Alfredo Pasquarello

List of Publications by Year
in descending order

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339 papers	37,081 citations	10984 71 h-index	3105 187 g-index

370 all docs	370 docs citations	370 times ranked	30859 citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
2	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. Physical Review B, 1993, 47, 10142-10153.	3.2	1,303
3	Identification of Raman Defect Lines as Signatures of Ring Structures in Vitreous Silica. Physical Review Letters, 1998, 80, 5145-5147.	7.8	377
4	Organic Cathode for Aqueous Zn-Ion Batteries: Taming a Unique Phase Evolution toward Stable Electrochemical Cycling. Chemistry of Materials, 2018, 30, 3874-3881.	6.7	373
5	Finite-size supercell correction schemes for charged defect calculations. Physical Review B, 2012, 86, .	3.2	371
6	First Solvation Shell of the Cu(II) Aqua Ion: Evidence for Fivefold Coordination. Science, 2001, 291, 856-859.	12.6	358
7	Accurate theory of excitons in GaAs-Ga1â^'xAlxAs quantum wells. Physical Review B, 1990, 42, 8928-8938.	3.2	356
8	Ab initiomolecular dynamics ford-electron systems: Liquid copper at 1500 K. Physical Review Letters, 1992, 69, 1982-1985.	7.8	346
9	Fully Unconstrained Approach to Noncollinear Magnetism: Application to Small Fe Clusters. Physical Review Letters, 1998, 80, 3622-3625.	7.8	331
10	Ab initioMolecular Dynamics in a Finite Homogeneous Electric Field. Physical Review Letters, 2002, 89, 157602.	7.8	322
11	sp2/sp3hybridization ratio in amorphous carbon from C1score-level shifts: X-ray photoelectron spectroscopy and first-principles calculation. Physical Review B, 2001, 65, .	3.2	313
12	Structural and Electronic Properties of Liquid and Amorphous SiO2: AnAb InitioMolecular Dynamics Study. Physical Review Letters, 1995, 74, 4682-4685.	7.8	266
13	Defect Energy Levels in Density Functional Calculations: Alignment and Band Gap Problem. Physical Review Letters, 2008, 101, 046405.	7.8	263
14	Defect levels through hybrid density functionals: Insights and applications. Physica Status Solidi (B): Basic Research, 2011, 248, 775-789.	1.5	253
15	Interface structure between silicon and its oxide by first-principles molecular dynamics. Nature, 1998, 396, 58-60.	27.8	230
16	Band Offsets at Semiconductor-Oxide Interfaces from Hybrid Density-Functional Calculations. Physical Review Letters, 2008, 101, 106802.	7.8	229
17	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. Physical Review B, 1996, 53, 1180-1185.	3.2	228
18	Oxygen vacancy in monoclinic HfO2: A consistent interpretation of trap assisted conduction, direct electron injection, and optical absorption experiments. Applied Physics Letters, 2006, 89, 262904.	3.3	224

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19	Hole subbands in strained GaAs-Ga1â^'xAlxAs quantum wells: Exact solution of the effective-mass equation. Physical Review B, 1987, 36, 5887-5894.	3.2	223
20	Theory of Si 2pcore-level shifts at the Si(001)-SiO2interface. Physical Review B, 1996, 53, 10942-10950.	3.2	211
21	Structure and Hyperfine Parameters ofE1â€²Centers inÎ±-Quartz and in VitreousSiO2. Physical Review Letters, 1997, 78, 887-890.	7.8	207
22	Oxide versus Nonoxide Cathode Materials for Aqueous Zn Batteries: An Insight into the Charge Storage Mechanism and Consequences Thereof. ACS Applied Materials & Interfaces, 2019, 11, 674-682.	8.0	199
23	Effect of Metal Elements in Catalytic Growth of Carbon Nanotubes. Physical Review Letters, 2008, 100, 156102.	7.8	189
24	Model of vitreousSiO2generated by anab initiomolecular-dynamics quench from the melt. Physical Review B, 1995, 52, 12690-12695.	3.2	180
25	Si2pCore-Level Shifts at the Si(001)-SiO2Interface: A First-Principles Study. Physical Review Letters, 1995, 74, 1024-1027.	7.8	179
26	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	177
27	Raman scattering intensities in Î±-quartz: A first-principles investigation. Physical Review B, 2001, 63, .	3.2	173
28	Si-O-Si bond-angle distribution in vitreous silica from first-principles29SiNMR analysis. Physical Review B, 2000, 62, R4786-R4789.	3.2	167
29	Band Offsets at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Si</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Interface: Insights from Many-Body Perturbation Theory. Physical Review Letters, 2008, 100, 186401.	7.8	154
30	Defect levels of dangling bonds in silicon and germanium through hybrid functionals. Physical Review B, 2008, 78, .	3.2	147
31	Band-edge problem in the theoretical determination of defect energy levels: The O vacancy in ZnO as a benchmark case. Physical Review B, 2011, 84, .	3.2	143
32	Nitrogen Incorporation atSi(001)â^'SiO2Interfaces: Relation between N1sCore-Level Shifts and Microscopic Structure. Physical Review Letters, 1997, 79, 5174-5177.	7.8	142
33	Dynamical Charge Tensors and Infrared Spectrum of AmorphousSiO2. Physical Review Letters, 1997, 79, 1766-1769.	7.8	141
34	Finite-Size Supercell Correction for Charged Defects at Surfaces and Interfaces. Physical Review Letters, 2013, 110, 095505.	7.8	141
35	Ring Currents in Icosahedral C60. Science, 1992, 257, 1660-1661.	12.6	140
36	Migration of oxygen vacancy in HfO2 and across the HfO2â•SiO2 interface: A first-principles investigation. Applied Physics Letters, 2007, 91, .	3.3	134

