

# Alexander A Demkov

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9212090/publications.pdf>

Version: 2024-02-01

240  
papers

7,965  
citations

53660

45  
h-index

62479

80  
g-index

242  
all docs

242  
docs citations

242  
times ranked

8007  
citing authors



#	ARTICLE	IF	CITATIONS
19	Tunable giant nonlinear optical susceptibility in BaSnO <sub>3</sub> quantum wells. <i>Physical Review B</i> , 2021, 104, .	1.1	2
20	Epitaxial, electro-optically active barium titanate thin films on silicon by chemical solution deposition. <i>Journal of the American Ceramic Society</i> , 2020, 103, 1209-1218.	1.9	17
21	Dielectric breakdown in epitaxial BaTiO <sub>3</sub> thin films. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2020, 38, 044007.	0.6	3
22	Preparation of clean MgO surface by oxygen plasma: Comparison with standard substrate cleaning procedures. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2020, 38, .	0.6	5
23	Controlling spin-polarized carriers at the interface via the ferroelectric field effect. <i>Physical Review B</i> , 2020, 102, .		
24	Design rules for strong electro-optic materials. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	27
25	Composition and annealing effects on the linear electro-optic response of solution-deposited barium strontium titanate. <i>Journal of the American Ceramic Society</i> , 2020, 103, 5700-5705.	1.9	9
26	Stoichiometry, band alignment, and electronic structure of Eu <sub>2</sub> O <sub>3</sub> thin films studied by direct and inverse photoemission: A reevaluation of the electronic band structure. <i>Journal of Applied Physics</i> , 2020, 127, 074101.	1.1	7
27	Deal-Grove-like thermal oxidation of Si (001) buried under a thin layer of SrTiO <sub>3</sub> . <i>Journal of Applied Physics</i> , 2020, 127, .	1.1	5
28	Role of template layers for heteroepitaxial growth of lanthanum oxide on GaN(0001) via atomic layer deposition. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020, 38, .	0.9	5
29	Epitaxial integration of ferroelectric and conductive perovskites on silicon. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020, 38, .	0.9	5
30	Ferroelectric domain architecture and poling of BaTiO <sub>3</sub> on Si. <i>Physical Review Materials</i> , 2020, 4, .		
31	First-Principles Modeling of Interface Effects in Oxides. , 2020, , 1119-1149.		0
32	Atomic layer deposition of epitaxial ferroelectric barium titanate on Si(001) for electronic and photonic applications. <i>Journal of Applied Physics</i> , 2019, 126, .	1.1	19
33	Epitaxial BaSnO <sub>3</sub> and SrSnO <sub>3</sub> perovskite growth on SrTiO <sub>3</sub> (001) via atomic layer deposition. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2019, 37, 050902.	0.9	5
34	Ultra-Low-Power Tuning in Hybrid Barium Titanate-Silicon Nitride Electro-optic Devices on Silicon. <i>ACS Photonics</i> , 2019, 6, 2677-2684.	3.2	37
35	Band offset modulation in Si-EuO heterostructures via controlled interface formation. <i>Physical Review B</i> , 2019, 100, .	1.1	7
36	Growth of NbO <sub>2</sub> thin films on GaN(0001) by molecular beam epitaxy. <i>Thin Solid Films</i> , 2019, 691, 137603.	0.8	2

