Peter Sushko

List of Publications by Year in Descending Order

182 papers	7,826 citations	43 h-index	84 g-index
191 ext. papers	8,558 ext. citations	6.1 avg, IF	5.73 L-index

#	Paper	IF	Citations
182	Effect of loading path on grain misorientation and geometrically necessary dislocation density in polycrystalline aluminum under reciprocating shear. *Computational Materials Science*, **2022**, 205, 111221	3.2	0
181	An Approach for the Microstructure-Sensitive Simulation of Shear-Induced Deformation and Recrystallization in Al Si Alloys. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2022**, 53, 1450	2.3	
180	Formation and dissociation of shear-induced high-energy dislocations: insight from molecular dynamics simulations. *Modelling and Simulation in Materials Science and Engineering*, **2022**, 30, 025012	2	0
179	Extended Shear Deformation of the Immiscible Cu-Nb Alloy Resulting in Nanostructuring and Oxygen Ingress with Enhancement in Mechanical Properties.. *ACS Omega*, **2022**, 7, 13721-13736	3.9	1
178	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. *Chemical Reviews*, **2021**, 121, 4962-4998	68.1	12
177	Shear-Deformation-Induced Modification of Defect Structures and Hierarchical Microstructures in Miscible and Immiscible Alloys. *Microscopy and Microanalysis*, **2021**, 27, 3106-3108	0.5	
176	Tuning Electronic Properties of 2D Materials Using Metal Adsorbates: Cu at WTe Edges. *Journal of Physical Chemistry Letters*, **2021**, 12, 6596-6603	6.4	0
175	Ship-in-a-Bottle Synthesis of High Concentration of N Molecules in a Cage-Structured Electride. *Journal of Physical Chemistry Letters*, **2021**, 12, 1295-1299	6.4	2
174	Defect-Induced Magnetic Skyrmion in a Two-Dimensional Chromium Triiodide Monolayer. *Jacs Au*, **2021**, 1, 1362-1367		4
173	Lattice misorientation evolution and grain refinement in Al-Si alloys under high-strain shear deformation. *Materialia*, **2021**, 18, 101146	3.2	3
172	Understanding the Electronic Structure Evolution of Epitaxial LaNiFeO Thin Films for Water Oxidation. *Nano Letters*, **2021**, 21, 8324-8331	11.5	6
171	Air-Stable Calcium Cyanamide-Supported Ruthenium Catalyst for Ammonia Synthesis and Decomposition. *ACS Applied Energy Materials*, **2020**, 3, 6573-6582	6.1	11
170	Hole-Trapping-Induced Stabilization of Ni in SrNiO /LaFeO Superlattices. *Advanced Materials*, **2020**, 32, e2005003	24	13
169	Extreme shear-deformation-induced modification of defect structures and hierarchical microstructure in an Al Si alloy. *Communications Materials*, **2020**, 1,	6	10
168	Extracting band edge profiles at semiconductor heterostructures from hard-x-ray core-level photoelectron spectra. *Scientific Reports*, **2020**, 10, 13028	4.9	7
167	Structure and Electronic Properties of [Ca24Al28O64]4+ 4e Surfaces: Opportunities for Termination-Controlled Electron Transfer. *Journal of Physical Chemistry C*, **2019**, 123, 6030-6036	3.8	5
166	Charge Transfer and Built-in Electric Fields between a Crystalline Oxide and Silicon. *Physical Review Letters*, **2019**, 123, 026805	7.4	15

165	Hole-induced electronic and optical transitions in La1−xSrxFeO3 epitaxial thin films. *Physical Review Materials*, **2019**, 3,	3.2	20
164	Influence of crystalline order and defects on the absolute work functions and electron affinities of TiO2- and SrO-terminated nSrTiO3(001). *Physical Review Materials*, **2019**, 3,	3.2	8
