Alexander L Shluger

List of Publications by Year
in descending order

276 papers	13,167 citations	24978 57 h-index	31759 101 g-index
277 all docs	277 docs citations	277 times ranked	10195 citing authors

#	Article	IF	Citations
1	Vacancy and interstitial defects in hafnia. Physical Review B, 2002, 65, .	1.1	560
2	Recommended Methods to Study Resistive Switching Devices. Advanced Electronic Materials, 2019, 5, 1800143.	2.6	452
3	Theories of scanning probe microscopes at the atomic scale. Reviews of Modern Physics, 2003, 75, 1287-1331.	16.4	432
4	Relative energies of surface and defect states: ab initio calculations for the MgO (001) surface. Surface Science, 2000, 450, 153-170.	0.8	336
5	Structure and electrical levels of point defects in monoclinic zirconia. Physical Review B, 2001, 64, .	1.1	307
6	Negative oxygen vacancies in HfO2 as charge traps in high-k stacks. Applied Physics Letters, 2006, 89, 082908.	1.5	295
7	Crystallographic phase transition and high-T_csuperconductivity in LaFeAsO:F. Superconductor Science and Technology, 2008, 21, 125028.	1.8	230
8	Atom-resolved imaging of ordered defect superstructures at individual grain boundaries. Nature, 2011, 479, 380-383.	13.7	219
9	Recent Trends in Surface Characterization and Chemistry with Highâ€Resolution Scanning Force Methods. Advanced Materials, 2011, 23, 477-501.	11.1	214
10	Atomically resolved edges and kinks of NaCl islands on Cu(111): Experiment and theory. Physical Review B, 2000, 62, 2074-2084.	1.1	213
11	Theoretical study of the stabilization of cubic-phaseZrO2by impurities. Physical Review B, 1994, 49, 11560-11571.	1.1	202
12	Spectroscopic properties of oxygen vacancies in monoclinicHfO2calculated with periodic and embedded cluster density functional theory. Physical Review B, 2007, 75, .	1.1	196
13	Electron Localization and a Confined Electron Gas in Nanoporous Inorganic Electrides. Physical Review Letters, 2003, 91, 126401.	2.9	192
14	Trapping, self-trapping and the polaron family. Journal of Physics Condensed Matter, 2007, 19, 255208.	0.7	182
15	The interaction of oxygen vacancies with grain boundaries in monoclinic HfO2. Applied Physics Letters, 2009, 95, .	1.5	178
16	Spectroscopy of low-coordinated surface sites:â€,Theoretical study of MgO. Physical Review B, 1999, 59, 2417-2430.	1.1	164
17	Unambiguous Interpretation of Atomically Resolved Force Microscopy Images of an Insulator. Physical Review Letters, 2001, 86, 2373-2376.	2.9	156
18	Silicon Oxide (SiO_x): A Promising Material for Resistance Switching?. Advanced Materials, 2018, 30, e1801187.	11.1	156

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19	Small polarons in real crystals: concepts and problems. Journal of Physics Condensed Matter, 1993, 5, 3049-3086.	0.7	151
20	Mechanism of Interstitial Oxygen Diffusion in Hafnia. Physical Review Letters, 2002, 89, 225901.	2.9	146
21	Electronic Properties of Structural Defects at the MgO (001) Surface. Journal of Physical Chemistry B, 2002, 106, 2269-2276.	1.2	140
22	Model of noncontact scanning force microscopy on ionic surfaces. Physical Review B, 1999, 59, 2436-2448.	1.1	134
23	Paramagnetic Defect Centers at the MgO Surface. An Alternative Model to Oxygen Vacancies. Journal of the American Chemical Society, 2003, 125, 738-747.	6.6	134
24	Theoretical Prediction of Intrinsic Self-Trapping of Electrons and Holes in Monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2007, 99, 155504.	2.9	133
25	Asymmetry and long-range character of lattice deformation by neutral oxygen vacancy in Î±-quartz. Physical Review B, 2002, 66, .	1.1	131
