Martti J Puska

List of Publications by Citations

224 papers	13,157 citations	58 h-index	109 g-index
231 ext. papers	13,991 ext. citations	4 avg, IF	6.16 L-index

#	Paper	IF	Citations
224	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. *Journal of Physics Condensed Matter*, **2010**, 22, 253202	1.8	1092
223	Theory of positrons in solids and on solid surfaces. *Reviews of Modern Physics*, **1994**, 66, 841-897	40.5	851
222	Interatomic interactions in the effective-medium theory. *Physical Review B*, **1987**, 35, 7423-7442	3.3	768
221	Defect spectroscopy with positrons: a general calculational method. *Journal of Physics F: Metal Physics*, **1983**, 13, 333-346		665
220	Atoms embedded in an electron gas: Immersion energies. *Physical Review B*, **1981**, 24, 3037-3047	3.3	329
219	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
218	Theoretical and experimental study of positron annihilation with core electrons in solids. *Physical Review B*, **1996**, 54, 2397-2409	3.3	221
217	Screening of positrons in semiconductors and insulators. *Physical Review B*, **1989**, 39, 7666-7679	3.3	220
216	Convergence of supercell calculations for point defects in semiconductors: Vacancy in silicon. *Physical Review B*, **1998**, 58, 1318-1325	3.3	210
215	Positron trapping in semiconductors. *Physical Review B*, **1990**, 41, 9980-9993	3.3	206
214	Atoms embedded in an electron gas: Phase shifts and cross sections. *Physical Review B*, **1983**, 27, 6121-6128	3.3	205
213	Identification of vacancy defects in compound semiconductors by core-electron annihilation: Application to InP. *Physical Review B*, **1995**, 51, 4176-4185	3.3	195
212	Photoabsorption of atoms inside C60. *Physical Review A*, **1993**, 47, 1181-1186	2.6	191
211	Calculation of positron states and annihilation in solids: A density-gradient-correction scheme. *Physical Review B*, **1996**, 53, 16201-16213	3.3	181
210	Gradient correction for positron states in solids. *Physical Review B*, **1995**, 51, 7341-7344	3.3	173
209	Positron affinities for elemental metals. *Journal of Physics Condensed Matter*, **1989**, 1, 6081-6094	1.8	173
208	Time-dependent density-functional theory in the projector augmented-wave method. *Journal of Chemical Physics*, **2008**, 128, 244101	3.9	158

207	Electronic polarizability of small metal spheres. *Physical Review B*, **1985**, 31, 3486-3495	3.3	158
206	Real-space electronic-structure calculations: Combination of the finite-difference and conjugate-gradient methods. *Physical Review B*, **1995**, 51, 14057-14061	3.3	152
205	Linear-scaling self-consistent implementation of the van der Waals density functional. *Physical Review B*, **2009**, 79,	3.3	149
204	Quantum Motion of Chemisorbed Hydrogen on Ni Surfaces. *Physical Review Letters*, **1983**, 51, 1081-1084	7.4	145
203	Theory of hydrogen and helium impurities in metals. *Physical Review B*, **1984**, 29, 5382-5397	3.3	138
202	Vacancy-formation energies for fcc and bcc transition metals. *Physical Review B*, **1995**, 51, 9526-9532	3.3	130
201	Multigrid method for electronic structure calculations. *Physical Review B*, **2001**, 63,	3.3	120
200	Electron transport through monovalent atomic wires. *Physical Review B*, **2004**, 69,	3.3	119
199	Momentum distributions of electron-positron pairs annihilating at vacancy clusters in Si. *Physical Review B*, **1998**, 57, 7621-7627	3.3	117
198	Electron-positron Car-Parrinello methods: Self-consistent treatment of charge densities and ionic relaxations. *Physical Review B*, **1995**, 52, 10947-10961	3.3	115
197	Repulsive interaction of the helium atom with a metal surface. *Physical Review B*, **1984**, 29, 2314-2316	3.3	113
196	Positron states in Si and GaAs. *Physical Review B*, **1988**, 38, 9874-9880	3.3	108
195	Generalized tight-binding transport model for graphene nanoribbon-based systems. *Physical Review B*, **2010**, 81,	3.3	106
194	Impurity effects in quantum dots: Toward quantitative modeling. *Physical Review B*, **2004**, 70,	3.3	104
193	Ab initio study of fully relaxed divacancies in GaAs. *Physical Review B*, **1996**, 53, 3813-3819	3.3	96
192	Effect of Alkali Metal Atom Doping on the CuInSe2-Based Solar Cell Absorber. *Journal of Physical Chemistry C*, **2017**, 121, 15516-15528	3.8	95
191	Modeling the momentum distributions of annihilating electron-positron pairs in solids. *Physical Review B*, **2006**, 73,	3.3	94
190	Electronic structure and positron states at vacancies in Si and GaAs. *Physical Review B*, **1986**, 34, 2695-2705	3.3	93

