Kalevi Kokko

List of Publications by Year
in descending order

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		430442	500791
127	1,345	18	28
papers	citations	h-index	g-index

127	127	127	1325
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interatomic Feâ€“Cr potential for modeling kinetics on Fe surfaces. Computational Materials Science, 2022, 203, 110840.	1.4	1
2	Atomic-Scale Modification of Oxidation Phenomena on the Ge(100) Surface by Si Alloying. ACS Materials Au, 2022, 2, 204-214.	2.6	1
3	Effects of thermal vacuum nitridation of Si(100) surface via NH3 exposure. Thin Solid Films, 2022, 757, 139392.	0.8	1
4	Oxygen adsorption on (100) surfaces in Feâ€“Cr alloys. Scientific Reports, 2021, 11, 6046.	1.6	7
5	Passivation of IIIâ€“V surfaces with crystalline oxidation. Applied Physics Reviews, 2021, 8, .	5.5	23
6	Observation of Si 2p Coreâ€Level Shift in Si/Highâ€Îº Dielectric Interfaces Containing a Negative Charge. Advanced Electronic Materials, 2021, 7, 2100034.	2.6	7
7	Atomic and electronic structures of Si/Ge(100) interfaces studied by high-resolution photoelectron spectroscopy and scanning tunneling microscopy. Physical Review B, 2021, 103, .	1.1	1
8	Stabilization of unstable and metastable InP native oxide thin films by interface effects. Applied Surface Science, 2021, 567, 150848.	3.1	2
9	Optimization of SiO2 with GHA and basin hopping. Computational Materials Science, 2021, , 111011.	1.4	1
10	Dimer-vacancy defects on Si(1Â0Â0): The role of nickel impurity. Applied Surface Science, 2020, 506, 144647.	3.1	2
11	Decreasing Interface Defect Densities via Silicon Oxide Passivation at Temperatures Below 450 Â°C. ACS Applied Materials & Interfaces, 2020, 12, 46933-46941.	4.0	6
12	Density Functional Theory description of the order-disorder transformation in Fe-Ni. Scientific Reports, 2019, 9, 8172.	1.6	22
13	First-principles investigations of the magnetic phase diagram of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Gd</mml:mi><mml:mrow><mml:mn>1</mml:mn> Physical Review B, 2019, 99, .	1.1	9
14	Unusual oxidation-induced core-level shifts at the HfO2/InP interface. Scientific Reports, 2019, 9, 1462.	1.6	9
15	Observation of Crystalline Oxidized Silicon Phase. Advanced Materials Interfaces, 2019, 6, 1802033.	1.9	3
16	Density functional theory description of random Cu-Au alloys. Physical Review B, 2019, 99, .	1.1	5
17	Space partitioning of exchange-correlation functionals with the projector augmented-wave method. Journal of Chemical Physics, 2019, 150, 054101.	1.2	8
18	Optimizing Atomic Structures through Geno-Mathematical Programming. Communications in Computational Physics, 2019, 25, .	0.7	1