#	ARTICLE	IF	CITATIONS
37	Electron pairing by remote-phonon scattering in oxide-supported graphene. Physical Review B, 2019, 100, .	1.1	0
38	Monolithic integration of transition metal oxide multiple quantum wells on silicon (001). Journal of Applied Physics, 2019, 125, 155302.	1.1	7
39	Dynamic Waveguiding in Silicon-Integrated Barium Titanate Thin Films. , 2019, , .		0
40	Epitaxial Oxides on Glass: A Platform for Integrated Oxide Devices. ACS Applied Nano Materials, 2019, 2, 7713-7718.	2.4	8
41	First-Principles Modeling of Interface Effects in Oxides. , 2019, , 1-30.		0
42	Large Pockels effect in micro- and nanostructured barium titanate integrated on silicon. Nature Materials, 2019, 18, 42-47.	13.3	311
43	Rare-earth adatoms on GaN (0001). Physical Review Materials, 2019, 3, .	0.9	3
44	Designing near-infrared electro-optical devices from the SrTiO <sub>3</sub> /LaAlO <sub>3</sub> materials system. Optical Materials Express, 2019, 9, 2982.	1.6	9
45	Electron accumulation and charge neutrality level at the Eu/EuO interface. Physical Review Materials, 2019, 3, .	0.9	0
46	Theoretical investigation of the band alignment of graphene on a polar $\text{SrTiO}_3$ surface. Physical Review B, 2018, 97, .	1.1	11
47	Surface structure analysis of Eu Zintl template on Ge(001). Surface Science, 2018, 674, 94-102.	0.8	9
48	Polarization retention in ultra-thin barium titanate films on Ge(001). Applied Physics Letters, 2018, 112, .	1.5	7
49	Spin-polarized two-dimensional electron gas: <i>Ab initio</i> study of EuO interface with oxygen-deficient $\text{SrTiO}_3$ . Physical Review B, 2018, 97, .	1.1	9
50	Effect of SrTiO <sub>3</sub> oxygen vacancies on the conductivity of LaTiO <sub>3</sub> /SrTiO <sub>3</sub> heterostructures. Journal of Applied Physics, 2018, 124, 185303.	1.1	22
51	EuO epitaxy by oxygen scavenging on SrTiO <sub>3</sub> (001): Effect of SrTiO <sub>3</sub> thickness and temperature. Journal of Applied Physics, 2018, 124, .	1.1	7
52	Piezoelectric modulation of nonlinear optical response in BaTiO <sub>3</sub> thin film. Applied Physics Letters, 2018, 113, 132902.	1.5	13
53	An EELS signal-from-background separation algorithm for spectral line-scan/image quantification. Ultramicroscopy, 2018, 195, 25-31.	0.8	6
54	Monolithic integration of patterned BaTiO <sub>3</sub> thin films on Ge wafers. Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, 2018, 36, .	0.6	6

#	ARTICLE	IF	CITATIONS
55	Large positive linear magnetoresistance in the two-dimensional t <sub>2g</sub> electron gas at the EuO/SrTiO <sub>3</sub> interface. Scientific Reports, 2018, 8, 7721.	1.6	40
56	Crystalline SrZrO <sub>3</sub> deposition on Ge (001) by atomic layer deposition for high- <i>k</i> dielectric applications. Journal of Applied Physics, 2018, 124, .	1.1	9
57	Quantum Confinement in Oxide Heterostructures: Room-Temperature Intersubband Absorption in SrTiO <sub>3</sub> /LaAlO <sub>3</sub> Multiple Quantum Wells. ACS Nano, 2018, 12, 7682-7689.	7.3	15
58	The MBE growth of arbitrarily thick SrTiO <sub>3</sub> /LaAlO <sub>3</sub> quantum well heterostructures for use in next-generation optoelectronic devices. Journal of Applied Physics, 2018, 124, .	1.1	9
59	Strain enhancement of the electro-optical response in BaTiO <sub>3</sub> films integrated on SrTiO <sub>3</sub> films. First-principles study of the linear electro-optical response in strained BaTiO <sub>3</sub> films. Physical Review Materials, 2018, 2, .	1.1	21
60	Microstructure and ferroelectricity of BaTiO <sub>3</sub> thin films on Si for integrated photonics. Nanotechnology, 2017, 28, 075706.	0.9	14
61	Zintl layer formation during perovskite atomic layer deposition on Ge (001). Journal of Chemical Physics, 2017, 146, 052817.	1.2	11
62	Ge(001) surface cleaning methods for device integration. Applied Physics Reviews, 2017, 4, .	5.5	42
63	Effect of oxygen vacancies and strain on the phonon spectrum of HfO <sub>2</sub> thin films. Journal of Applied Physics, 2017, 121, .	1.1	10
64	Scavenging of oxygen from SrTiO <sub>3</sub> during oxide thin film deposition and the formation of interfacial 2DEGs. Journal of Applied Physics, 2017, 121, .	1.1	50
65	Recent studies of oxide-semiconductor heterostructures using aberration-corrected scanning transmission electron microscopy. Journal of Materials Research, 2017, 32, 912-920.	1.2	7
66	Temperature dependence of the morphology and electronic structure of ultrathin platinum on TiO <sub>2</sub> -terminated SrTiO <sub>3</sub> (001). Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, 2017, 35, 061203.	0.6	1
67	Microstructure and ferroelectricity of barium titanate thin films on Si for integrated photonics. , 2017, , .		0
68	Epitaxial growth of barium titanate thin films on germanium via atomic layer deposition. Journal of Crystal Growth, 2017, 476, 6-11.	0.7	13
69	Cubic crystalline erbium oxide growth on GaN(0001) by atomic layer deposition. Journal of Applied Physics, 2017, 122, .	1.1	10
70	Orientation dependence of the work function for metal nanocrystals. Journal of Chemical Physics, 2017, 147, 214301.	1.2	21
71	Hexagonal to monoclinic phase transformation in Eu <sub>2</sub> O <sub>3</sub> thin films grown on GaN (0001). Applied Physics Letters, 2017, 111, .	1.5	9
72			