189	Electron and positron energy levels in solids. *Physical Review B*, **1987**, 36, 7786-7794	3.3	92
188	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
187	Evaluation of some basic positron-related characteristics of SiC. *Physical Review B*, **1996**, 54, 2512-2517	3.3	84
186	Spontaneous Magnetization of Simple Metal Nanowires. *Physical Review Letters*, **1998**, 80, 3336-3339	7.4	83
185	Three real-space discretization techniques in electronic structure calculations. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 1016-1053	1.3	82
184	Direct evidence of impurity decoration of Ga vacancies in GaN from positron annihilation spectroscopy. *Physical Review B*, **2006**, 73,	3.3	81
183	Hydrogen chemisorbed on nickel surfaces: A wave-mechanical treatment of proton motion. *Surface Science*, **1985**, 157, 413-435	1.8	81
182	Positron Surface States on Clean and Oxidized Al and in Surface Vacancies. *Physical Review Letters*, **1983**, 50, 281-284	7.4	80
181	Native defects and self-diffusion in GaSb. *Journal of Applied Physics*, **2002**, 91, 4988-4994	2.5	79
180	First-principles calculations of interstitial boron in silicon. *Physical Review B*, **2000**, 61, 8155-8161	3.3	79
179	Identification of Vacancy-Impurity Complexes in Highly n-Type Si. *Physical Review Letters*, **1999**, 82, 1883-1886	7.4	77
178	Electronic structures of point defects in III-V compound semiconductors. *Journal of Physics Condensed Matter*, **1989**, 1, 7347-7366	1.8	77
177	Ab-initio calculation of positron annihilation rates in solids. *Journal of Physics Condensed Matter*, **1991**, 3, 3455-3469	1.8	76
176	Electronic structure of rectangular quantum dots. *Physical Review B*, **2003**, 67,	3.3	74
175	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	6.4	73
174	Heavy Alkali Treatment of Cu(In,Ga)Se2 Solar Cells: Surface versus Bulk Effects. *Advanced Energy Materials*, **2020**, 10, 1903752	21.8	68
173	First-principles study of fully relaxed vacancies in GaAs. *Physical Review B*, **1992**, 45, 4122-4130	3.3	63
172	Vacancy recovery and vacancy-hydrogen interaction in niobium and tantalum studied by positrons. *Physical Review B*, **1985**, 32, 4326-4331	3.3	62