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37	Origin of the High-Frequency Doublet in the Vibrational Spectrum of Vitreous SiO2. Science, 1997, 275, 1925-1927.	12.6	133
38	First-principles study of dynamical and dielectric properties of tetragonal zirconia. Physical Review B, 2001, 64, .	3.2	129
39	First-principles investigation of high-Îºdielectrics: Comparison between the silicates and oxides of hafnium and zirconium. Physical Review B, 2004, 69, .	3.2	129
40	Theory of atomic-scale dielectric permittivity at insulator interfaces. Physical Review B, 2005, 71, .	3.2	128
41	Concentration of Small Ring Structures in Vitreous Silica from a First-Principles Analysis of the Raman Spectrum. Physical Review Letters, 2003, 90, 027401.	7.8	127
42	Alignment of defect levels and band edges through hybrid functionals: Effect of screening in the exchange term. Physical Review B, 2010, 81, .	3.2	124
43	Nonempirical dielectric-dependent hybrid functional with range separation for semiconductors and insulators. Physical Review Materials, 2018, 2, .	2.4	122
44	Origin of low electronâ€“hole recombination rate in metal halide perovskites. Energy and Environmental Science, 2018, 11, 101-105.	30.8	113
45	Hybrid-functional calculations with plane-wave basis sets: Effect of singularity correction on total energies, energy eigenvalues, and defect energy levels. Physical Review B, 2009, 80, .	3.2	112
46	Self-compensation due to point defects in Mg-doped GaN. Physical Review B, 2016, 93, .	3.2	111
47	Structurally relaxed models of the Si(001)â€“SiO2 interface. Applied Physics Letters, 1996, 68, 625-627.	3.3	110
48	Ring currents in topologically complex molecules: Application toC60,C70, and their hexa-anions. Physical Review A, 1993, 47, 1783-1789.	2.5	109
49	Magnetoresistive junctions based on epitaxial graphene and hexagonal boron nitride. Physical Review B, 2009, 80, .	3.2	109
50	Dangling Bond Defects atSiâ^'SiO2Interfaces: Atomic Structure of thePb1Center. Physical Review Letters, 2000, 85, 2773-2776.	7.8	104
51	A hybrid density functional study of lithium in ZnO: Stability, ionization levels, and diffusion. Physical Review B, 2009, 80, .	3.2	104
52	Dynamic structure factor of vitreous silica from first principles: Comparison to neutron-inelastic-scattering experiments. Physical Review B, 1998, 57, 14133-14140.	3.2	100
53	Band offsets of lattice-matched semiconductor heterojunctions through hybrid functionals andG0W0. Physical Review B, 2014, 89, .	3.2	100
54	Predictive Determination of Band Gaps of Inorganic Halide Perovskites. Journal of Physical Chemistry Letters, 2017, 8, 5507-5512.	4.6	98