26	Hydrogen Cycle on CeO₂ (111) Surfaces:â€‰ Density Functional Theory Calculations. Journal of Physical Chemistry C, 2007, 111, 15337-15341.	1.5	131
27	Electron-trapping polycrystalline materials with negative electron affinity. Nature Materials, 2008, 7, 859-862.	13.3	122
28	From Insulator to Electride:Â A Theoretical Model of Nanoporous Oxide 12CaOÂ·7Al2O3. Journal of the American Chemical Society, 2007, 129, 942-951.	6.6	115
29	Hydride ions in oxide hosts hidden by hydroxide ions. Nature Communications, 2014, 5, 3515.	5.8	108
30	Roadmap on multiscale materials modeling. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 043001.	0.8	100
31	Nature of intrinsic and extrinsic electron trapping in SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 89, .	1.1	96
32	Contrast formation in atomic resolution scanning force microscopy on CaF2(111): experiment and theory. Journal of Physics Condensed Matter, 2001, 13, 2061-2079.	0.7	93
33	A microscopic mechanism of dielectric breakdown in SiO2 films: An insight from multi-scale modeling. Journal of Applied Physics, 2017, 121, .	1.1	93
34	Modeling charge self-trapping in wide-gap dielectrics: Localization problem in local density functionals. Physical Review B, 2003, 67, .	1.1	87
35	Application of molecular models to electronic structure calculations of defects in oxide crystals. I. Parametrization of the modified INDO method. Theoretica Chimica Acta, 1985, 66, 355-363.	0.9	85
36	Hydrogen-Induced Rupture of Strained Siâ”€O Bonds in Amorphous Silicon Dioxide. Physical Review Letters, 2015, 114, 115503.	2.9	82

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37	Role of tip structure and surface relaxation in atomic resolution dynamic force microscopy:CaF2(111)as a reference surface. Physical Review B, 2002, 66, .	1.1	79
38	Mg clusters on MgO surfaces: study of the nucleation mechanism with MIES and ab initio calculations. Faraday Discussions, 1999, 114, 173-194.	1.6	77
39	Positive and Negative Oxygen Vacancies in Amorphous Silica. ECS Transactions, 2009, 19, 3-17.	0.3	77
40	Theoretical and experimental investigation of force imaging at the atomic scale on alkali halide crystals. Physical Review B, 1994, 49, 4915-4930.	1.1	70
41	Atomic and ionic processes of silicon oxidation. Physical Review B, 2001, 63, .	1.1	70
42	Structure and properties of defects in amorphous silica: new insights from embedded cluster calculations. Journal of Physics Condensed Matter, 2005, 17, S2115-S2140.	0.7	69
43	The origin of negative charging in amorphous Al₂O₃ films: the role of native defects. Nanotechnology, 2019, 30, 205201.	1.3	68
44	Electron-Injection-Assisted Generation of Oxygen Vacancies in Monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>HfO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m Physical Review Applied, 2015, 4, .	1.5	67
45	Atomistic theory of the interaction between AFM tips and ionic surfaces. Journal of Physics Condensed Matter, 1994, 6, 1825-1846.	0.7	66
46	Electron trapping at neutral divacancy sites on the MgO surface. Journal of Chemical Physics, 2002, 117, 2844-2851.	1.2	63
47	Quantum-chemical simulation of impurity-induced trapping of a hole: (Li)0centre in MgO. Journal of Physics C: Solid State Physics, 1986, 19, 4183-4199.	1.5	62
48	The model of a triplet self-trapped exciton in crystalline SiO2. Journal of Physics C: Solid State Physics, 1988, 21, L431-L434.	1.5	62
49	Ionic and electronic processes at ionic surfaces induced by atomic-force-microscope tips. Physical Review B, 1997, 56, 15332-15344.	1.1	62