163	Probing energy landscapes in multilayer heterostructures: Challenges and opportunities. *APL Materials*, **2019**, 7, 110904	5.7	2
162	Electronic Structure and Band Alignment of LaMnO3/SrTiO3 Polar/Nonpolar Heterojunctions. *Advanced Materials Interfaces*, **2019**, 6, 1801428	4.6	11
161	Onset of phase separation in the double perovskite oxide La2MnNiO6. *Physical Review B*, **2018**, 97,	3.3	3
160	Interconversion of intrinsic defects in SrTiO3(001). *Physical Review B*, **2018**, 97,	3.3	13
159	Layer-resolved band bending at the nSrTiO3(001)/pGe(001) interface. *Physical Review Materials*, **2018**, 2,	3.2	16
158	Direct Visualization of Li Dendrite Effect on LiCoO Cathode by In Situ TEM. *Small*, **2018**, 14, e1803108	11	28
157	Interface properties and built-in potential profile of a LaCrO3/SrTiO3 superlattice determined by standing-wave excited photoemission spectroscopy. *Physical Review B*, **2018**, 98,	3.3	17
156	Formation, Structural Variety, and Impact of Antiphase Boundaries on Li Diffusion in LiCoO Thin-Film Cathodes. *Journal of Physical Chemistry Letters*, **2018**, 9, 5515-5520	6.4	12
155	Electronic and Optical Properties of a Semiconducting Spinel (Fe2CrO4). *Advanced Functional Materials*, **2017**, 27, 1605040	15.6	14
154	Probing the Origin of Interfacial Carriers in SrTiO3LaCrO3 Superlattices. *Chemistry of Materials*, **2017**, 29, 1147-1155	9.6	17
153	The effects of core-level broadening in determining band alignment at the epitaxial SrTiO3(001)/p-Ge(001) heterojunction. *Applied Physics Letters*, **2017**, 110, 082104	3.4	21
152	Structure and stability of CaH2 surfaces: on the possibility of electron-rich surfaces in metal hydrides for catalysis. *Journal of Materials Chemistry A*, **2017**, 5, 5550-5558	13	17
151	Low-Dimensional Oxygen Vacancy Ordering and Diffusion in SrCrO. *Journal of Physical Chemistry Letters*, **2017**, 8, 1757-1763	6.4	11
150	Effect of doping and chemical ordering on the optoelectronic properties of complex oxides: FeO-VO solid solutions and hetero-structures. *Physical Chemistry Chemical Physics*, **2017**, 19, 1097-1107	3.6	4
149	Formation of Oxygen Radical Sites on MoVNbTeOx by Cooperative Electron Redistribution. *Journal of the American Chemical Society*, **2017**, 139, 12342-12345	16.4	29
148	An Ultrathin Single Crystalline Relaxor Ferroelectric Integrated on a High Mobility Semiconductor. *Nano Letters*, **2017**, 17, 6248-6257	11.5	9

147	Rattling of Oxygen Ions in a Sub-Nanometer-Sized Cage Converts Terahertz Radiation to Visible Light. *ACS Nano*, **2017**, 11, 12358-12364	16.7	11
146	Multimodal Imaging of Cation Disorder and Oxygen Deficiency-Mediated Phase Separation in Double Perovskite Oxides. *Microscopy and Microanalysis*, **2017**, 23, 1678-1679	0.5	1
145	Dynamic interface rearrangement in LaFeO3/n□SrTiO3 heterojunctions. *Physical Review Materials*, **2017**, 1,	3.2	14
144	Monochromated STEM-EELS Analysis of Interface-Induced Polarization in LaCrO3-SrTiO3 Superlattices **2016**, 972-973		
143	Electron anions and the glass transition temperature. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 10007-12	11.5	14
142	Defect compensation by Cr vacancies and oxygen interstitials in Ti4+-doped Cr2O3 epitaxial thin films. *Physical Review B*, **2016**, 94,	3.3	18
141	Spectroscopic properties of oxygen vacancies in LaAlO3. *Physical Review B*, **2016**, 93,	3.3	11