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19	Electronic structure and relative stability of the coherent and semi-coherent HfO2/III-V interfaces. Applied Surface Science, 2018, 427, 243-252.	3.1	6
20	<scp>K</scp>ullbackâ€“<scp>L</scp>eibler and relative <scp>F</scp>isher information as descriptors of locality. International Journal of Quantum Chemistry, 2018, 118, e25557.	1.0	6
21	Imaging empty states on the Ge(100) surface at 12 K. Physical Review B, 2018, 98, .	1.1	2
22	Oxidation-Induced Changes in the ALD-Al₂O₃/InAs(100) Interface and Control of the Changes for Device Processing. ACS Applied Materials & Interfaces, 2018, 10, 44932-44940.	4.0	6
23	Crystalline and oxide phases revealed and formed on InSb(111)B. Scientific Reports, 2018, 8, 14382.	1.6	11
24	Gradient-level and nonlocal density functional descriptions of Cu-Au intermetallic compounds. European Physical Journal B, 2018, 91, 1.	0.6	5
25	Surface doping of Ga In1â^'As semiconductor crystals with magnesium. Materialia, 2018, 2, 33-36.	1.3	0
26	Variation of magnetic properties of Sr₂FeMoO₆ due to oxygen vacancies. Journal of Physics Condensed Matter, 2018, 30, 305801.	0.7	21
27	Tuning the probability of defect formation via substrate strains in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>Fe</mml:mi><mml:msub><mml:mi>MoO</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math> films. Physical Review Materials, 2018, 2, .	2.9	7
28	Decreasing Defectâ€State Density of Al₂O₃/Ga_xIn_{1â^'}_xAs Device Interfaces with InO_x Structures. Advanced Materials Interfaces, 2017, 4, 1700722.	1.9	4
29	Local variation in Bi crystal sites of epitaxial GaAsBi studied by photoelectron spectroscopy and first-principles calculations. Applied Surface Science, 2017, 396, 688-694.	3.1	5
30	Stacking fault energy of C-alloyed steels: The effect of magnetism. Acta Materialia, 2017, 122, 72-81.	3.8	30
31	Toward the Atomically Abrupt Interfaces of SiO_x/Semiconductor Junctions. Advanced Materials Interfaces, 2016, 3, 1500510.	1.9	3
32	First-principles prediction of the deformation modes in austenitic Fe-Cr-Ni alloys. Applied Physics Letters, 2016, 108, .	1.5	17
33	Comparison of Chemical, Electronic, and Optical Properties of Mg-Doped AlGaN. Journal of Physical Chemistry C, 2016, 120, 28591-28597.	1.5	4
34	Orderâ€“disorder transition of alloys. Philosophical Magazine, 2016, 96, 3697-3710.	0.7	0
35	Exchange-Correlation Catastrophe in Cu-Au: A Challenge for Semilocal Density Functional Approximations. Physical Review Letters, 2016, 117, 066401.	2.9	12
36	Directional Youngâ€™s modulus of single-crystal and cold-rolled titanium fromab initiocalculations: Preferred crystal orientation due to cold rolling. Philosophical Magazine, 2016, 96, 2736-2751.	0.7	0

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37	Origin of Fermi-level pinning and its control on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math>-type Ge(100) surface. Physical Review B, 2016, 94, .	1.1	12
38	Quantitative description of short-range order and its influence on the electronic structure in Ag-Pd alloys. Journal of Physics Condensed Matter, 2016, 28, 305501.	0.7	3
39	Sr/Si(100)(1 Ã— 2) reconstruction as a template for the growth of crystalline high-k films on silicon: Atomic structure and reactivity. Surface Science, 2016, 646, 140-145.	0.8	7
40	Thermally assisted oxidation of GaSb(100) and the effect of initial oxide phases. Applied Surface Science, 2016, 369, 520-524.	3.1	4
41	Assessing the elastic properties and ductility of Feâ€“Crâ€“Al alloys fromab initiocalculations. Philosophical Magazine, 2016, 96, 122-133.	0.7	10
42	Alternative to the Kohn-Sham equations: The Pauli potential differential equation. Physical Review A, 2015, 92, .	1.0	11
43	Observation of unusual metal-semiconductor interaction and metal-induced gap states at an oxide-semiconductor interface: The case of epitaxial BaO/Ge(100) junction. Physical Review B, 2015, 92, .	1.1	7
44	Thermodynamics of the pseudobinary GaAs1-xBix (0Ââ‰ÂxÂâ‰Â1) alloys studied by different exchange-correlation functionals, special quasi-random structures and Monte Carlo simulations. Computational Condensed Matter, 2015, 5, 7-13.	0.9	5
45	Oxidized crystalline (3 Ã— 1)-O surface phases of InAs and InSb studied by high-resolution photoelectron spectroscopy. Applied Physics Letters, 2015, 106, .	1.5	10
46	Line shape and composition of the In 3d5/2 core-level photoemission for the interface analysis of In-containing IIIâ€“V semiconductors. Applied Surface Science, 2015, 329, 371-375.	3.1	5
47	Synthesis and properties of crystalline thin film of antimony trioxide on the Si(1 0 0) substrate. Applied Surface Science, 2015, 349, 259-263.	3.1	13
48	Oxidation of GaSb(100) and its control studied by scanning tunneling microscopy and spectroscopy. Applied Physics Letters, 2015, 107, 061601.	1.5	8
49	Effects of thinning and heating for TiO2/AlInP junctions. Journal of Electron Spectroscopy and Related Phenomena, 2015, 205, 6-9.	0.8	0
50	Oxidation of the GaAs semiconductor at the Al₂O₃/GaAs junction. Physical Chemistry Chemical Physics, 2015, 17, 7060-7066.	1.3	12
51	Cusp relation for the Pauli potential. Physical Review A, 2014, 90, .	1.0	12
52	Atomic structure and thermally induced transformation of the crystalline BaO/Si(100) junction. Physical Review B, 2014, 90, .	1.1	13
53	Unveiling and controlling the electronic structure of oxidized semiconductor surfaces: Crystalline oxidized InSb(100)(1 Ã— 2)-O. Physical Review B, 2014, 90, .	1.1	10
54	Flexibility of the quasi-non-uniform exchange-correlation approximation. Physical Review B, 2014, 89, .	1.1	23