50	Wavelength selective excitation of surface oxygen anions on highly dispersed MgO. Journal of Chemical Physics, 2002, 116, 1707-1712.	1.2	62
51	Theoretical models of hydrogen-induced defects in amorphous silicon dioxide. Physical Review B, 2015, 92, .	1.1	62
52	Nanoporous Crystal 12CaOÂ·7Al2O3:Â A Playground for Studies of Ultraviolet Optical Absorption of Negative Ions. Journal of Physical Chemistry B, 2007, 111, 1946-1956.	1.2	61
53	Shear dynamics of nanoconfined ionic liquids. Physical Chemistry Chemical Physics, 2014, 16, 8247-8256.	1.3	60
54	A relationship between three-dimensional surface hydration structures and force distribution measured by atomic force microscopy. Nanoscale, 2016, 8, 7334-7342.	2.8	59

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55	Theoretical studies of atomic emission and defect formation by electronic excitation at the (100) surface of NaCl. Physical Review B, 1993, 47, 10760-10768.	1.1	58
56	Functionalized Truxenes: Adsorption and Diffusion of Single Molecules on the KBr(001) Surface. ACS Nano, 2010, 4, 3429-3439.	7.3	58
57	Model of self-trapped excitons in alkali halides. Physical Review B, 1993, 47, 6226-6240.	1.1	57
58	Intramolecular Dipole Coupling and Depolarization in Selfâ€Assembled Monolayers. Advanced Functional Materials, 2008, 18, 2228-2236.	7.8	57
59	Oxygen ion conduction in 12CaOÂ·7Al2O3: O2â˜' conduction mechanism and possibility of Oâ˜' fast conductionâ˜†. Solid State Ionics, 2009, 180, 550-555.	1.3	57
60	Relation between image charge and potential alignment corrections for charged defects in periodic boundary conditions. Journal of Chemical Physics, 2018, 149, 024103.	1.2	57
61	Role of disorder in incorporation energies of oxygen atoms in amorphous silica. Physical Review B, 2001, 63, .	1.1	56
62	Chemical Resolution at Ionic Crystal Surfaces Using Dynamic Atomic Force Microscopy with Metallic Tips. Physical Review Letters, 2011, 106, 216102.	2.9	56
63	Two-Dimensional Polaronic Behavior in the Binary Oxides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>m</mml:mi><mml:mtext mathvariant="normal">â˜'</mml:mtext><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>m</mml:mi><mml:mtext mathvariant="normal">â˜'</mml:mtext><mml:msub><mml:mi>ZrO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 116403.	2.9	56
64	Structural dynamics of laser-irradiated gold nanofilms. Physical Review B, 2013, 88, .	1.1	56
65	Hydride Ion as a Two-Electron Donor in a Nanoporous Crystalline Semiconductor 12CaOÂ·7Al2O3. Journal of Physical Chemistry B, 2005, 109, 23836-23842.	1.2	55
66	Inside Powders:Â A Theoretical Model of Interfaces between MgO Nanocrystallites. Journal of the American Chemical Society, 2007, 129, 8600-8608.	6.6	55
67	Intrinsic charge trapping in amorphous oxide films: status and challenges. Journal of Physics Condensed Matter, 2018, 30, 233001.	0.7	55
68	Theoretical study of Na-atom emission from NaCl (100) surfaces. Physical Review B, 1994, 49, 11364-11373.	1.1	54
69	Energies and Dynamics of Photoinduced Electron and Hole Processes on MgO Powders. Journal of Physical Chemistry B, 2002, 106, 12478-12482.	1.2	54
70	Role of water in atomic resolution AFM in solutions. Physical Chemistry Chemical Physics, 2011, 13, 12584.	1.3	54
71	Physics of Nanomechanical Biosensing on Cantilever Arrays. Advanced Materials, 2008, 20, 3848-3853.	11.1	53
72	Effect of Molecular and Lattice Structure on Hydrogen Transfer in Molecular Crystals of Diamino-dinitroethylene and Triamino-trinitrobenzene. Journal of Physical Chemistry A, 2008, 112, 4496-4500.	1.1	53