140	Interface-Induced Polarization in SrTiO3-LaCrO3 Superlattices. *Advanced Materials Interfaces*, **2016**, 3, 1500779	4.6	24
139	Quasi 2D Ultrahigh Carrier Density in a Complex Oxide Broken-Gap Heterojunction. *Advanced Materials Interfaces*, **2016**, 3, 1500432	4.6	27
138	Competing Pathways for Nucleation of the Double Perovskite Structure in the Epitaxial Synthesis of La2MnNiO6. *Chemistry of Materials*, **2016**, 28, 3814-3822	9.6	22
137	Modelling the local atomic structure of molybdenum in nuclear waste glasses with ab initio molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 26125-26132	3.6	10
136	Predictive Control over Charge Density in the Two-Dimensional Electron Gas at the Polar-Nonpolar NdTiO_{3}/SrTiO_{3} Interface. *Physical Review Letters*, **2016**, 117, 106803	7.4	38
135	Electronic structure and optical properties of □(Fe1-xVx)2O3 solid-solution thin films. *Applied Physics Letters*, **2015**, 106, 041905	3.4	10
134	Electride support boosts nitrogen dissociation over ruthenium catalyst and shifts the bottleneck in ammonia synthesis. *Nature Communications*, **2015**, 6, 6731	17.4	400
133	Hole-induced insulator-to-metal transition in La1□SrxCrO3 epitaxial films. *Physical Review B*, **2015**, 91,	3.3	60
132	Interface Promoted Reversible Mg Insertion in Nanostructured Tin-Antimony Alloys. *Advanced Materials*, **2015**, 27, 6598-605	24	67
131	Multi-scale Simulations of Metal-Semiconductor Nanoscale Contacts. *Journal of Physics: Conference Series*, **2015**, 647, 012030	0.3	2
130	Mechanisms of formation of chemical bonding and defect formation at the a-SiO2/BaTiO3 interfaces. *Journal of Physics Condensed Matter*, **2015**, 27, 475006	1.8	3

129	Perovskite Sr-Doped LaCrO3 as a New p-Type Transparent Conducting Oxide. *Advanced Materials*, **2015**, 27, 5191-5	24	125
128	Dominance of Interface Chemistry over the Bulk Properties in Determining the Electronic Structure of Epitaxial Metal/Perovskite Oxide Heterojunctions. *Chemistry of Materials*, **2015**, 27, 4093-4098	9.6	3
127	Electronic and magnetic properties of epitaxial perovskite SrCrO(0 0 1). *Journal of Physics Condensed Matter*, **2015**, 27, 245605	1.8	8
126	Structure and ionic diffusion of alkaline-earth ions in mixed cation glasses A2O2MO4SiO2 with molecular dynamics simulations. *Journal of Non-Crystalline Solids*, **2015**, 422, 57-63	3.9	7
125	Realizing the full potential of insertion anodes for Mg-ion batteries through the nanostructuring of Sn. *Nano Letters*, **2015**, 15, 1177-82	11.5	70
124	Enhanced N2 dissociation on Ru-loaded inorganic electride. *Journal of the American Chemical Society*, **2014**, 136, 2216-9	16.4	42
123	Hydride ions in oxide hosts hidden by hydroxide ions. *Nature Communications*, **2014**, 5, 3515	17.4	85
122	Reversible nano-structuring of SrCrO3- through oxidation and reduction at low temperature. *Nature Communications*, **2014**, 5, 4669	17.4	51
121	Impact of lattice mismatch and stoichiometry on the structure and bandgap of (Fe,Cr)2O3 epitaxial thin films. *Journal of Physics Condensed Matter*, **2014**, 26, 135005	1.8	25
120	Effect of metal intermixing on the Schottky barriers of Mo(100)/GaAs(100) interfaces. *Journal of Applied Physics*, **2014**, 116, 193703	2.5	4
119	Band-Gap Reduction and Dopant Interaction in Epitaxial La,Cr Co-doped SrTiO3Thin Films. *Chemistry of Materials*, **2014**, 26, 7073-7082	9.6	45