171	Theoretical Aspects of Positrons in Imperfect Solids. *Physica Status Solidi A*, **1987**, 102, 11-29		61
170	Electronic stopping power from first-principles calculations with account for core electron excitations and projectile ionization. *Physical Review B*, **2014**, 89,	3.3	59
169	Computational analysis of positron experiments. *Journal of Physics F: Metal Physics*, **1984**, 14, 1299-1316		59
168	3d impurities in Al: density functional results. *Journal of Physics F: Metal Physics*, **1980**, 10, L123-L127		59
167	Resistive Switching in All-Oxide Ferroelectric Tunnel Junctions with Ionic Interfaces. *Advanced Materials*, **2016**, 28, 6852-9	24	59
166	Vortex clusters in quantum dots. *Physical Review Letters*, **2004**, 93, 116802	7.4	58
165	Indium and phosphorus vacancies and antisites in InP. *Physical Review B*, **1994**, 49, 5253-5262	3.3	55
164	Positron states in YBa2Cu3O7-x. *Journal of Physics Condensed Matter*, **1989**, 1, 3727-3732	1.8	55
163	Stability of large vacancy clusters in silicon. *Physical Review B*, **2002**, 65,	3.3	54
162	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
161	First-principles calculation of positron annihilation characteristics at metal vacancies. *Physical Review B*, **1996**, 54, 15016-15024	3.3	51
160	First-principles calculation of positron lifetimes and affinities in perfect and imperfect transition-metal carbides and nitrides. *Physical Review B*, **1994**, 49, 10947-10957	3.3	51
159	Electronic polarizability of small sodium clusters. *Physical Review B*, **1986**, 33, 4289-4290	3.3	51
158	Correlation effects for electron-positron momentum density in solids. *Physical Review B*, **1997**, 56, 7136-7142	3.3	48
157	First-principles study of He in Si. *Physical Review B*, **1992**, 46, 12806-12809	3.3	48
156	Quantized Evolution of the Plasmonic Response in a Stretched Nanorod. *Physical Review Letters*, **2015**, 115, 236804	7.4	46
155	Testing of two-dimensional local approximations in the current-spin and spin-density-functional theories. *Physical Review B*, **2003**, 67,	3.3	46
154	Atoms embedded in an electron gas: Beyond the local-density approximation. *Physical Review B*, **1991**, 43, 12221-12233	3.3	46

153	pH-Dependent Distribution of Functional Groups on Titanium-Based MXenes. *ACS Nano*, **2019**, 13, 9171-9181	16.7	45
152	Comment on the Positron Surface-State Lifetime. *Physical Review Letters*, **1984**, 53, 1298-1298	7.4	45
151	Interfacial oxide growth at silicon–high-k oxide interfaces: First principles modeling of the Si–HfO2 interface. *Journal of Applied Physics*, **2006**, 100, 043708	2.5	44
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149	All-electron density functional theory and time-dependent density functional theory with high-order finite elements. *Journal of Chemical Physics*, **2009**, 131, 054103	3.9	43
148	Positron annihilation in II-VI compound semiconductors: theory. *Journal of Physics Condensed Matter*, **1994**, 6, 8809-8827	1.8	43
147	Plasmon-Induced Direct Hot-Carrier Transfer at Metal-Acceptor Interfaces. *ACS Nano*, **2019**, 13, 3188-3195	16.7	42
146	Calculation of valence electron momentum densities using the projector augmented-wave method. *Journal of Physics and Chemistry of Solids*, **2005**, 66, 1128-1135	3.9	41
145	Positron localization effects on the Doppler broadening of the annihilation line: Aluminum as a case study. *Physical Review B*, **2005**, 72,	3.3	40
144	Role of van der Waals forces in the adsorption and diffusion of organic molecules on an insulating surface. *Physical Review B*, **2009**, 80,	3.3	38
143	Quantum size effects in Pb islands on Cu(111): Electronic structure calculations. *Physical Review B*, **2004**, 69,	3.3	38
142	Energetics of positron states trapped at vacancies in solids. *Physical Review B*, **2007**, 76,	3.3	37
141	Crystals from metallic clusters: A first-principles calculation. *Physical Review B*, **1993**, 48, 1981-1983	3.3	37
140	Vibrational Properties of Metal Phosphorus Trichalcogenides from First-Principles Calculations. *Journal of Physical Chemistry C*, **2017**, 121, 27207-27217	3.8	36
139	MIKA: Multigrid-based program package for electronic structure calculations. *International Journal of Quantum Chemistry*, **2003**, 91, 171-176	2.1	35
138	Conductance oscillations in metallic nanocontacts. *Physical Review B*, **2002**, 66,	3.3	35
137	Self-consistent study of electron confinement to metallic thin films on solid surfaces. *Physical Review B*, **2005**, 71,	3.3	34
136	Electronic structure of cylindrical simple-metal nanowires in the stabilized jellium model. *Physical Review B*, **1999**, 59, 12652-12660	3.3	34