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73	Self-trapping holes and excitons in the bulk and on the (100) surfaces of MgO. Journal of Physics Condensed Matter, 1991, 3, 8027-8036.	0.7	52
74	Enhanced N₂ Dissociation on Ru-Loaded Inorganic Electride. Journal of the American Chemical Society, 2014, 136, 2216-2219.	6.6	52
75	Nanoscale Transformations in Metastable, Amorphous, Siliconâ€Rich Silica. Advanced Materials, 2016, 28, 7486-7493.	11.1	52
76	Simple Model for DNA Adsorption onto a Mica Surface in 1:1 and 2:1 Electrolyte Solutions. Langmuir, 2006, 22, 7678-7688.	1.6	51
77	Shaping the Morphology of Gold Nanoparticles by CO Adsorption. Journal of Physical Chemistry C, 2007, 111, 18848-18852.	1.5	51
78	Interaction of Organic Molecules with the TiO2(110) Surface:Â Ab Inito Calculations and Classical Force Fields. Journal of Physical Chemistry B, 2006, 110, 4853-4862.	1.2	50
79	Effect of charged and excited states on the decomposition of 1,1-diamino-2,2-dinitroethylene molecules. Journal of Chemical Physics, 2007, 126, 234711.	1.2	50
80	A mechanism for Frenkel defect creation in amorphous SiO₂facilitated by electron injection. Nanotechnology, 2016, 27, 505207.	1.3	50
81	Self-lubrication in scanning-force-microscope image formation on ionic surfaces. Physical Review B, 1997, 56, 12482-12489.	1.1	49
82	Optical and EPR properties of point defects at a crystalline silica surface:Ab initioembedded-cluster calculations. Physical Review B, 2007, 75, .	1.1	49
83	Calibration of embedded-cluster method for defect studies in amorphous silica. Physical Review B, 2004, 69, .	1.1	48
84	Laser Control of Desorption through Selective Surface Excitation. Journal of Physical Chemistry B, 2005, 109, 19563-19578.	1.2	48
85	Diffusion and aggregation of oxygen vacancies in amorphous silica. Journal of Physics Condensed Matter, 2017, 29, 245701.	0.7	48
86	Mechanism of Contrast Formation in Atomic Force Microscopy in Water. Physical Review Letters, 2010, 105, 196101.	2.9	47
87	Origin of the Asymmetry in the Magnitude of the Statistical Variability of n- and p-Channel Poly-Si Gate Bulk MOSFETs. IEEE Electron Device Letters, 2008, 29, 913-915.	2.2	46
88	Nonthermal solid-to-solid phase transitions in tungsten. Physical Review B, 2014, 90, .	1.1	46
89	Electron Trapping at Point Defects on Hydroxylated Silica Surfaces. Physical Review Letters, 2007, 99, 136801.	2.9	45
90	Effect of Protons on the Optical Properties of Oxide Nanostructures. Journal of the American Chemical Society, 2007, 129, 12491-12496.	6.6	45

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91	Mechanism of laser assisted field evaporation from insulating oxides. Ultramicroscopy, 2011, 111, 567-570.	0.8	45
92	Identification of intrinsic electron trapping sites in bulk amorphous silica from ab initio calculations. Microelectronic Engineering, 2013, 109, 68-71.	1.1	44
93	Dynamical simulations of an electronically induced solid-solid phase transformation in tungsten. Physical Review B, 2015, 92, .	1.1	44
94	Intrinsic electron traps in atomic-layer deposited HfO2 insulators. Applied Physics Letters, 2016, 108, .	1.5	44
95	Deep electron and hole polarons and bipolarons in amorphous oxide. Physical Review B, 2016, 94, .	1.1	44
96	Modelling of oxygen vacancy aggregates in monoclinic HfO₂: can they contribute to conductive filament formation?. Journal of Physics Condensed Matter, 2015, 27, 415401.	0.7	43