118	Multi-scale simulations of a Mo/n+GaAs Schottky contact for nano-scale III-V MOSFETs. *Semiconductor Science and Technology*, **2014**, 29, 054003	1.8	6
117	Neutral and Charged Oxygen Vacancies Induce Two-Dimensional Electron Gas Near SiO2/BaTiO3 Interfaces. *Journal of Physical Chemistry Letters*, **2013**, 4, 333-7	6.4	14
116	Activation and splitting of carbon dioxide on the surface of an inorganic electride material. *Nature Communications*, **2013**, 4, 2378	17.4	126
115	Optical Absorption and Band Gap Reduction in (Fe1-xCrx)2O3 Solid Solutions: A First-Principles Study. *Journal of Physical Chemistry C*, **2013**, 117, 25504-25512	3.8	38
114	Multiband optical absorption controlled by lattice strain in thin-film LaCrO3. *Physical Review Letters* , **2013**, 110, 077401	7.4	33
113	Li-Ion Batteries: Oxygen Vacancies and Ordering of d-levels Control Voltage Suppression in Oxide Cathodes: the Case of Spinel LiNi0.5Mn1.5O4-(Adv. Funct. Mater. 44/2013). *Advanced Functional Materials*, **2013**, 23, 5454-5454	15.6	2
112	Dendrite-free lithium deposition via self-healing electrostatic shield mechanism. *Journal of the American Chemical Society*, **2013**, 135, 4450-6	16.4	1374

111	Localized directed orbitals representing chemical bonds in ion-covalent crystals. *International Journal of Quantum Chemistry*, **2013**, 113, 1868-1876	2.1	3
110	The Impacts of Cation Stoichiometry and Substrate Surface Quality on Nucleation, Structure, Defect Formation, and Intermixing in Complex Oxide Heteroepitaxy□aCrO3 on SrTiO3(001). *Advanced Functional Materials*, **2013**, 23, 2953-2963	15.6	41
109	Oxygen Vacancies and Ordering of d-levels Control Voltage Suppression in Oxide Cathodes: the Case of Spinel LiNi0.5Mn1.5O4-□*Advanced Functional Materials*, **2013**, 23, 5530-5535	15.6	55
108	Surface Decoration of MgO Nanocubes with Sulfur Oxides: Experiment and Theory. *Journal of Physical Chemistry C*, **2013**, 117, 7727-7735	3.8	14
107	Mechanisms of Photodesorption of Br Atoms from CsBr Surfaces. *Journal of Physical Chemistry C*, **2013**, 117, 13502-13509	3.8	6
106	Interfaces: Ultralow Contact Resistance at an Epitaxial Metal/Oxide Heterojunction Through Interstitial Site Doping (Adv. Mater. 29/2013). *Advanced Materials*, **2013**, 25, 3926-3926	24	
105	Multi-Scale Simulation of Transport via a Mo/n+-GaAs Schottky Contact. *Materials Research Society Symposia Proceedings*, **2013**, 1553, 1		1
104	Ultralow contact resistance at an epitaxial metal/oxide heterojunction through interstitial site doping. *Advanced Materials*, **2013**, 25, 4001-5	24	21
103	Optical absorption and spectral photoconductivity in □(Fe□xCrx)□□□solid-solution thin films. *Journal of Physics Condensed Matter*, **2013**, 25, 392002	1.8	28
102	Selective response of mesoporous silicon to adsorbants with nitro groups. *Chemistry - A European Journal*, **2012**, 18, 2912-22	4.8	6
101	Models of triplet self-trapped excitons in SiO2, HfO2, and HfSiO4. *Physical Review B*, **2012**, 85,	3.3	18
100	Defect-mediated lattice relaxation and domain stability in ferroelectric oxides. *Physical Review Letters*, **2012**, 109, 117601	7.4	29
99	Tuning optical properties of complex oxides: examples of 12CaO.7Al2O3 mayenite and LaCrO3 perovskite **2012**,		1
98	High-performance LiNi0.5Mn1.5O4 spinel controlled by Mn3+ concentration and site disorder. *Advanced Materials*, **2012**, 24, 2109-16	24	371