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55	Oxygen Diffusion through the Disordered Oxide Network during Silicon Oxidation. Physical Review Letters, 2002, 88, 125901.	7.8	92
56	Structural and electronic properties of small copper clusters: a first principles study. Chemical Physics Letters, 1995, 238, 215-221.	2.6	91
57	Pressure-Induced Structural Changes in LiquidSiO2fromAb InitioSimulations. Physical Review Letters, 2002, 89, 245504.	7.8	91
58	First-principles study of structural, electronic, dynamical, and dielectric properties of zircon. Physical Review B, 2001, 63, .	3.2	87
59	Transition Structure at theSi(100)â^'SiO2Interface. Physical Review Letters, 2003, 90, 186101.	7.8	86
60	Multiscale modeling of oxygen diffusion through the oxide during silicon oxidation. Physical Review B, 2004, 70, .	3.2	86
61	Charge transition levels of carbon-, oxygen-, and hydrogen-related defects at the SiC/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>interface through hybrid functionals. Physical Review B, 2011, 84, .	3.2	86
62	Metal adatoms on graphene and hexagonal boron nitride: Towards rational design of self-assembly templates. Physical Review B, 2010, 82, .	3.2	84
63	Dielectric Discontinuity at Interfaces in the Atomic-Scale Limit: Permittivity of Ultrathin Oxide Films on Silicon. Physical Review Letters, 2003, 91, 267601.	7.8	82
64	Accurate band gaps of extended systems via efficient vertex corrections in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:n Physical Review B, 2015, 92, .	3.2	81
65	Structural and electronic properties of small Cun clusters using generalized-gradient approximations within density functional theory. Journal of Chemical Physics, 1998, 109, 6626-6630.	3.0	78
66	Short- and intermediate-range structure of liquid GeSe2. Physical Review B, 2001, 64, .	3.2	77
67	Effect of Subband Coupling on Exciton Binding Energies and Oscillator Strengths in GaAs-Ga _{1-x} Al _x As Quantum Wells. Europhysics Letters, 1988, 6, 259-264.	2.0	76
68	Assessing the accuracy of hybrid functionals in the determination of defect levels: Application to the As antisite in GaAs. Physical Review B, 2011, 84, .	3.2	76
69	Nonempirical hybrid functionals for band gaps and polaronic distortions in solids. Physical Review B, 2018, 97, .	3.2	75
70	Microscopic Structure of LiquidGeSe2: The Problem of Concentration Fluctuations over Intermediate Range Distances. Physical Review Letters, 1998, 80, 2342-2345.	7.8	74
71	Band-edge levels in semiconductors and insulators: Hybrid density functional theory versus many-body perturbation theory. Physical Review B, 2012, 86, .	3.2	74
72	Alignment of Redox Levels at Semiconductorâ€“Water Interfaces. Chemistry of Materials, 2018, 30, 94-111.	6.7	74

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73	Atomic-Scale Simulation of Electrochemical Processes at Electrode/Water Interfaces under Referenced Bias Potential. Journal of Physical Chemistry Letters, 2018, 9, 1880-1884.	4.6	72
74	Density-functional perturbation theory for lattice dynamics with ultrasoft pseudopotentials. Physical Review B, 1997, 56, R11369-R11372.	3.2	71
75	Electronic Levels of Excess Electrons in Liquid Water. Journal of Physical Chemistry Letters, 2017, 8, 2055-2059.	4.6	70
76	Dielectric Constants of Zr Silicates: A First-Principles Study. Physical Review Letters, 2002, 89, 117601.	7.8	68
77	Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions. Journal of Chemical Physics, 2015, 142, 034501.	3.0	68
78	Reaction of the Oxygen Molecule at theSi(100)â˜SiO2Interface During Silicon Oxidation. Physical Review Letters, 2004, 93, 086102.	7.8	67
79	Band offsets at the Ge/GeO2 interface through hybrid density functionals. Applied Physics Letters, 2009, 94, 141911.	3.3	67
80	Correspondence of defect energy levels in hybrid density functional theory and many-body perturbation theory. Physical Review B, 2013, 88, .	3.2	67
81	Band-edge positions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mm Effects of starting point and self-consistency. Physical Review B, 2014, 90, .	3.2	67
82	First Principles Study of Photoelectron Spectra ofCunâ˜Clusters. Physical Review Letters, 1995, 75, 2104-2107.	7.8	66
83	Atomistic structure of the Si(100)â€“SiO2 interface: A synthesis of experimental data. Applied Physics Letters, 2003, 83, 1417-1419.	3.3	65
84	Infrared spectra of jennite and tobermorite from first-principles. Cement and Concrete Research, 2014, 60, 11-23.	11.0	65
85	Role of Polarons in Water Splitting: The Case of BiVO₄. ACS Energy Letters, 2018, 3, 1693-1697.	17.4	65
86	Structural and electronic properties of an abrupt<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi><mml:mtext>â˜</mml:mtext><mml:mi>SiC</mml:mi><mml model: Classical molecular dynamics simulations and density functional calculations. Physical Review B, 2007, 76, .	3.2	64
87	AbÂinitio Electronic Structure of Liquid Water. Physical Review Letters, 2016, 117, 186401.	7.8	64
88	Origin of the first sharp diffraction peak in the structure factor of disordered network-forming systems: Layers or voids?. Journal of Chemical Physics, 2001, 114, 7976-7979.	3.0	63
89	Fraction of Boroxol Rings in Vitreous Boron Oxide from a First-Principles Analysis of Raman and NMR Spectra. Physical Review Letters, 2005, 95, 137401.	7.8	63
90	Band alignments and defect levels in Siâ€“HfO2 gate stacks: Oxygen vacancy and Fermi-level pinning. Applied Physics Letters, 2008, 92, .	3.3	63

