic Structure Calculations Using Multiple Graphics Processing Units (GPUs). <i>Lecture Notes in Computer Science</i> , <b>2013</b> , 63-76	0.9	12
43	Effect of edge plasmons on the optical properties of MoS <sub>2</sub> monolayer flakes. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	11
42	A hierarchical dualscale study of bisphenol-A-polycarbonate on a silicon surface: structure, dynamics and impurity diffusion. <i>Soft Matter</i> , <b>2011</b> , 7, 6457	3.6	11
41	Modeling charge-imbalanced NaNbO <sub>3</sub> /SrTiO <sub>3</sub> superlattices: Lattice relaxation and metallicity. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	11
40	Boston et al. Reply:. <i>Physical Review Letters</i> , <b>2011</b> , 106,	7.4	11
39	Effect of Cu impurities on wet etching of Si(110): formation of trapezoidal hillocks. <i>New Journal of Physics</i> , <b>2008</b> , 10, 013033	2.9	11
38	Time-dependent simulation of Czochralski silicon crystal growth. <i>Journal of Crystal Growth</i> , <b>1997</b> , 180, 468-476	1.6	9
37	Density-functional molecular dynamics studies of biologically relevant iron and cobalt complexes with macrocyclic ligands. <i>Coordination Chemistry Reviews</i> , <b>2008</b> , 252, 1497-1513	23.2	9
36	Developments in the density-functional theory of electronic structure. <i>Current Opinion in Solid State and Materials Science</i> , <b>1999</b> , 4, 493-498	12	9
35	Thermodynamic Considerations of the Role of Hydrogen in Sublimation Growth of Silicon Carbide. <i>Journal of the Electrochemical Society</i> , <b>1997</b> , 144, 1024-1027	3.9	8

34	Adsorption of metal impurities on H-terminated Si surfaces and their influence on the wet chemical etching of Si. <i>Journal of Physics Condensed Matter</i> , <b>2008</b> , 20, 485005	1.8	7
33	Atomistic approach for simulating plasmons in nanostructures. <i>Applied Physics A: Materials Science and Processing</i> , <b>2014</b> , 115, 427-431	2.6	6
32	The effect of interstitial hydrogen on the electronic structure of the B2 FeAl alloy. <i>Physica Status Solidi (B): Basic Research</i> , <b>2007</b> , 244, 3684-3694	1.3	6
31	Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3. <i>Solid State Ionics</i> , <b>2004</b> , 168, 291-298	3.3	6
30	Supercell Methods for Defect Calculations. <i>Topics in Applied Physics</i> , 29-68	0.5	6
29	Berseneva, Krasheninnikov, and Nieminen Reply:. <i>Physical Review Letters</i> , <b>2011</b> , 107,	7.4	5
28	NosHoover molecular-dynamics study of self-pipe-diffusion in gold using many-atom interactions. <i>Physical Review B</i> , <b>1994</b> , 50, 6450-6452	3.3	5
27	Fast convergence to equilibrium for long-chain polymer melts using a MD/continuum hybrid method. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 154115	3.9	4
26	Quantum Chemical Study of Effects Produced by Nb- and La-Doping in BaTiO3. <i>Key Engineering Materials</i> , <b>2001</b> , 206-213, 1325-1328	0.4	4
25	Cluster calculations for H2dissociation on Cu and Ni. <i>Physica Scripta</i> , <b>1988</b> , 37, 141-144	2.6	4
24	Effect of Magnetic Ordering on the Stability of NiMnTa(CoCu) Alloys Along the Tetragonal Deformation Path. <i>IEEE Transactions on Magnetics</i> , <b>2017</b> , 53, 1-6	2	3
23	Energy Dissipation of AFM Studied by MD/Continuum Coupling Model. <i>E-Journal of Surface Science and Nanotechnology</i> , <b>2014</b> , 12, 339-342	0.7	3
22	Ferromagnetism in MgTiO3-Ti2O3 Solid Solutions. <i>Materials Science Forum</i> , <b>2011</b> , 700, 23-27	0.4	3
21	The Effect of Compound Composition and Strain on Vacancies in Si/SiGe Heterostructures. <i>Solid State Phenomena</i> , <b>2005</b> , 108-109, 457-462	0.4	3
20	Computational model for noncontact atomic force microscopy: energy dissipation of cantilever. <i>Journal of Physics Condensed Matter</i> , <b>2016</b> , 28, 375001	1.8	2
19	Formation of Vacancies and Divacancies in Plane-Stressed Silicon. <i>Solid State Phenomena</i> , <b>2005</b> , 108-109, 433-438	0.4	2
18	Stability of the maximum-density droplet state in quantum dots: a quantum Monte Carlo study. <i>Physica B: Condensed Matter</i> , <b>2000</b> , 284-288, 1776-1777	2.8	2
17	First-Principles Simulations of Vacancies and Antisites in InP. <i>Materials Science Forum</i> , <b>1993</b> , 143-147, 1305-1310	0.4	2

16	Electronic Structure and Positron Trapping in Semiconductors. <i>Materials Science Forum</i> , <b>1994</b> , 175-178, 279-286	0.4	2
15	Electronic Properties of Two-Dimensional Systems. <i>Physica Scripta</i> , <b>1988</b> , T23, 54-58	2.6	2
14	Analysis of Tip Stability in Adhesion Process in AFM Using Potential Energy Surface: Stability Versus Dissipation. <i>E-Journal of Surface Science and Nanotechnology</i> , <b>2018</b> , 16, 132-136	0.7	1
13	Atomic Force Microscopy Simulation by MD/Continuum Coupling Method. <i>Integrated Ferroelectrics</i> , <b>2014</b> , 155, 33-38	0.8	1
12	Mechanical Properties of Silicon Microstructures <b>2010</b> , 179-219		1
11	Dynamics of Biomolecules From First Principles. <i>Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems</i> , <b>2010</b> , 1, 557-573		1
10	AB Initio Studies of Atomic-Scale Defects in GaN and AlN. <i>Materials Science Forum</i> , <b>1997</b> , 258-263, 1119-1124	1.4	1
9	Stability of Tip in Adhesion Process on Atomic Force Microscopy Studied by Coupling Computational Model. <i>Applied Science and Convergence Technology</i> , <b>2017</b> , 26, 6-10	0.8	1
8	Grid-Based Projector-Augmented Wave Method <b>2016</b> , 191-210		
7	Simulated coating of carbon nanotube networks by a beam of carbon atoms. <i>Physica Status Solidi (B): Basic Research</i> , <b>2012</b> , 249, 317-323	1.3	
6	Metastable Antisite Pair in GaAs. <i>Materials Science Forum</i> , <b>1997</b> , 258-263, 969-974	0.4	
5	Chemical Reactions in Bulk and on Surfaces <b>1997</b> , 413-416		
4	Mechanisms of Diffusion and Dissociation of E-Centers in Silicon. <i>Defect and Diffusion Forum</i> , <b>2005</b> , 237-240, 1129-1134	0.7	
3	Defects and Diffusion: First- Principles Modeling. <i>Defect and Diffusion Forum</i> , <b>2001</b> , 194-199, 261-278	0.7	
2	Effect of electromagnetic environment on transport of composite fermions in a narrow constriction between compressible quantum Hall liquids. <i>Physica B: Condensed Matter</i> , <b>2000</b> , 284-288, 1730-1731	2.8	
1	Considerations on the Crystal Morphology in the Sublimation Growth of SiC. <i>Materials Science Forum</i> , <b>2000</b> , 338-342, 95-98	0.4	