135	Positron states in fullerites and other carbon phases. *Journal of Physics Condensed Matter*, **1992**, 4, L149-L156		34
134	Carbon-vacancy interaction in alpha iron: interpretation of positron annihilation results. *Journal of Physics F: Metal Physics*, **1982**, 12, L211-L216		33
133	Native point defect energetics in GaSb: Enabling p-type conductivity of undoped GaSb. *Physical Review B*, **2012**, 86,	3.3	32
132	Nonadiabatic Ehrenfest molecular dynamics within the projector augmented-wave method. *Journal of Chemical Physics*, **2012**, 136, 144103	3.9	32
131	Analysis of electron-positron momentum spectra of metallic alloys as supported by first-principles calculations. *Physical Review B*, **2007**, 75,	3.3	32
130	Positron states at vacancy-impurity pairs in semiconductors. *Physical Review B*, **1989**, 40, 12523-12526	3.3	32
129	Bound and free self-interstitial defects in graphite and bilayer graphene: A computational study. *Physical Review B*, **2011**, 84,	3.3	31
128	Metastable defect complexes in GaAs. *Physical Review B*, **1996**, 54, 7909-7916	3.3	31
127	Rectangular quantum dots in high magnetic fields. *Physical Review B*, **2004**, 69,	3.3	30
126	Nonequilibrium electron transport in two-dimensional nanostructures modeled using Green functions and the finite-element method. *Physical Review B*, **2004**, 69,	3.3	30
125	Vacancy-impurity complexes in highly Sb-doped Si grown by molecular beam epitaxy. *Physical Review Letters*, **2005**, 94, 165501	7.4	30
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123	Microscopic identification of native donor Ga-vacancy complexes in Te-doped GaAs. *Physical Review B*, **1999**, 60, 1464-1467	3.3	30
122	Embedded-atom calculations of Auger and x-ray photoemission shifts for metallic elements. *Physical Review B*, **1982**, 25, 67-77	3.3	30
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120	Spontaneous magnetization of aluminum nanowires deposited on the NaCl(100) surface. *Physical Review B*, **2002**, 66,	3.3	28
119	Phosphorus vacancy in InP: A negative-U center. *Physical Review B*, **1993**, 47, 6381-6384	3.3	28
118	Positron trapping rate into small vacancy clusters and light substitutional impurities. *Journal of Physics F: Metal Physics*, **1987**, 17, 2235-2248		28

117	Broken symmetry in density-functional theory: Analysis and cure. *Physical Review B*, **2004**, 69,	3.3	27
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115	Nitrogen-impurity□ative-defect complexes in ZnSe. *Physical Review B*, **1998**, 57, 12174-12180	3.3	26
114	Excitation of hydrogen motion inside a nickel vacancy. *Physical Review Letters*, **1985**, 55, 852-855	7.4	26
113	Theory and Applications of Generalized Pipek-Mezey Wannier Functions. *Journal of Chemical Theory and Computation*, **2017**, 13, 460-474	6.4	25
112	Electron transport in edge-disordered graphene nanoribbons. *Physical Review B*, **2011**, 83,	3.3	25
111	Positron affinity for precipitates in reactor pressure vessel steels. *Nuclear Engineering and Design*, **1995**, 158, 149-156	1.8	25
110	First-Principles Modeling of Point Defects and Complexes in Thin-Film Solar-Cell Absorber CuInSe2. *Advanced Electronic Materials*, **2017**, 3, 1600353	6.4	24
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105	Nanoplasmonics simulations at the basis set limit through completeness-optimized, local numerical basis sets. *Journal of Chemical Physics*, **2015**, 142, 094114	3.9	22
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102	Effect of the surrounding oxide on the photoabsorption spectra of Si nanocrystals. *Physical Review B*, **2009**, 79,	3.3	20
101	Stability of vortex structures in quantum dots. *Physical Review B*, **2005**, 71,	3.3	20
100	Observation of Ga vacancies and negative ions in undoped and Mg-doped GaN bulk crystals. *Physica B: Condensed Matter*, **1999**, 273-274, 33-38	2.8	20