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91	Proton Diffusion Mechanism in AmorphousSiO2. Physical Review Letters, 2006, 97, 155901.	7.8	62
92	Redox levels in aqueous solution: Effect of van der Waals interactions and hybrid functionals. Journal of Chemical Physics, 2015, 143, 244508.	3.0	62
93	Validity of the bond-energy picture for the energetics atSiâ^'SiO2interfaces. Physical Review B, 2000, 62, R16326-R16329.	3.2	61
94	Atomic structure of the two intermediate phase glasses<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiSe</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:ms xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>GeSe</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:m Physical Review B, 2009, 79, .	3.2	61
95	Structural, Dynamical, and Electronic Properties of Liquid Water: A Hybrid Functional Study. Journal of Physical Chemistry B, 2016, 120, 7456-7470.	2.6	61
96	Medium-range structure of vitreous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu through first-principles investigation of vibrational spectra. Physical Review B, 2009, 79, .	3.2	60
97	Intermediate Range Order and Bonding Character in Disordered Network-Forming Systems. Journal of the American Chemical Society, 1999, 121, 2943-2944.	13.7	59
98	Magnetism of carbon clusters. Physical Review B, 1994, 50, 16459-16463.	3.2	58
99	Nitrogen bonding configurations at nitrided Si(001) surfaces andSi(001)â^'SiO2interfaces: A first-principles study of core-level shifts. Physical Review B, 2001, 63, .	3.2	58
100	Medium-Range Structural Properties of Vitreous Germania Obtained through First-Principles Analysis of Vibrational Spectra. Physical Review Letters, 2005, 95, 075505.	7.8	57
101	Vibrational spectra of vitreous germania from first-principles. Physical Review B, 2006, 74, .	3.2	56
102	Short and intermediate range order in amorphous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ge</mml:mi><mml:msub><mml:mi mathvariant="normal">Se</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2008, 77, .	3.2	55
103	Diffusion mechanism of Cu adatoms on a Cu(001) surface. Surface Science, 1994, 306, L575-L578.	1.9	54
104	Infrared Spectra at Surfaces and Interfaces from First Principles: Evolution of the Spectra across theSi(100)â^'SiO2Interface. Physical Review Letters, 2005, 95, 187402.	7.8	53
105	Binding energies of excited shallow acceptor states in GaAs/Ga1â^'xAlxAs quantum wells. Physical Review B, 1989, 40, 5602-5612.	3.2	52
106	Origin of Fine Structure in Si2pPhotoelectron Spectra at Silicon Surfaces and Interfaces. Physical Review Letters, 2006, 96, 157601.	7.8	51
107	Absolute Energy Levels of Liquid Water. Journal of Physical Chemistry Letters, 2018, 9, 3212-3216.	4.6	51
108	Comparison of structurally relaxed models of the Si(001)-SiO2 interface based on different crystalline oxide forms. Applied Surface Science, 1996, 104-105, 317-322.	6.1	50