97	Spectroscopic characterization of a multiband complex oxide: Insulating and conducting cement 12CaO□7Al2O3. *Physical Review B*, **2012**, 85,	3.3	19
96	Structure and properties of oxygen centers in CaF2 crystals from ab initio embedded cluster calculations. *Physical Review B*, **2011**, 84,	3.3	17
95	Embedding and atomic orbitals hybridization. *International Journal of Quantum Chemistry*, **2011**, 111, 2602-2619	2.1	6
94	Models of stoichiometric and oxygen-deficient surfaces of subnanoporous 12CaO□7Al 2 O 3. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2011**, 467, 2066-2083	2.4	26

93	Optical properties of nanocrystal interfaces in compressed MgO nanopowders. *ACS Nano*, **2011**, 5, 3003-16	26.7	42
92	Exciton-Driven Highly Hyperthermal O-Atom Desorption from Nanostructured CaO. *Journal of Physical Chemistry C*, **2011**, 115, 692-699	3.8	5
91	Band alignment, built-in potential, and the absence of conductivity at the LaCrO3/SrTiO3(001) heterojunction. *Physical Review Letters*, **2011**, 107, 206802	7.4	89
90	Cation mixing, band offsets and electric fields at LaAlO3/SrTiO3(001) heterojunctions with variable La:Al atom ratio. *Surface Science*, **2011**, 605, 1381-1387	1.8	71
89	Embedding and atomic orbitals hybridization **2011**, 111, 2602		1
88	(Invited) Photoluminescence Properties of Alkaline-Earth Oxide Nanoparticles. *ECS Transactions*, **2010**, 28, 67-80	1	5
87	Interaction of Intercalated Li+ Ions with Oxygen Vacancies in Rutile TiO2. *ECS Transactions*, **2010**, 28, 299-306	1	4
86	The Structure and Decomposition Chemistry of Isomer Defects in a Crystalline DADNE. *Journal of Energetic Materials*, **2010**, 28, 128-139	1.6	6
85	General Purpose Electrostatic Embedding Potential. *Journal of Chemical Theory and Computation*, **2010**, 6, 1323-1333	6.4	26
84	Fromab initioproperties of the Si-SiO2interface, to electrical characteristics of metal-oxide-semiconductor devices. *Journal of Physics: Conference Series*, **2010**, 242, 012010	0.3	2
83	Thermodynamic instability at the stoichiometric LaAlO3/SrTiO3(001) interface. *Journal of Physics Condensed Matter*, **2010**, 22, 312201	1.8	68
82	QM/MM method for metal-organic interfaces. *Journal of Computational Chemistry*, **2010**, 31, 2955-66	3.5	9
81	Instability, intermixing and electronic structure at the epitaxial LaAlO3/SrTiO3(001) heterojunction. *Surface Science Reports*, **2010**, 65, 317-352	12.9	241
80	Tuning Photoluminescence Properties of Alkaline-earth Oxide Nanoparticles by Site-selective Functionalization and Doping. *ECS Transactions*, **2009**, 25, 131-139	1	2
79	Positive and Negative Oxygen Vacancies in Amorphous Silica. *ECS Transactions*, **2009**, 19, 3-17	1	66
78	Oxygen ion conduction in 12CaO□7Al2O3: O2□conduction mechanism and possibility of O□fast conduction?. *Solid State Ionics*, **2009**, 180, 550-555	3.3	49
77	Excitons in potassium bromide: A study using embedded time-dependent density functional theory and equation-of-motion coupled cluster methods. *Chemical Physics Letters*, **2009**, 470, 353-357	2.5	26
76	Excitation, Ionization, and Desorption: How Sub-Band Gap Photons Modify the Structure of Oxide Nanoparticles. *Journal of Physical Chemistry C*, **2009**, 113, 1274-1279	3.8	14

75	Impact of Body-Thickness-Dependent Band Structure on Scaling of Double-Gate MOSFETs: A DFT/NEGF Study. *IEEE Nanotechnology Magazine*, **2009**, 8, 159-166	2.6	22