#	ARTICLE	IF	CITATIONS
73	Integration of ferroelectric BaTiO <sub>3</sub> with Ge: The role of a SrTiO <sub>3</sub> buffer layer investigated using aberration-corrected STEM. Applied Physics Letters, 2017, 110, .	1.5	5
74	Multi-layered NiO <sub>y</sub> /NbO <sub>x</sub> /NiO <sub>y</sub> fast drift-free threshold switch with high Ion/Ioff ratio for selector application. Scientific Reports, 2017, 7, 4068.	1.6	59
75	ELNES spectrum unmixing and mapping for oxide/oxide interfaces.. Microscopy and Microanalysis, 2017, 23, 1588-1589.	0.2	0
76	Aberration-corrected STEM Imaging and EELS Mapping of BaTiO <sub>3</sub> /SrTiO <sub>3</sub> Interfacial Defects. Microscopy and Microanalysis, 2017, 23, 1598-1599.	0.2	0
77	ELNES analysis of $\hat{1}^3$ -Al <sub>2</sub> O <sub>3</sub> /SrTiO <sub>3</sub> and LaTiO <sub>3</sub> /SrTiO <sub>3</sub> interfaces. Microscopy and Microanalysis, 2016, 22, 1660-1661.	0.2	0
78	Characterization of a ferroelectric BaTiO <sub>3</sub> /SrTiO <sub>3</sub> heterostructure with interface-induced polarization. Microscopy and Microanalysis, 2016, 22, 1508-1509.	0.2	0
79	Monolithic integration of perovskites on Ge(001) by atomic layer deposition: a case study with SrHf <sub>x</sub> Ti <sub>1-x</sub> O <sub>3</sub> . MRS Communications, 2016, 6, 125-132.	0.8	13
80	Surface-hydrogen-induced metallization and rumpling in thin $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \langle \text{mml:mrow} \langle \text{mml:mi} \text{BaTi} \langle \text{mml:msub} \langle \text{mml:mi} \text{mathvariant="normal"} \rangle \text{O} \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ films. Physical Review B, 2016, 94, .	1.1	3
81	Mechanism of oxidation protection of the Si(001) surface by sub-monolayer Sr template. Journal of Applied Physics, 2016, 120, .	1.1	17
82	Structural characterization of niobium oxide thin films grown on SrTiO <sub>3</sub> (111) and (La,Sr)(Al,Ta)O <sub>3</sub> (111) substrates. Journal of Applied Physics, 2016, 120, 245302.	1.1	16
83	Anti-phase boundaries at the SrTiO <sub>3</sub> /Si(001) interface studied using aberration-corrected scanning transmission electron microscopy. Applied Physics Letters, 2016, 108, .	1.5	16
84	Spectral identification scheme for epitaxially grown single-phase niobium dioxide. Journal of Applied Physics, 2016, 119, .	1.1	11
85	Theoretical modeling and experimental observations of the atomic layer deposition of SrO using a cyclopentadienyl Sr precursor. Journal of Chemical Physics, 2016, 145, 064701.	1.2	3
86	Spin-polarized, orbital-selected hole gas at the EuO/Pt interface. Journal of Applied Physics, 2016, 119, .	1.1	6
87	Spectrum and phase mapping across the epitaxial $\hat{1}^3$ -Al <sub>2</sub> O <sub>3</sub> /SrTiO <sub>3</sub> interface. Applied Physics Letters, 2016, 108, .	1.5	9
88	Ferroelectric Oxides on Sili. Materials and Energy, 2016, , 403-454.	2.5	1
89	Theoretical study of negative optical mode splitting in LaAlO <sub>3</sub> . Physical Review B, 2016, 93, .	1.1	4
90	Contradictory nature of Co doping in ferroelectric BaTiO <sub>3</sub> . Physical Review B, 2016, 94, .	1.1	8