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109	On the Electronic and Optical Properties of Metalâ€“Organic Frameworks: Case Study of MIL-125 and MIL-125-NH₂. Journal of Physical Chemistry C, 2020, 124, 4065-4072.	3.1	50
110	Atomistic models of the Si(100)â€“SiO2interface: structural, electronic and dielectric properties. Journal of Physics Condensed Matter, 2005, 17, S2065-S2074.	1.8	48
111	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. Npj Computational Materials, 2019, 5, .	8.7	48
112	First-principles modeling of paramagnetic Si dangling-bond defects in amorphousSiO2. Physical Review B, 2002, 66, .	3.2	47
113	First principles investigation of defects at interfaces between silicon and amorphous high-Îº oxides. Microelectronic Engineering, 2007, 84, 2022-2027.	2.4	47
114	First-principles determination of defect energy levels through hybrid density functionals andGW. Journal of Physics Condensed Matter, 2015, 27, 133202.	1.8	47
115	Electronic and dielectric properties of a suboxide interlayer at the siliconâ€“oxide interface in MOS devices. Surface Science, 2005, 586, 183-191.	1.9	46
116	Energetics of native point defects in GaN: A density-functional study. Microelectronic Engineering, 2015, 147, 51-54.	2.4	46
117	pH-Dependent Surface Chemistry from First Principles: Application to the BiVO₄(010)â€“Water Interface. ACS Applied Materials & Interfaces, 2018, 10, 10011-10021.	8.0	46
118	Infrared and Raman spectra of disordered materials from first principles. Diamond and Related Materials, 2005, 14, 1255-1261.	3.9	45
119	Defect levels of carbon-related defects at the SiC/SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>interface from hybrid functionals. Physical Review B, 2011, 83, .	3.2	45
120	Comparison of vacancy and antisite defects in GaAs and InGaAs through hybrid functionals. Journal of Physics Condensed Matter, 2012, 24, 045801.	1.8	45
121	First principles molecular dynamics calculation of the structure and acidity of a bulk zeolite. Chemical Physics Letters, 1994, 226, 245-250.	2.6	44
122	Band gaps and dielectric constants of amorphous hafnium silicates: A first-principles investigation. Applied Physics Letters, 2007, 90, 082907.	3.3	44
123	Absolute deformation potentials of two-dimensional materials. Physical Review B, 2016, 94, .	3.2	44
124	Comprehensive modeling of the band gap and absorption spectrum of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiVO</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> Physical Review Materials, 2017, 1, .	2.4	44
125	Supported Fe Nanoclusters: Evolution of Magnetic Properties with Cluster Size. Physical Review Letters, 2003, 90, 247202.	7.8	43
126	Intrinsic defects in GaAs and InGaAs through hybrid functional calculations. Physica B: Condensed Matter, 2012, 407, 2833-2837.	2.7	43

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127	Picture of the wet electron: a localized transient state in liquid water. Chemical Science, 2019, 10, 7442-7448.	7.4	43
128	Gauge-invariant two-photon transitions in quantum wells. Physical Review B, 1988, 38, 6206-6210.	3.2	42
129	First-principles study of NH3 exposed Si(001)2Ã—1: Relation between N 1s core-level shifts and atomic structure. Applied Physics Letters, 2000, 76, 553-555.	3.3	42
130	First principles investigation of defect energy levels at semiconductor-oxide interfaces: Oxygen vacancies and hydrogen interstitials in the Siâ€“SiO2â€“HfO2 stack. Journal of Applied Physics, 2009, 105, 061603.	2.5	41
131	Oxygen defects in amorphous Al2O3: A hybrid functional study. Applied Physics Letters, 2016, 109, .	3.3	41
132	pH-Dependent Catalytic Reaction Pathway for Water Splitting at the BiVO₄â€“Water Interface from the Band Alignment. ACS Energy Letters, 2018, 3, 829-834.	17.4	41
133	First-principles investigation of the structural and vibrational properties of vitreousGeSe2. Physical Review B, 2007, 75, .	3.2	40
134	Structural assignments of NMR chemical shifts in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ge</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> via first-principles calculations for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><m. Physical Review B, 2010, 82, .	3.2	40
135	SpherosiloxaneH8Si8O12clusters on Si(001): First-principles calculation of Si2pcore-level shifts. Physical Review B, 1996, 54, R2339-R2342.	3.2	38
136	Charge fluctuations and concentration fluctuations at intermediate-range distances in the disordered network-forming materialsSiO2,SiSe2, andGeSe2. Physical Review B, 2004, 70, .	3.2	38
137	Surface Polarons Reducing Overpotentials in the Oxygen Evolution Reaction. ACS Catalysis, 2018, 8, 5847-5851.	11.2	37
138	Structural Composition of First-Neighbor Shells in GeSe₂ and GeSe₄ Glasses from a First-Principles Analysis of NMR Chemical Shifts. Journal of Physical Chemistry C, 2011, 115, 7755-7759.	3.1	36
139	Nonempirical hybrid functionals for band gaps of inorganic metal-halide perovskites. Physical Review Materials, 2019, 3, .	2.4	35
140	Dynamical monopoles and dipoles in a condensed molecular system: The case of liquid water. Physical Review B, 2003, 68, .	3.2	34
141	Polarizability and dielectric constant in density-functional supercell calculations with discretek-point samplings. Physical Review B, 2003, 68, .	3.2	34
142	Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal. Chemical Physics, 1998, 233, 343-352.	1.9	33
143	Identification of defect levels at As/oxide interfaces through hybrid functionals. Microelectronic Engineering, 2011, 88, 1436-1439.	2.4	32
144	Carbon rehybridization at the graphene/SiC(0001) interface: Effect on stability and atomic-scale corrugation. Physical Review B, 2012, 85, .	3.2	32