97	Role of hydrogen in volatile behaviour of defects in SiO ₂ -based electronic devices. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2016, 472, 20160009.	1.0	43
98	Photoluminescence from Au ion-implanted nanoporous single-crystal12CaOâ˜7Al2O3. Physical Review B, 2006, 73, .	1.1	42
99	Intrinsic Resistance Switching in Amorphous Silicon Suboxides: The Role of Columnar Microstructure. Scientific Reports, 2017, 7, 9274.	1.6	41
100	Mechanisms of Oxygen Vacancy Aggregation in SiO2 and HfO2. Frontiers in Physics, 2019, 7, .	1.0	41
101	Two types of self-trapped excitons in alkali halide crystals. Physical Review B, 1991, 44, 1499-1508.	1.1	40
102	Modeling disorder in amorphous silica with embedded clusters:â€ƒThe peroxy bridge defect center. Physical Review B, 2001, 64, .	1.1	39
103	Controlled Manipulation of Atoms in Insulating Surfaces with the Virtual Atomic Force Microscope. Physical Review Letters, 2007, 98, 028101.	2.9	39
104	Structure and properties of intrinsic and extrinsic defects in black phosphorus. Nanoscale, 2018, 10, 19536-19546.	2.8	38
105	Electronic structure of excited states at low-coordinated surface sites of MgO. Surface Science, 1999, 421, L157-L165.	0.8	37
106	Oxygen vacancies in cubic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> studied by anab initioembedded cluster method. Physical Review B, 2008, 78, .	1.1	37
107	The effect of van der Waals interactions on the properties of intrinsic defects in graphite. Carbon, 2010, 48, 4145-4161.	5.4	37
108	Dipoleâ"Dipole Interactions and the Structure of Self-Assembled Monolayers. Journal of Physical Chemistry B, 2007, 111, 4019-4025.	1.2	36

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109	Electron and hole trapping in polycrystalline metal oxide materials. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 2043-2053.	1.0	36
110	Determination of transient atomic structure of laser-excited materials from time-resolved diffraction data. Applied Physics Letters, 2013, 103, .	1.5	36
111	Using Metallic Noncontact Atomic Force Microscope Tips for Imaging Insulators and Polar Molecules: Tip Characterization and Imaging Mechanisms. ACS Nano, 2014, 8, 5339-5351.	7.3	36
112	One-center trapping of the holes in alkali halide crystals. Physical Review B, 1996, 54, 962-969.	1.1	35
113	Selective laser desorption of ionic surfaces: Resonant surface excitation of KBr. Journal of Chemical Physics, 2001, 115, 9463-9472.	1.2	35
114	Unambiguous Determination of the Adsorption Geometry of a Metalâ^'Organic Complex on a Bulk Insulator. Nano Letters, 2010, 10, 2965-2971.	4.5	35
115	Simulation of defect processes: experiences with the self-trapped exciton. Modelling and Simulation in Materials Science and Engineering, 1993, 1, 673-692.	0.8	34
116	Theoretical simulation of localized holes in MgO. Journal of Physics Condensed Matter, 1992, 4, 5711-5722.	0.7	33
117	Embedded cluster calculations of metal complex impurity defects: properties of the iron cyanide in NaCl. Journal of Physics Condensed Matter, 2000, 12, 8257-8266.	0.7	33
118	Lateral and friction forces originating during force microscope scanning of ionic surfaces. Surface Science, 1995, 343, 273-287.	0.8	32
119	Towards chemical identification in atomic-resolution noncontact AFM imaging with silicon tips. Physical Review B, 2003, 68, .	1.1	32
120	Structure and diffusion of intrinsic defects, adsorbed hydrogen, and water molecules at the surface of alkali-earth fluorides calculated using density functional theory. Physical Review B, 2009, 80, .	1.1	32