#	ARTICLE	IF	CITATIONS
91	A Low-Leakage Epitaxial High- $\hat{\nu}$ Gate Oxide for Germanium Metal-oxide Semiconductor Devices. ACS Applied Materials & Interfaces, 2016, 8, 5416-5423.	4.0	9
92	Final-state effect on x-ray photoelectron spectrum of nominally $d^{10}$ -doped transition metal oxides. Physical Review B, 2015, 92, .	1.1	29
93	Quench dynamics of Anderson impurity model using configuration interaction method. Physical Review B, 2015, 92, .	1.1	6
94	Early stages of the Schottky barrier formation in submonolayer Pt on $SrTiO_3(001)$ . Physical Review B, 2015, 92, .	1.1	4
95	Nature of the metal-insulator transition in $NbO_2$ . Physical Review B, 2015, 92, .	1.1	47
96	Atomic layer deposition of perovskite oxides and their epitaxial integration with Si, Ge, and other semiconductors. Applied Physics Reviews, 2015, 2, .	5.5	76
97	Quasi-two-dimensional electron gas at the interface of $\hat{\nu}$ - $Al_2O_3/SrTiO_3$ heterostructures grown by atomic layer deposition. Journal of Applied Physics, 2015, 118, .	1.1	30
98	Structure, thermodynamics, and crystallization of amorphous hafnia. Journal of Applied Physics, 2015, 118, .	1.1	12
99	Investigation of Co-Doped $BaTiO_3$ by Atomic-Resolution EELS. Microscopy and Microanalysis, 2015, 21, 2077-2078.	0.2	0
100	Oxygen Vacancies at the $\hat{\nu}$ - $Al_2O_3/STO$ Heterointerface Grown by Atomic Layer Deposition. Materials Research Society Symposia Proceedings, 2015, 1730, 14.	0.1	0
101	Characterization of Two-Dimensional Electron Gas at the $\gamma$ - $Al_2O_3/SrTiO_3$ Interface. Microscopy and Microanalysis, 2015, 21, 1309-1310.	0.2	0
102	Cross-Sectional Characterization of $SrTiO_3/Si(001)$ Interfaces using Aberration-Corrected STEM. Microscopy and Microanalysis, 2015, 21, 1305-1306.	0.2	0
103	Quantum confinement in transition metal oxide quantum wells. Applied Physics Letters, 2015, 106, .	1.5	17
104	Integrated films of transition metal oxides for information technology. Microelectronic Engineering, 2015, 147, 285-289.	1.1	12
105	Atomic layer deposition of crystalline $SrHfO_3$ directly on Ge (001) for high- $k$ dielectric applications. Journal of Applied Physics, 2015, 117, .	1.1	43
106	Optical properties of transition metal oxide quantum wells. Journal of Applied Physics, 2015, 117, .	1.1	12
107	Carrier density modulation in a germanium heterostructure by ferroelectric switching. Nature Communications, 2015, 6, 6067.	5.8	75
108	Hydroxyapatite: Vibrational spectra and monoclinic to hexagonal phase transition. Journal of Applied Physics, 2015, 117, 074701.	1.1	15

#	ARTICLE	IF	CITATIONS
109	Analysis of the Pockels effect in ferroelectric barium titanate thin films on Si(0 0 1). <i>Microelectronic Engineering</i> , 2015, 147, 215-218.	1.1	34
110	Localized states induced by an oxygen vacancy in rutile TiO <sub>2</sub> . <i>Journal of Applied Physics</i> , 2015, 117, .	1.1	34
111	Quasi-two-dimensional electron gas at the epitaxial alumina/SrTiO <sub>3</sub> interface: Control of oxygen vacancies. <i>Journal of Applied Physics</i> , 2015, 117, .	1.1	37
112	Switchable conductivity at the ferroelectric interface: Nonpolar oxides. <i>Physical Review B</i> , 2015, 91, .	1.1	78
113	A silicon-based photocathode for water reduction with an epitaxial SrTiO <sub>3</sub> protection layer and a nanostructured catalyst. <i>Nature Nanotechnology</i> , 2015, 10, 84-90.	15.6	353
114	Band alignment in visible-light photo-active CoO/SrTiO <sub>3</sub> (001) heterostructures. <i>Journal of Applied Physics</i> , 2014, 116, .	1.1	10
115	A Chemical Route to Monolithic Integration of Crystalline Oxides on Semiconductors. <i>Advanced Materials Interfaces</i> , 2014, 1, 1400081.	1.9	40
116	Integration of Functional Oxides with Semiconductors. , 2014, , .		69
117	Epitaxial <i>c</i> -axis oriented BaTiO <sub>3</sub> thin films on SrTiO <sub>3</sub> -buffered Si(001) by atomic layer deposition. <i>Applied Physics Letters</i> , 2014, 104, .	1.5	59
118	Electronic and optical properties of NbO <sub>2</sub> . <i>Journal of Applied Physics</i> , 2014, 116, .	1.1	67
119	Epitaxy of polar semiconductor Co <sub>3</sub> O <sub>4</sub> (110): Growth, structure, and characterization. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	27
120	Atomic and electronic structure of the ferroelectric BaTiO <sub>3</sub> /Ge(001) interface. <i>Applied Physics Letters</i> , 2014, 104, .	1.5	45
121	Band gap of epitaxial in-plane-dimerized single-phase NbO <sub>2</sub> films. <i>Applied Physics Letters</i> , 2014, 104, 092901.	1.5	40
122	Incorporation of La in epitaxial SrTiO <sub>3</sub> thin films grown by atomic layer deposition on SrTiO <sub>3</sub> -buffered Si (001) substrates. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	15
123	Oxygen and nitrogen diffusion in $\delta$ -hafnium from first principles. <i>Applied Physics Letters</i> , 2014, 104, .	1.5	9
124	Assessing hafnium on hafnia as an oxygen getter. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	37
125	Critical differences in the surface electronic structure of Ge(001) and Si(001): <i>Ab initio</i> theory and angle-resolved photoemission spectroscopy. <i>Physical Review B</i> , 2014, 89, .	1.1	31
126	Structural, optical, and electrical properties of strained La-doped SrTiO <sub>3</sub> films. <i>Journal of Applied Physics</i> , 2014, 116, .	1.1	53