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55	Synthesis and Characterization of Layered Tin Monoxide Thin Films with Monocrystalline Structure on IIIâ€“V Compound Semiconductor. Advanced Materials Interfaces, 2014, 1, 1300022.	1.9	2
56	Does Bi form clusters in GaAs1 â^'xBixalloys?. Semiconductor Science and Technology, 2014, 29, 115007.	1.0	11
57	Atomic-Level Understanding of Interfaces in the Synthesis of Crystalline Oxides on Semiconductors: Sr- and Ba/Si(100)(2 Ã— 3) Reconstructions. Journal of Physical Chemistry C, 2014, 118, 1894-1902.	1.5	12
58	Short-range correlations in binary alloys: Spin model approach to AgcAu1â^'c and AgcPd1â^'c. Journal of Alloys and Compounds, 2014, 614, 408-414.	2.8	1
59	Bismuth-containing c(4Ã—4) surface structure of the GaAs(100) studied by synchrotron-radiation photoelectron spectroscopy and ab initio calculations. Journal of Electron Spectroscopy and Related Phenomena, 2014, 193, 34-38.	0.8	3
60	Magnetic origin of the chemical balance in alloyed Feâ€“Cr stainless steels: First-principles and Ising model study. Computational Materials Science, 2014, 92, 135-140.	1.4	1
61	Photoemission and density functional theory study of Ge(100): Clean surface and Yb-induced (2Ã—4) reconstruction. Surface Science, 2013, 615, 88-96.	0.8	6
62	Ab initio study of the surface properties of austenitic stainless steel alloys. Surface Science, 2013, 609, 190-194.	0.8	13
63	Ab initioinvestigation of the elastic properties of Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>Fe. Physical Review B, 2013, 88, .	1.1	14
64	Adhesion of the ironâ€“chromium oxide interface from first-principles theory. Journal of Physics Condensed Matter, 2013, 25, 495501.	0.7	10
65	Growth and properties of crystalline barium oxide on the GaAs(100) substrate. Applied Physics Letters, 2013, 103, .	1.5	5
66	Formation and destabilization of Ga interstitials in GaAsN: Experiment and theory. Physical Review B, 2012, 86, .	1.1	12
67	Elastic anomalies and long/short-range ordering effects: A first-principles investigation of the AgcPd1â^'csolid solution. Physical Review B, 2012, 86, .	1.1	8
68	Quasi-non-uniform gradient-level exchange-correlation approximation for metals and alloys. Physical Review B, 2012, 86, .	1.1	17
69	Structure of ordered oxide on InAs(100) surface. Surface Science, 2012, 606, 1837-1841.	0.8	5
70	Surface core-level shifts on Ge(111)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>c</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>2</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>8</mml:mn><mml:mo) TjET Qq0 0 0 rgBT /Ov 2011, 83, .		
71	Initial Oxidation of Feâ€“Al and Feâ€“Crâ€“Al Alloys: Cr as an Alumina Booster. Oxidation of Metals, 2011, 76, 331-346.	1.0	31
72	Tin-stabilized (1Ã—2) and (1Ã—4) reconstructions on GaAs(100) and InAs(100) studied by scanning tunneling microscopy, photoelectron spectroscopy, and ab initio calculations. Surface Science, 2011, 605, 883-888.	0.8	2