74	Modeling proton transfer and polarons in a molecular crystal diamino-dinitroethylene. *Physical Review B*, **2009**, 80,	3.3	16
73	Modelling of electron and hole trapping in oxides. *Modelling and Simulation in Materials Science and Engineering*, **2009**, 17, 084004	2	46
72	Oxygen vacancies in cubic ZrO2 nanocrystals studied by an ab initio embedded cluster method. *Physical Review B*, **2008**, 78,	3.3	37
71	Crystallographic phase transition and high-Tcsuperconductivity in LaFeAsO:F. *Superconductor Science and Technology*, **2008**, 21, 125028	3.1	212
70	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, 4496-500	2.8	45
69	Mechanism of phase transitions and electronic density of states in LaFeAsO1−xFx and SmFeAsO1−xFx from ab initio density functional calculations. *Physical Review B*, **2008**, 78,	3.3	10
68	Atomistic mesh generation for the simulation of nanoscale metal-oxide-semiconductor field-effect transistors. *Physical Review E*, **2008**, 77, 056702	2.4	2
67	Tetragonal–Orthorhombic Phase Transition and F-Doping Effects on the Crystal Structure in the Iron-Based High-TcSuperconductor LaFeAsO. *Journal of the Physical Society of Japan*, **2008**, 77, 32-35	1.5	7
66	Si–SiO2 interface band-gap transition effects on MOS inversion layer. *Physica Status Solidi (A) Applications and Materials Science*, **2008**, 205, 1290-1295	1.6	21
65	Energy and site selectivity in O-atom photodesorption from nanostructured MgO. *Surface Science*, **2008**, 602, 1968-1973	1.8	20
64	Insulator–conductor transition in 12CaO·7Al2O3 films: On the stability of the crystal lattice under Ar+ bombardment. *Thin Solid Films*, **2008**, 516, 1350-1353	2.2	4
63	Inside powders: a theoretical model of interfaces between MgO nanocrystallites. *Journal of the American Chemical Society*, **2007**, 129, 8600-8	16.4	51
62	Nanoporous crystal 12CaO.7Al2O3: a playground for studies of ultraviolet optical absorption of negative ions. *Journal of Physical Chemistry B*, **2007**, 111, 1946-56	3.4	57
61	Transient Atomic Configurations of Supported Gold Nanocrystallites at Finite Temperature. *Journal of Physical Chemistry C*, **2007**, 111, 2823-2826	3.8	11
60	Effect of charged and excited states on the decomposition of 1,1-diamino-2,2-dinitroethylene molecules. *Journal of Chemical Physics*, **2007**, 126, 234711	3.9	43
59	From insulator to electride: a theoretical model of nanoporous oxide 12CaO.7Al2O3. *Journal of the American Chemical Society*, **2007**, 129, 942-51	16.4	105
58	Optical and EPR properties of point defects at a crystalline silica surface: Ab initio embedded-cluster calculations. *Physical Review B*, **2007**, 75,	3.3	45

57	Electronic structure of insulator-confined ultra-thin Si channels. *Microelectronic Engineering*, **2007**, 84, 2043-2046	2.5	12
56	Electronic structure and spectroscopic properties of interstitial anions in the nanoporous complex oxide 12CaO·7Al2O3. *Physica Status Solidi (A) Applications and Materials Science*, **2007**, 204, 663-669	1.6	8
55	Dynamics of low-coordinated surface atoms on gold nanocrystallites. *Journal of Chemical Physics*, **2007**, 126, 154704	3.9	9
54	Electron trapping at point defects on hydroxylated silica surfaces. *Physical Review Letters*, **2007**, 99, 136801	7.4	41
53	Structure and spectroscopic properties of trapped holes in silica. *Journal of Non-Crystalline Solids*, **2007**, 353, 599-604	3.9	35