#	ARTICLE	IF	CITATIONS
127	(Invited) Resistive Switching Characteristics and Controllable Quantized Conductance in Single-Crystal Anatase TiO <sub>2</sub> on Si (001). ECS Transactions, 2014, 64, 147-152.	0.3	1
128	Role of oxygen vacancies in room-temperature ferromagnetism in cobalt-substituted SrTiO <sub>3</sub> . Physical Review B, 2014, 90, .	2.9	16
129	Consequences of Oxygen-Vacancy Correlations at the Surface of SrTiO <sub>3</sub> . Physical Review Letters, 2014, 113, 157602.	2.9	16
130	Highly Controllable and Stable Quantized Conductance and Resistive Switching Mechanism in Single-Crystal TiO <sub>2</sub> Resistive Memory on Silicon. Nano Letters, 2014, 14, 4360-4367.	4.5	121
131	Monolithic integration of rare-earth oxides and semiconductors for on-silicon technology. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2014, 32, .	0.9	15
132	Efficient and stable orbital-searching algorithm for the configuration interaction method and its application to quantum impurity problems. Physical Review B, 2014, 90, .	1.1	5
133	Epitaxy: A Chemical Route to Monolithic Integration of Crystalline Oxides on Semiconductors (Adv.) Tj ETQq1 1 0.784314 rgBT /Overl	1.9	1
134	Growing SrTiO <sub>3</sub> on Si (001) by Molecular Beam Epitaxy. , 2014, , 115-158.		1
135	Critical Issues in Oxide-Semiconductor Heteroepitaxy. , 2014, , 25-44.		1
136	Integration of Functional Oxides on SrTiO <sub>3</sub> /Si Pseudo-Substrates. , 2014, , 159-203.		0
137	Switching of ferroelectric polarization in epitaxial BaTiO <sub>3</sub> films on silicon without a conducting bottom electrode. Nature Nanotechnology, 2013, 8, 748-754.	15.6	218
138	Bandgap engineering in perovskite oxides: Al-doped SrTiO <sub>3</sub> . Applied Physics Letters, 2013, 103, .	1.5	22
139	First principles study of hydroxyapatite surface. Journal of Chemical Physics, 2013, 139, 044714.	1.2	40
140	Electron Correlation in Oxygen Vacancy in SrTiO <sub>3</sub> . Physical Review Letters, 2013, 111, 217601.	2.9	104
141	Atomic layer deposition of photoactive CoO/SrTiO <sub>3</sub> and CoO/TiO <sub>2</sub> on Si(001) for visible light driven photoelectrochemical water oxidation. Journal of Applied Physics, 2013, 114, .	1.1	29
142	Epitaxial growth of LaAlO <sub>3</sub> on SrTiO <sub>3</sub> -buffered Si (001) substrates by atomic layer deposition. Journal of Crystal Growth, 2013, 363, 150-157.	0.7	31
143	Metal-induced charge transfer, structural distortion, and orbital order in SrTiO <sub>3</sub> thin films. Physical Review B, 2013, 87, .	1.1	12
144	Oxygen vacancy-mediated room-temperature ferromagnetism in insulating cobalt-substituted SrTiO <sub>3</sub> epitaxially integrated with silicon. Physical Review B, 2013, 87, .	1.1	26