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73	First-principles atomistic study of surfaces of Fe-rich Feâ€“Cr. Journal of Physics Condensed Matter, 2011, 23, 265004.	0.7	23
74	Dimer-T<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>reconstruction of the Sm/Si(100)(<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.1	5
75	surface studied by high-resolution photoelectron spectroscopy and density functional theory calcul Oxidized In-containing III-V(100) surfaces: Formation of crystalline oxide films and semiconductor-oxide interfaces. Physical Review B, 2011, 83, .	1.1	32
76	Effect of long-range order on elastic properties of Pd<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn mathvariant="bold">0</mml:mn><mml:mo>.</mml:mo><mml:mn mathvariant="bold">5</mml:mn></mml:mrow></mml:msub></mml:math>Ag<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn mathvariant="bold">0</mml:mn><mml:mo>.</mml:mo><mml:mn mathvariant="	1.1	16
77	Ultrathin (1Ã—2)-Sn layer on GaAs(100) and InAs(100) substrates: A catalyst for removal of amorphous surface oxides. Applied Physics Letters, 2011, 98, .	1.5	3
78	Core-level shifts of the c(8Ã—2)-reconstructed InAs(100) and InSb(100) surfaces. Journal of Electron Spectroscopy and Related Phenomena, 2010, 177, 52-57.	0.8	13
79	Ab initioand scanning tunneling microscopy study of an indium-terminated GaAs(100) surface: An indium-induced surface reconstruction change in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>c</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>8</mml:mn><mml:mn	1.1	18
80	Physical Review B, 2010, 81, . Bismuth-stabilized<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>c</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>2</mml:mn><mml:mn on a InSb(100) substrate: Violation of the electron counting model. Physical Review B, 2010, 81, .	1.1	19
81	High temperature oxidation of Feâ€“Al and Feâ€“Crâ€“Al alloys: The role of Cr as a chemically active element. Corrosion Science, 2010, 52, 3394-3404.	3.0	154
82	Ab initiostudy of the phase stability in paramagnetic duplex steel alloys. Physical Review B, 2009, 79, .	1.1	14
83	Stability and structure of rare-earth metal and Ba-induced reconstructions on a Si(100) surface. Physical Review B, 2009, 80, .	1.1	9
84	Ab initiostudy of the elastic anomalies in Pd-Ag alloys. Physical Review B, 2009, 79, .	1.1	29
85	Core-level shifts of InP(100)(2Ã—4) surface: Theory and experiment. Surface Science, 2009, 603, 2664-2668.	0.8	5
86	Surface core-level shift of Pd at the AgcPd1â^'c(111) surface: Nonlinear subsurface effects. Surface Science, 2007, 601, 5419-5423.	0.8	4
87	The chemical potential in surface segregation calculations: AgPd alloys. Surface Science, 2006, 600, 904-913.	0.8	30
88	Reactivity of Pd doped Ag surfaces. Vacuum, 2004, 74, 169-172.	1.6	1
89	Polarization dependent X-ray spectra of MgB2. Journal of Alloys and Compounds, 2004, 362, 139-142.	2.8	4
90	Structure and reactivity of Pd doped Ag surfaces. Surface Science, 2003, 529, 403-409.	0.8	8

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91	Electronic structure of the intermetallic compound Gd3Pd. Journal of Alloys and Compounds, 2003, 350, 5-8.	2.8	5
92	Electronic structures of AuMg and AuZn. Journal of Electron Spectroscopy and Related Phenomena, 2001, 113, 167-174.	0.8	11
93	The electronic structure of K2NiF4 and K2CoF4: beyond LSDA. Solid State Communications, 2001, 117, 583-588.	0.9	4
94	One-dimensional magnetism of Rh chains on the Ag(001) surface. Physical Review B, 2000, 62, 6415-6420.	1.1	20
95	within the LSDA +Uapproach. Journal of Physics Condensed Matter, 1999, 11, 2341-2349.	0.7	43
96	Surface alloys of CuAu I: charge transfer and the electronic density of states. Journal of Physics Condensed Matter, 1999, 11, 6685-6692.	0.7	3
97	From x-ray-absorption near-edge structures to thed-hole population in Pd-Ag alloys. Physical Review B, 1999, 60, 4659-4664.	1.1	15
98	Structure and stability of clusters on metal surfaces. Physics of the Solid State, 1999, 41, 1216-1221.	0.2	4
99	Filmâ€“substrate interface mixing in the energetic deposition of Ag on Cu(001). Surface Science, 1999, 442, 420-430.	0.8	17
100	Low-temperature specific heat of near-equiatomic Ni-rich B19â€²-TiNi-alloys. Solid State Communications, 1998, 108, 567-571.	0.9	3
101	Molecular dynamics simulation of Co thin films growth on Cu(001). Surface Science, 1998, 400, 54-62.	0.8	35
102	Some ground-state properties of 3d and 4d metals studied using the generalized gradient approximation. Journal of Physics Condensed Matter, 1998, 10, 1285-1291.	0.7	11
103	Effects of changes in the translational symmetry of VRu on the electronic density of states. Journal of Physics Condensed Matter, 1998, 10, 6073-6081.	0.7	0
104	Magnetic states in mixedFeX(X=3d)clusters on the Ag(001) surface. Physical Review B, 1998, 57, 15585-15590.	1.1	15
105	K-emission spectra of Zn, ZnS, and ZnSe within dipole and quadrupole approximations. Physical Review B, 1998, 58, 1272-1278.	1.1	7
106	Step roughening effect on adatom diffusion. Physical Review B, 1997, 56, 12135-12138.	1.1	35
107	First-principles calculations for work function and surface energy of thin lithium films. Surface Science, 1996, 348, 168-174.	0.8	54
108	The x-ray -emission band and the electronic structure of Zn, ZnS and ZnSe crystals. Journal of Physics Condensed Matter, 1996, 8, 6791-6801.	0.7	6