52	Effect of protons on the optical properties of oxide nanostructures. *Journal of the American Chemical Society*, **2007**, 129, 12491-6	16.4	43
51	Atomistic Mesh Generation for the Simulation of Semiconductor Devices **2007**, 97-100		
50	Site-specific laser modification of MgO nanoclusters: Towards atomic-scale surface structuring. *Physical Review B*, **2006**, 74,	3.3	24
49	Photoluminescence from Au ion-implanted nanoporous single-crystal 12CaO·7Al2O3. *Physical Review B*, **2006**, 73,	3.3	39
48	Role of hydrogen atoms in the photoinduced formation of stable electron centers in H-doped 12CaO·7Al2O3. *Physical Review B*, **2006**, 73,	3.3	39
47	Optical absorption and luminescence energies of F centers in CaO from ab initio embedded cluster calculations. *Journal of Chemical Physics*, **2006**, 125, 074710	3.9	27
46	Mechanisms of oxygen ion diffusion in a nanoporous complex oxide 12CaO·7Al2O3. *Physical Review B*, **2006**, 73,	3.3	52
45	Probing electron transfer dynamics at MgO surfaces by Mg-atom desorption. *Journal of Physical Chemistry B*, **2006**, 110, 18093-6	3.4	11
44	Laser control of desorption through selective surface excitation. *Journal of Physical Chemistry B*, **2005**, 109, 19563-78	3.4	46
43	Hydride ion as a two-electron donor in a nanoporous crystalline semiconductor 12CaO.7Al2O3. *Journal of Physical Chemistry B*, **2005**, 109, 23836-42	3.4	48
42	Spectroscopic features of dimer and dangling bondE? centres in amorphous silica. *Journal of Physics Condensed Matter*, **2005**, 17, 1311-1318	1.8	15
41	Structure and properties of defects in amorphous silica: new insights from embedded cluster calculations. *Journal of Physics Condensed Matter*, **2005**, 17, S2115-S2140	1.8	62
40	Chemistry at corners and edges: generation and adsorption of H atoms on the surface of MgO nanocubes. *Journal of Chemical Physics*, **2005**, 123, 64714	3.9	33

39	Oxygen vacancies in amorphous silica: structure and distribution of properties. *Microelectronic Engineering*, **2005**, 80, 292-295	2.5	42
38	A mechanism of photo-induced desorption of oxygen atoms from MgO nano-crystals. *Surface Science*, **2005**, 593, 210-220	1.8	27
37	Localisation assisted by the lattice relaxation and the optical absorption of extra-framework electrons in 12CaO·Al2O3. *Materials Science and Engineering C*, **2005**, 25, 722-726	8.3	15
36	Optical properties and transformation mechanism of oxygen centres and their aggregates in CaF2 crystals. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2005**, 2, 392-396		11
35	The effect of the α-quartz lattice on the optical absorption and stretching frequency of the interstitial O2 molecule. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2005**, 2, 503-506		4
34	Photoinduced generation of electron anions in H-doped nanoporous oxide 12CaO·7Al2O3: Toward an optically controlled formation of electrides. *Applied Physics Letters*, **2005**, 86, 092101	3.4	42
33	Correlation between the atomic structure, formation energies, and optical absorption of neutral oxygen vacancies in amorphous silica. *Physical Review B*, **2005**, 71,	3.3	36
32	Modeling of the structure and properties of oxygen vacancies in amorphous silica. *Physical Review B*, **2004**, 70,	3.3	79
31	Laser control of product electronic state: desorption from alkali halides. *Journal of Chemical Physics* , **2004**, 120, 2456-63	3.9	13