#	ARTICLE	IF	CITATIONS
145	Wetting at the BaTiO <sub>3</sub> /Pt interface. Journal of Applied Physics, 2013, 113, 184102.	1.1	10
146	Epitaxial strontium titanate films grown by atomic layer deposition on SrTiO <sub>3</sub> -buffered Si(001) substrates. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2013, 31, .	0.9	44
147	Voltage-controlled ferromagnetism and magnetoresistance in LaCoO <sub>3</sub> /SrTiO <sub>3</sub> heterostructures. Journal of Applied Physics, 2013, 114, .	1.1	13
148	Preparation of a clean Ge(001) surface using oxygen plasma cleaning. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2013, 31, .	0.6	37
149	(Invited) Monolithic Integration of Oxides on Semiconductors. ECS Transactions, 2013, 54, 255-269.	0.3	17
150	Combined in-situ photoemission spectroscopy and density functional theory of the Sr Zintl template for oxide heteroepitaxy on Si(001). Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2013, 31, 04D107.	0.6	7
151	Schottky barrier at the AlN/metal junction. Journal of Applied Physics, 2013, 113, . Lattice distortion effects on topological phases in (LaNiO <sub>3</sub> ) <sub>1-x</sub> (Sr <sub>2-x</sub> TiO <sub>7</sub> ) <sub>x</sub> /Overlock 10 Tf 50 487 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow>	1.1	6
152	xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow>		

#	ARTICLE	IF	CITATIONS
163	Band engineering in silicide alloys. Physical Review B, 2012, 85, .	1.1	10
164	First-principles study of Zintl aluminide SrAl <sub>2</sub> . Physical Review B, 2012, 85, .	1.1	11
165	Electronic structure of oxygen vacancies in $\text{SrTiO}_3$ and $\text{LaAlO}_3$ . Physical Review B, 2012, 86, .	1.1	146
166	Growth of epitaxial oxides on silicon using atomic layer deposition: Crystallization and annealing of TiO <sub>2</sub> on SrTiO <sub>3</sub> -buffered Si(001). Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, 2012, 30, 04E111.	0.6	19
167	Orbital ordering under reduced symmetry in transition metal perovskites: Oxygen vacancy in $\text{SrTiO}_3$ . Physical Review B, 2012, 86, .	1.1	72
168	Orbital ordering under reduced symmetry in transition metal perovskites: Oxygen vacancy in $\text{SrTiO}_3$ . Physical Review B, 2012, 86, .	1.1	49
169	First-principles study of the biominerals hydroxyapatite. Physical Review B, 2011, 84, .	1.1	91
170	Work function engineering in silicides: Chlorine doping in NiSi. Journal of Applied Physics, 2011, 109, 083703.	1.1	7
172	Emerging physics of oxide heterostructures. Physica Status Solidi (B): Basic Research, 2011, 248, 2076-2081.	0.7	5
173	Advances and applications in the Fermi level pinning molecular dynamics formalism. Physica Status Solidi (B): Basic Research, 2011, 248, 1989-2007.	0.7	207
174	Strain-induced ferromagnetism in LaCoO <sub>3</sub> : Theory and growth on Si (100). Microelectronic Engineering, 2011, 88, 1444-1447.	1.1	15
175	First-principles study of polar LaAlO <sub>3</sub> (001) surface stabilization by point defects. Physical Review B, 2011, 84, .	1.1	34
176	Band alignment at the SiO <sub>2</sub> /HfO <sub>2</sub> interface: Group IIIA versus group IIIB metal dopants. Physical Review B, 2011, 84, .	1.1	19
177	Epitaxial integration of ferromagnetic correlated oxide LaCoO <sub>3</sub> with Si (100). Applied Physics Letters, 2011, 98, .	1.5	64
178	Formation of single-orientation epitaxial islands of TiSi <sub>2</sub> on Si(001) using Sr passivation. Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, 2011, 29, .	0.6	4
179	Resonant inelastic charge transfer in short alanine bridges. Physical Review B, 2010, 81, .	1.1	2
180	Spin-polarized two-dimensional electron gas through electrostatic doping in $\text{LaAlO}_3$ . Physical Review B, 2010, 82, .	1.1	27