99	Hydrogen and deuterium decoration of In-vacancy complexes in nickel. *Physical Review B*, **1987**, 35, 6059-6063	3.3	20
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97	Modeling Bi-induced changes in the electronic structure of GaAs1−xBix alloys. *Physical Review B*, **2013**, 88,	3.3	19
96	Origin of band gap bowing in dilute GaAs1−xNx and GaP1−xNx alloys: A real-space view. *Physical Review B*, **2013**, 88,	3.3	19
95	Spin-Dependence in Asymmetric, V-Shaped-Notched Graphene Nanoribbons. *Journal of Low Temperature Physics*, **2008**, 153, 393-398	1.3	19
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91	Image potential states of supported metallic nanoislands. *Physical Review B*, **2007**, 76,	3.3	17
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89	Shell and supershell structures of nanowires: A quantum-mechanical analysis. *Physical Review B*, **2001**, 64,	3.3	17
88	Role of elastic and electronic interactions in trapping of hydrogen by impurities in transition metals. *Physical Review B*, **1985**, 31, 7612-7616	3.3	17
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79	Atomic relaxations around vacancy clusters in molybdenum and their effects on trapped-positron lifetime. *Physical Review B*, **1988**, 37, 6-11	3.3	14
78	Computed positron lifetimes in vacancies and vacancy-iron clusters in gold. *Radiation Effects*, **1983**, 79, 305-312		13
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74	Effect of edge plasmons on the optical properties of MoS2 monolayer flakes. *Physical Review B*, **2017**, 96,	3.3	11
73	Electronic transport in graphene-based structures: An effective cross-section approach. *Physical Review B*, **2012**, 85,	3.3	11
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70	Positron annihilation at paramagnetic defects in semiconductors. *Journal of Physics Condensed Matter*, **1993**, 5, L307-L314	1.8	11
69	Enhancing conductivity of metallic carbon nanotube networks by transition metal adsorption. *Journal of Chemical Physics*, **2015**, 142, 054705	3.9	10
68	Full-correlation single-particle positron potentials for a positron and positronium interacting with atoms. *Physical Review A*, **2014**, 89,	2.6	10
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65	Core Polarizabilities in Metals. *Physica Scripta*, **1982**, 25, 952-956	2.6	10
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44	First-Principles Study of Excited State Evolution in a Protected Gold Complex. *Journal of Physical Chemistry C*, **2013**, 117, 11837-11842	3.8	6
43	Metastability of the antistructure pair in GaAs. *Physical Review B*, **1997**, 55, 6914-6917	3.3	6
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39	Plasmon Excitations in Mixed Metallic Nanoarrays. *ACS Nano*, **2019**, 13, 5344-5355	16.7	5
38	Impact of Ga-V Codoping on Interfacial Electron Transfer in Dye-Sensitized TiO2. *Journal of Physical Chemistry Letters*, **2015**, 6, 2603-7	6.4	5
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36	Charge Transfer at the Hybrid Interfaces in the Presence of Water: A Theoretical Study. *Journal of Physical Chemistry C*, **2015**, 119, 28347-28352	3.8	5
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