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145	Vibrational spectra of vitreous SiO₂and vitreous GeO₂from first principles. Journal of Physics Condensed Matter, 2007, 19, 415112.	1.8	30
146	Dangling bond charge transition levels in AlAs, GaAs, and InAs. Applied Physics Letters, 2010, 97, .	3.3	30
147	Electron trapping in substoichiometric germanium oxide. Applied Physics Letters, 2010, 97, .	3.3	30
148	Note: Assessment of the SCAN+rVV10 functional for the structure of liquid water. Journal of Chemical Physics, 2017, 147, 216101.	3.0	30
149	Breakdown of intermediate-range order in liquid GeSe2at high temperatures. Journal of Physics Condensed Matter, 2000, 12, L697-L704.	1.8	29
150	Effect of improved band-gap description in density functional theory on defect energy levels in -quartz. Physica B: Condensed Matter, 2007, 401-402, 670-673.	2.7	29
151	Fermi-level pinning through defects at GaAs/oxide interfaces: A density functional study. Physical Review B, 2015, 92, .	3.2	29
152	Accurate optical spectra through time-dependent density functional theory based on screening-dependent hybrid functionals. Physical Review Research, 2020, 2, .	3.6	29
153	Modeling of the Raman spectrum of vitreous silica: concentration of small ring structures. Physica B: Condensed Matter, 2002, 316-317, 572-574.	2.7	28
154	Noncollinear magnetism in liquid oxygen: A first-principles molecular dynamics study. Physical Review B, 2004, 70, .	3.2	28
155	Electron and Hole Polarons at the BiVO4â€“Water Interface. ACS Applied Materials & Interfaces, 2019, 11, 18423-18426.	8.0	28
156	Binding energies of ground and excited states of shallow acceptors in GaAs/Ga1â^'xAlxAs quantum wells. Physical Review B, 1990, 42, 5349-5352.	3.2	27
157	Microscopic origin of concentration fluctuations over intermediate range distances in network-forming disordered systems. Physical Review B, 2007, 75, .	3.2	27
158	Accuracy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m for calculating defect energy levels in solids. Physical Review B, 2017, 96, .	3.2	27
159	Interpretation of photoelectron spectra inCunâ^'clusters including thermal and final-state effects: The case ofCu7â^'. Physical Review B, 1996, 54, 8913-8918.	3.2	26
160	Dielectric effect of a thin SiO2 interlayer at the interface between silicon and high-k oxides. Microelectronic Engineering, 2004, 72, 299-303.	2.4	26
161	Mechanism suppressing charge recombination at iodine defects in CH3NH3PbI3 by polaron formation. Journal of Materials Chemistry A, 2018, 6, 16863-16867.	10.3	26
162	First-principles electronic structure study of Ti-PTCDA contacts. Physical Review B, 2002, 65, .	3.2	25