121	Calculation of adiabatic barriers for cation diffusion in Li2O and LiCl crystals. Modelling and Simulation in Materials Science and Engineering, 1992, 1, 29-38.	0.8	31
122	Laser-induced reactions in crystals:â€ƒFemtosecond pump-probe spectroscopy andab initiocalculations of self-trapped excitons and holes in KBr. Physical Review B, 2000, 61, 5392-5402.	1.1	31
123	F and F⁺ Centers on MgO/Ag(100) or MgO/Mo(100) Ultrathin Films:â€‰ Are They Stable?. Journal of Physical Chemistry C, 2008, 112, 3857-3865.	1.5	31
124	Intrinsic electron trapping in amorphous oxide. Nanotechnology, 2018, 29, 125703.	1.3	31
125	Reactivity of (H+)(eâ^') color centers at the MgO surface: formation of O2â^' and N2â^' radical anions. Surface Science, 2003, 542, 293-306.	0.8	30
126	Determination of surface exciton energies by velocity resolved atomic desorption. Surface Science, 2004, 564, 62-70.	0.8	30

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127	Interactions of hydrogen with amorphous hafnium oxide. Physical Review B, 2017, 95, .	1.1	30
128	Contrast mechanism in non-contact SFM imaging of ionic surfaces. Applied Surface Science, 1999, 140, 327-332.	3.1	29
129	Measuring Site-Specific Clusterâ^'Surface Bond Formation. Journal of the American Chemical Society, 2005, 127, 17863-17866.	6.6	29
130	Manipulation of defects on oxide surfaces via barrier reduction induced by atomic force microscope tips. Physical Review B, 2006, 73, .	1.1	29
131	Multiscale model of the manipulation of single atoms on insulating surfaces using an atomic force microscope tip. Physical Review B, 2007, 76, .	1.1	29
132	Siâ€“SiO₂ interface bandâ€gap transition â€“ effects on MOS inversion layer. Physica Status Solidi (A) Applications and Materials Science, 2008, 205, 1290-1295.	0.8	29
133	The behaviour of oxygen at metal electrodes in HfO2 based resistive switching devices. Microelectronic Engineering, 2013, 109, 346-350.	1.1	29
134	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mi>b</mml:mi></mml:mrow></mml:ma <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>i</mml:mi><mml:mi>n</mml:mi><mml:mi>i</mml:mi><m treatment of silicon-hydrogen bond rupture at <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Si</mml:mi><mml:mo>/</mml:mo><mml:mi	1.1	29
135	Interaction of Silicon Dangling Bonds with Insulating Surfaces. Physical Review Letters, 2004, 92, 036101.	2.9	28
136	Effect of electric field on migration of defects in oxides: Vacancies and interstitials in bulk MgO. Physical Review B, 2018, 98, .	1.1	28
137	Theoretical modeling of charge trapping in crystalline and amorphous Al₂O₃. Journal of Physics Condensed Matter, 2017, 29, 314005.	0.7	27
138	First principles calculations of optical properties for oxygen vacancies in binary metal oxides. Journal of Chemical Physics, 2019, 150, 044702.	1.2	27
139	Optical transitions of theHcenters in alkali halides. Physical Review B, 1995, 52, 4017-4028.	1.1	26
140	Models of image contrast in scanning force microscopy on insulators. Journal of Physics Condensed Matter, 1999, 11, R295-R322.	0.7	26
141	Modelling atomic scale manipulation with the non-contact atomic force microscope. Nanotechnology, 2006, 17, 5866-5874.	1.3	26
142	Dynamical processes at oxide surfaces studied with the virtual atomic force microscope. Physical Review B, 2007, 76, .	1.1	26
143	Hole Trapping at Surfaces of m-ZrO₂ and m-HfO₂ Nanocrystals. Journal of Physical Chemistry C, 2012, 116, 25888-25897.	1.5	26
144	Properties of intrinsic point defects and dimers in hexagonal boron nitride. Journal of Physics Condensed Matter, 2020, 32, 055706.	0.7	26