#	ARTICLE	IF	CITATIONS
181	Hafnia: Energetics of thin films and nanoparticles. Journal of Applied Physics, 2010, 107, .	1.1	36
182	Interfacial magnetoelectric coupling in tricomponent superlattices. Physical Review B, 2010, 81, .	1.1	69
183	Theory of HfO <sub>2</sub> -Based High-k Dielectric Gate Stacks. , 2010, , 51-92.		1
184	Extended Frenkel pairs and band alignment at metal-oxide interfaces. Physical Review B, 2009, 79, .	1.1	31
185	Ab initio study of early stages of III-V epitaxy on high-index surfaces of group-IV semiconductors: In adsorption on Si(112). Physical Review B, 2009, 80, .	1.1	5
186	Absence of Critical Thickness in an Ultrathin Improper Ferroelectric Film. Physical Review Letters, 2009, 102, 107601.	2.9	70
187	Hafnia surface and high-k gate stacks. Materials Research Society Symposia Proceedings, 2009, 1155, 1.	0.1	0
188	Modeling complexity of a complex gate oxide. Microelectronic Engineering, 2009, 86, 1763-1766.	1.1	3
189	Magnetoelectric coupling and electric control of magnetization in ferromagnet/ferroelectric/normal-metal superlattices. Physical Review B, 2009, 80, .	1.1	92
190	Monoclinic to tetragonal transformations in hafnia and zirconia: A combined calorimetric and density functional study. Physical Review B, 2009, 80, .	1.1	109
191	Theory of the Sr-induced reconstruction of the Si (001) surface. Journal of Applied Physics, 2008, 103, 103710.	1.1	28
192	Ab initio study of atomic structure and Schottky barrier height at the $\text{GaAs}/\text{Ni}$ interface. Physical Review B, 2008, 77, .	1.1	11
193	Electronic, optical, and surface properties of PtSi thin films. Physical Review B, 2008, 78, .	1.1	33
194	Effects of aluminum incorporation on band alignment at the $\text{Si}/\text{O}_2/\text{HfO}_2/\text{Si}$ interface.	1.1	38
195	Combined experimental and theoretical study of thin hafnia films. Physical Review B, 2008, 78, .	1.1	32
196	Charge origin and localization at the $\text{Si}/\text{SiO}_2/\text{SrTiO}_3$ interface. Physical Review B, 2008, 78, .	1.1	189
197	Density Functional Theory of High-k Dielectric Gate Stacks. Nanostructure Science and Technology, 2008, , 171-190.	0.1	1
198	Electronic structure, elastic properties, surface energies, and work functions of NiGe and PtGe within the framework of density-functional theory for various surface terminations. Physical Review B, 2007, 75, .	1.1	23

#	ARTICLE	IF	CITATIONS
199	Fermi level pinning by defects in HfO <sub>2</sub> -metal gate stacks. Applied Physics Letters, 2007, 91, .	1.5	144
200	Spin-filtering multiferroic-semiconductor heterojunctions. Applied Physics Letters, 2007, 91, 202910.	1.5	10
201	Theoretical study of the insulator/insulator interface: Band alignment at the SiO <sub>2</sub> /HfO <sub>2</sub> junction. Physical Review B, 2007, 75, .	1.1	99
202	Inelastic resonant tunneling in $C_{60}$ molecular junctions. Physical Review B, 2007, 75, .	1.1	57
203	Density functional theory of high-k dielectric gate stacks. Microelectronics Reliability, 2007, 47, 686-693.	0.9	7
204	Thermodynamic stability and band alignment at a metal/high-k dielectric interface. Physical Review B, 2006, 74, .	1.1	60
205	Theoretical Investigation of the Band Alignment at the LaAlO <sub>3</sub> /SrTiO <sub>3</sub> Interface. Materials Research Society Symposia Proceedings, 2006, 966, 1.	0.1	1
206	Theoretical investigation of Pt/Si surface energies and work functions. Physical Review B, 2006, 73, .	1.1	41
207	Ab initio calculations of surface phase diagrams of silica polymorphs. Physical Review B, 2005, 71, .	1.1	17
208	Complex band structure and the band alignment problem at the Si/high-k dielectric interface. Physical Review B, 2005, 71, .	1.1	73
209	Difficulties of the microscopic theory of leakage current through ultra-thin oxide barriers: point defects. Physica Status Solidi (B): Basic Research, 2003, 239, 48-58.	0.7	28
210	Atomistic calculation of leakage current through ultra-thin metal-oxide barriers. Microelectronic Engineering, 2003, 69, 130-137.	1.1	6
211	Atomic and electronic structure of the Si/SrTiO <sub>3</sub> interface. Physical Review B, 2003, 68, .	1.1	129
212	The interface of epitaxial SrTiO <sub>3</sub> on silicon: in situ and ex situ studies. Applied Physics Letters, 2003, 82, 203-205.	1.5	93
213	Two-dimensional growth of high-quality strontium titanate thin films on Si. Journal of Applied Physics, 2003, 93, 4521-4525.	1.1	143
214	Displacement of surface arsenic atoms by insertion of oxygen atoms into As/Ga backbonds. Journal of Chemical Physics, 2003, 119, 9191-9198.	1.2	10
215	Steps on the (001) SrTiO <sub>3</sub> surface. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2002, 20, 1664.	1.6	20
216	Title is missing!. Journal of Computational Electronics, 2002, 1, 179-183.	1.3	7