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163	Ab initio study of charged states of H in amorphous SiO2. Microelectronic Engineering, 2005, 80, 288-291.	2.4	25
164	Alignment of hydrogen-related defect levels at the interface. Physica B: Condensed Matter, 2007, 401-402, 546-549.	2.7	25
165	Effect of the Solvent on the Oxygen Evolution Reaction at the TiO₂â€“Water Interface. Journal of Physical Chemistry C, 2019, 123, 18467-18474.	3.1	25
166	Finite-size corrections of defect energy levels involving ionic polarization. Physical Review B, 2020, 102, .	3.2	25
167	Structure of liquidGexSe1â^'xat the stiffness threshold composition. Physical Review B, 1998, 58, R14661-R14664.	3.2	24
168	Number of independent partial structure factors for a disorderedn-component system. Physical Review B, 1999, 59, 5-7.	3.2	24
169	Absence of charge-charge correlations at intermediate-range distances in disordered network-forming materials. Physical Review B, 2003, 68, .	3.2	24
170	Dielectric susceptibility of dipolar molecular liquids by ab initio molecular dynamics: application to liquid HCl. Chemical Physics Letters, 2004, 390, 193-198.	2.6	24
171	Redox Levels through Constant Fermi-Level ab Initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 1769-1777.	5.3	24
172	Electronic and structural characterization of barrier-type amorphous aluminium oxide. Electrochimica Acta, 2017, 224, 503-516.	5.2	24
173	Sizable Excitonic Effects Undermining the Photocatalytic Efficiency of Î²-Cu₂V₂O₇. Journal of Physical Chemistry Letters, 2018, 9, 5698-5703.	4.6	24
174	Adjustable potential probes for band-gap predictions of extended systems through nonempirical hybrid functionals. Physical Review B, 2019, 99, .	3.2	24
175	Density-functional perturbational theory for dielectric tensors in the ultrasoft pseudopotential scheme. Physical Review B, 2004, 69, .	3.2	23
176	Abrupt model interface for the 4H(1000)SiC-SiO2 interface. Microelectronic Engineering, 2005, 80, 38-41.	2.4	23
177	Equivalent oxide thickness of a thin oxide interlayer in gate insulator stacks on silicon. Applied Physics Letters, 2005, 86, 192901.	3.3	23
178	Comparison between various finite-size supercell correction schemes for charged defect calculations. Physica B: Condensed Matter, 2012, 407, 3063-3067.	2.7	23
179	Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets. Journal of Chemical Theory and Computation, 2016, 12, 3456-3462.	5.3	23
180	Theory of excitons in GaAsî—¸Ga1â^'xAlxAs quantum wells including valence band mixing. Superlattices and Microstructures, 1989, 5, 59-63.	3.1	22

#	Article	IF	Citations
181	Infrared transitions between shallow acceptor states in GaAs-Ga1â^'xAlxAs quantum wells. Physical Review B, 1991, 44, 1118-1127.	3.2	22
182	Hydrogen in Si(100)â€"SiO2â€"HfO2 gate stacks: Relevant charge states and their location. Applied Physics Letters, 2007, 91, .	3.3	22
183	Proton-Induced Fixed Positive Charge at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Si</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>100</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 662 Td (stretchy="fals mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Interfac Physical Review Letters, 2007, 99, 126102.	7.8	21
184	Vibrational amplitudes in vitreous silica. Physical Review B, 2000, 61, 3951-3959.	3.2	20
185	Mixed Wannier-Bloch Functions for Electrons and Phonons in Periodic Systems. Physical Review Letters, 2006, 96, 216403.	7.8	20
186	Band gaps of liquid water and hexagonal ice through advanced electronic-structure calculations. Physical Review Research, 2021, 3, .	3.6	20
187	Nitrogen 1s core-level shifts at the NH3 saturated Si(100)-2Ã—1 surface: a first-principles study. Surface Science, 2001, 490, L614-L618.	1.9	19
188	First-principles analysis of the Raman spectrum of vitreous silica: comparison with the vibrational density of states. Journal of Physics Condensed Matter, 2003, 15, S1547-S1552.	1.8	19
189	Modeling Phase Separation in Nonstoichiometric Silica. Physical Review Letters, 2004, 93, 135501.	7.8	19
190	Titanium oxides and silicates as high-Îº dielectrics: A first-principles investigation. International Journal of Quantum Chemistry, 2005, 101, 793-801.	2.0	19
191	Atomic-scale modelling of kinetic processes occurring during silicon oxidation. Journal of Physics Condensed Matter, 2005, 17, S2051-S2063.	1.8	19
192	Band alignment and chemical bonding at the GaAs/Al2O3 interface: A hybrid functional study. Applied Physics Letters, 2015, 107, .	3.3	19
193	Reaction pathway of oxygen evolution on Pt(1â€¯1â€¯1) revealed through constant Fermi level molecular dynamics. Journal of Catalysis, 2019, 375, 135-139.	6.2	19
194	Evaluation of Photocatalysts for Water Splitting through Combined Analysis of Surface Coverage and Energy-Level Alignment. ACS Catalysis, 2020, 10, 13186-13195.	11.2	19
195	Band alignment at <i>Î²</i> -Ga2O3/III-N (III = Al, Ga) interfaces through hybrid functional calculations. Applied Physics Letters, 2020, 117, .	3.3	19
196	Two-photon transitions to excitons in quantum wells. Physical Review B, 1990, 42, 9073-9079.	3.2	18
197	First-principles study of Siâ€‰2p core-level shifts at water and hydrogen covered Si(001)2Ã—1 surfaces. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1996, 14, 2809.	1.6	18
198	Modeling of Si 2p core-level shifts at Siâ€"(ZrO2)x(SiO2)1â^'x interfaces. Applied Physics Letters, 2002, 81, 4233-4235.	3.3	18