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145	Site-specific laser modification of MgO nanoclusters: Towards atomic-scale surface structuring. Physical Review B, 2006, 74, .	1.1	24
146	Electron correlation in the self-trapped hole and exciton in the NaCl crystal. Physical Review B, 1995, 52, 6254-6264.	1.1	23
147	Bonding of Methyl Phosphonate to TiO₂(110). Journal of Physical Chemistry C, 2010, 114, 16983-16988.	1.5	23
148	Models of triplet self-trapped excitons in SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, HfO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, and HfSiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	23
149	Effects of Oxide Roughness at Metal Oxide Interface: MgO on Ag(001). Journal of Physical Chemistry C, 2013, 117, 5075-5083.	1.5	23
150	Semiempirical Calculations of Defect Properties in LiF Crystal. Physica Status Solidi (B): Basic Research, 1981, 108, 673-681.	0.7	22
151	The semiempirical approach to electronic structure of ionic crystal surface. Journal of Physics C: Solid State Physics, 1982, 15, 847-861.	1.5	22
152	Semiempirical Calculations of Defect Properties in LiF Crystal. II. Electron and Hole Centres and Their Recombination. Physica Status Solidi (B): Basic Research, 1982, 109, 75-81.	0.7	22
153	Theoretical simulation of VK-centre migration in KCl. I. A quantum-chemical study. Journal of Physics Condensed Matter, 1992, 4, 7417-7428.	0.7	22
154	Properties of small clusters at ionic surfaces: (NaCl)nclusters (n=1â€“48) at the (100) MgO surface. Physical Review B, 1995, 51, 13631-13644.	1.1	22
155	Probing Organic Layers on the TiO2(110) Surface. Journal of Physical Chemistry B, 2005, 109, 4554-4560.	1.2	22
156	Energy and site selectivity in O-atom photodesorption from nanostructured MgO. Surface Science, 2008, 602, 1968-1973.	0.8	22
157	Structure and properties of oxygen centers in CaF<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>crystals fromab initioembedded cluster calculations. Physical Review B, 2011, 84, .	1.1	22
158	Calculating the Entropy Loss on Adsorption of Organic Molecules at Insulating Surfaces. Journal of Physical Chemistry C, 2016, 120, 3913-3921.	1.5	22
159	Making amorphous ZnO: Theoretical predictions of its structure and stability. Physical Review B, 2019, 99, .	1.1	22
160	Dielectric breakdown in HfO2 dielectrics: Using multiscale modeling to identify the critical physical processes involved in oxide degradation. Journal of Applied Physics, 2022, 131, .	1.1	21
161	A new model for the self-trapped exciton in alkali halides. Journal of Physics Condensed Matter, 1991, 3, 3125-3128.	0.7	20
162	(100) GaP surface charges, potentials, and stoichiometry; a quantum-chemical study. Journal of Physics Condensed Matter, 1994, 6, 4255-4268.	0.7	20

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163	Thermal fluctuations, localization, and self-trapping in a polar crystal: Combined shell-model molecular dynamics and quantum chemical approach. Physical Review B, 2001, 64, .	1.1	20
164	Quantitative modelling in scanning force microscopy on insulators. Applied Surface Science, 2002, 188, 306-318.	3.1	20
165	Polaron-like Charge Trapping in Oxygen Deficient and Disordered HfO2: Theoretical Insight. ECS Transactions, 2006, 3, 277-290.	0.3	20
166	Building Blocks for Molecular Devices:â€‰Organic Molecules on the MgO (001) Surface. Journal of Physical Chemistry C, 2007, 111, 15375-15381.	1.5	20
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