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109	Pressure-induced charge transfer in Li and Al alloys. Physical Review B, 1996, 53, 15393-15396.	1.1	0
110	Adsorbate-atom-induced relaxation of thin Li(001) films. Physical Review B, 1996, 54, 17078-17082.	1.1	1
111	Work function and surface energy of optimized lithium slabs. Physical Review B, 1995, 52, 1536-1539.	1.1	16
112	Surface relaxation of the clean and Mg-contaminated Li(100) surface. Physical Review B, 1995, 52, 7868-7871.	1.1	3
113	Theoretical investigation into a long-period anti-phase structure of Au3Zn. Journal of Physics Condensed Matter, 1995, 7, 5521-5527.	0.7	2
114	A first-principles study of the lattice distortion around a solute atom in BCC lithium. Journal of Physics Condensed Matter, 1995, 7, 2461-2471.	0.7	8
115	Local electronic structure of ordered Li-X (X=Na, Mg, Al) alloys under high pressure. Journal of Physics Condensed Matter, 1994, 6, 10247-10252.	0.7	3
116	XPS spectra and the electronic structure of CaCu and CaAg alloys. Physical Review B, 1994, 49, 14153-14159.	1.1	1
117	First principles study of the solute atom induced lattice distortion effects on bulk modulus and band structure in Li-alloys. Computational Materials Science, 1994, 2, 261-269.	1.4	5
118	A first principles study on the structure and the elastic properties of Li-Mg alloys. Journal of Physics Condensed Matter, 1993, 5, 3325-3332.	0.7	9
119	A band theoretical study on the electronic specific heat in the phase transition CuAuI to CuAu II. Journal of Physics Condensed Matter, 1991, 3, 5723-5728.	0.7	2
120	The core hole effect in the X-ray K-absorption spectrum of K. Physics Letters, Section A: General, Atomic and Solid State Physics, 1990, 145, 383-386.	0.9	1
121	The electronic structure of the CuAu II superlattice. Journal of Physics Condensed Matter, 1990, 2, 5253-5257.	0.7	8
122	A band theoretical explanation for the electronic specific heat of some copper-gold alloys. Journal of Physics Condensed Matter, 1990, 2, 4587-4593.	0.7	19
123	Determination of Electron Momentum Density from Electron Number Density. New Version of Semiclassical Transformation. Physica Status Solidi (B): Basic Research, 1989, 151, 139-144.	0.7	2
124	Fermi Level Density of States in Agïż¿Au Alloys. Nuclear Magnetic Spinâ€Lattice Relaxation Rate and Lowâ€Temperature Specific Heat. Physica Status Solidi (B): Basic Research, 1989, 153, 235-241.	0.7	10
125	Effects of Inhomogeneity in the Calculation of the Electron Momentum Density from the Electron Number Density. Physica Status Solidi (B): Basic Research, 1989, 156, K119.	0.7	1
126	Modeling of Steels and Steel Surfaces Using Quantum Mechanical First Principles Methods. Materials Science Forum, 0, 762, 445-450.	0.3	0

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127	Atomistic Study of Surfaces and Interfaces of Fe-Cr and Fe-Cr-Al Alloys. Materials Science Forum, 0, 762, 728-733.	0.3	2