#	ARTICLE	IF	CITATIONS
217	Theoretical Investigation of Ultrathin Gate Dielectrics. VLSI Design, 2001, 13, 135-143.	0.5	4
218	Theory of zeolite supralattices: Se in zeolite Linde type A. Journal of Physics Condensed Matter, 2001, 13, 10433-10457.	0.7	14
219	Further developments in the local-orbital density-functional-theory tight-binding method. Physical Review B, 2001, 64, .	1.1	232
220	Theoretical and experimental investigation of ultrathin oxynitrides and the role of nitrogen at the Si <sup>2</sup> /SiO <sub>2</sub> interface. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2000, 18, 2388.	1.6	30
221	Theoretical investigation of the initial reaction of the NO decomposition on the Si (100) (2 $\times$ 1) reconstructed surface. Journal of Chemical Physics, 2000, 113, 8237-8248.	1.2	10
222	Optical properties of bulk and thin-film SrTiO <sub>3</sub> on Si and Pt. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2000, 18, 2242.	1.6	106
223	Theoretical study of graphitic analogues of simple semiconductors. Modelling and Simulation in Materials Science and Engineering, 1999, 7, 929-938.	0.8	13
224	Growth Study and Theoretical Investigation of the Ultrathin Oxide/Si Heterojunction. Physical Review Letters, 1999, 83, 2038-2041.	2.9	97
225	The application of approximate density functionals to complex systems. International Journal of Quantum Chemistry, 1998, 69, 327-340.	1.0	46
226	Theoretical studies of Se clusters in zeolite LTA. Microporous and Mesoporous Materials, 1998, 21, 347-351.	2.2	4
227	Temperature-dependent <sup>23</sup> Na Knight shifts and sharply peaked structure in the electronic densities of states of Na-Si clathrates. Physical Review B, 1998, 57, 4172-4179.	1.1	44
228	Electronic structure of black sodalite. Physical Review B, 1998, 57, 15129-15139.	1.1	33
229	Model simulations of zeolite supralattices: Semiconductor Si clusters in sodalite. Physical Review B, 1997, 56, 10497-10504.	1.1	15
230	Structural Band Gap Engineering. Materials Research Society Symposia Proceedings, 1997, 486, 355.	0.1	3
231	Theoretical predictions of expanded-volume phases of GaAs. Physical Review B, 1997, 55, 6904-6913.	1.1	22
232	Recent Developments in the Theory of Supralattices. Chemistry of Materials, 1996, 8, 1793-1806.	3.2	12
233	Clusters stuffed inside frameworks: Electronic structure theory. Journal of Computer-Aided Materials Design, 1996, 3, 128-138.	0.7	3
234	Expanded-volume phases of silicon: Zeolites without oxygen. Physical Review B, 1996, 53, 11288-11291.	1.1	42

#	ARTICLE	IF	CITATIONS
235	Electronic structure approach for complex silicas. <i>Physical Review B</i> , 1995, 52, 1618-1630.	1.1	349
236	Chemisorption of In and Al on GaAs(110). <i>Journal of Applied Physics</i> , 1994, 76, 2918-2923.	1.1	0
237	Wide-band-gap Si in open fourfold-coordinated clathrate structures. <i>Physical Review B</i> , 1994, 49, 8048-8053.	1.1	258
238	Theoretical investigation of alkali-metal doping in Si clathrates. <i>Physical Review B</i> , 1994, 50, 17001-17008.	1.1	88
239	Energetics and electronic structure of the hypothetical cubic zincblende form of GeC. <i>Modelling and Simulation in Materials Science and Engineering</i> , 1993, 1, 741-754.	0.8	47
240	Theoretical investigation of random Si-C alloys. <i>Physical Review B</i> , 1993, 48, 2207-2214.	1.1	150