30	Determination of surface exciton energies by velocity resolved atomic desorption. *Surface Science*, **2004**, 564, 62-70	1.8	29
29	Calibration of embedded-cluster method for defect studies in amorphous silica. *Physical Review B*, **2004**, 69,	3.3	44
28	Calculation of relative concentrations of E? centres in amorphous silica. *Journal of Non-Crystalline Solids*, **2004**, 345-346, 703-709	3.9	7
27	Surface electronic spectra detected by atomic desorption. *Surface Science*, **2003**, 544, L683-L688	1.8	14
26	Reactivity of (H+)(e−) color centers at the MgO surface: formation of O2− and N2− radical anions. *Surface Science*, **2003**, 542, 293-306	1.8	27
25	Hopping and optical absorption of electrons in nano-porous crystal 12CaO·7Al2O3. *Thin Solid Films*, **2003**, 445, 161-167	2.2	63
24	Paramagnetic defect centers at the MgO surface. An alternative model to oxygen vacancies. *Journal of the American Chemical Society*, **2003**, 125, 738-47	16.4	125
23	Embedded Cluster Model: Application to Molecular Crystals. *Materials Research Society Symposia Proceedings*, **2003**, 800, 15		1
22	Electron localization and a confined electron gas in nanoporous inorganic electrides. *Physical Review Letters*, **2003**, 91, 126401	7.4	177

21	Modeling charge self-trapping in wide-gap dielectrics: Localization problem in local density functionals. *Physical Review B*, **2003**, 67,	3.3	76
20	Transient center photodecomposition in potassium bromide. *Applied Surface Science*, **2002**, 197-198, 581-586	6.7	3
19	Hydrogen defects in Forsterite: A test case for the embedded cluster method. *Journal of Chemical Physics*, **2002**, 116, 2628-2635	3.9	36
18	Embedding techniques for irradiation-induced defects in crystalline SiO/sub 2/. *IEEE Transactions on Nuclear Science*, **2002**, 49, 1383-1388	1.7	5
17	Control of laser desorption using tunable single pulses and pulse pairs. *Journal of Chemical Physics*, **2002**, 116, 8144-8151	3.9	16
16	Wavelength selective excitation of surface oxygen anions on highly dispersed MgO. *Journal of Chemical Physics*, **2002**, 116, 1707-1712	3.9	60
15	Electron trapping at neutral divacancy sites on the MgO surface. *Journal of Chemical Physics*, **2002**, 117, 2844-2851	3.9	62
14	Solid-state halogen atom source for chemical dynamics and etching. *Applied Physics Letters*, **2002**, 81, 1140-1142	3.4	8
13	Electronic Properties of Structural Defects at the MgO (001) Surface. *Journal of Physical Chemistry B*, **2002**, 106, 2269-2276	3.4	128
12	Energies and Dynamics of Photoinduced Electron and Hole Processes on MgO Powders. *Journal of Physical Chemistry B*, **2002**, 106, 12478-12482	3.4	52
11	Asymmetry and long-range character of lattice deformation by neutral oxygen vacancy in □quartz. *Physical Review B*, **2002**, 66,	3.3	115
10	Selective laser desorption of ionic surfaces: Resonant surface excitation of KBr. *Journal of Chemical Physics*, **2001**, 115, 9463-9472	3.9	35
9	Embedded cluster calculations of metal complex impurity defects: properties of the iron cyanide in NaCl. *Journal of Physics Condensed Matter*, **2000**, 12, 8257-8266	1.8	31
8	Relative energies of surface and defect states: ab initio calculations for the MgO (001) surface. *Surface Science*, **2000**, 450, 153-170	1.8	316
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