#	Article	IF	Citations
199	Ab InitioMolecular Dynamics Investigation of the Structure and the Noncollinear Magnetism in Liquid Oxygen: Occurrence ofO4Molecular Units. Physical Review Letters, 2002, 89, 197204.	7.8	18
200	Amorphous hafnium silicates: structural, electronic and dielectric properties. Microelectronic Engineering, 2007, 84, 2416-2419.	2.4	18
201	A hybrid functional scheme for defect levels and band alignments at semiconductorâ€“oxide interfaces. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 270-276.	1.8	18
202	Charge transition levels of nitrogen dangling bonds at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>SiO</mml:mt A first-principles study. Physical Review B, 2010, 81, .	3.2	18
203	Hole diffusion across leaky amorphous TiO₂coating layers for catalytic water splitting at photoanodes. Journal of Materials Chemistry A, 2018, 6, 11804-11810.	10.3	18
204	Si 2p core-level shifts in small molecules: a first principles study. Physica Scripta, 1996, T66, 118-120.	2.5	17
205	Cu++ and Li+ interaction with polyethylene oxide byab initiomolecular dynamics. Journal of Chemical Physics, 1998, 108, 9933-9936.	3.0	17
206	First-principle study of C 1s core-level shifts in amorphous carbon. Computational Materials Science, 2001, 22, 67-72.	3.0	17
207	Electronic properties of an epitaxial silicon oxynitride layer on a 6H-SiC(0001) surface: A first-principles investigation. Applied Physics Letters, 2007, 91, 061930.	3.3	17
208	Semiconductor defects at the interface. Physica B: Condensed Matter, 2007, 401-402, 556-559.	2.7	17
209	Theoretical calculations of shallow acceptor states in GaAs/AlxGa1â^'xAs quantum wells in the presence of an external magnetic field. Physical Review B, 1994, 50, 2393-2398.	3.2	16
210	Chemisorption pathways and Siâ€Š2p core-level shifts for the interaction of spherosiloxane clusters with Si(100): Implications for photoemission in Si/SiO2 systems. Applied Physics Letters, 2000, 76, 3873-3875.	3.3	16
211	Germanium core-level shifts at Ge/GeO<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>interfaces through hybrid functionals. Physical Review B, 2012, 85, .	3.2	16
212	Origin of Fermi-level pinning at GaAs surfaces and interfaces. Journal of Physics Condensed Matter, 2014, 26, 492202.	1.8	16
213	Polarization dependence of multiphoton transitions. Physical Review B, 1991, 43, 3837-3846.	3.2	15
214	Concentration fluctuations on intermediate range distances in liquid GeSe2: the critical role of ionicity. Computational Materials Science, 2000, 17, 115-121.	3.0	15
215	Carbon diffusion in CVD growth of carbon nanotubes on metal nanoparticles. Physica Status Solidi (B): Basic Research, 2008, 245, 2185-2188.	1.5	15
216	Charge state of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>O</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math during silicon oxidation through hybrid functional calculations. Physical Review B, 2008, 78, .	3.2	15

#	Article	IF	Citations
217	First principles study of substoichiometric germanium oxides. Microelectronic Engineering, 2009, 86, 1760-1762.	2.4	15
218	Vertex function compliant with the Ward identity for quasiparticle self-consistent calculations beyond <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m Physical Review B, 2021, 103, .	3.2	15
219	Small Electron Polarons in CsPbBr₃: Competition between Electron Localization and Delocalization. Chemistry of Materials, 2020, 32, 8393-8400.	6.7	15
220	Variational calculation of Fano linewidth: Application to excitons in quantum wells. Physical Review B, 1991, 44, 3162-3167.	3.2	14
221	First-principles simulation of vitreous systems. Current Opinion in Solid State and Materials Science, 2001, 5, 503-508.	11.5	14
222	Energy levels of candidate defects at SiCâˆ•SiO[sub 2] interfaces. AIP Conference Proceedings, 2010, , .	0.4	14
223	Formation of substoichiometric GeOx at the Geâ€“HfO2 interface. Applied Physics Letters, 2010, 97, 202908.	3.3	14
224	Band offsets at Ge/GeO2 interfaces: Effect of different interfacial bonding patterns. Microelectronic Engineering, 2011, 88, 1467-1470.	2.4	14
225	Oxygen evolution reaction: Bifunctional mechanism breaking the linear scaling relationship. Journal of Chemical Physics, 2020, 152, 104712.	3.0	14
226	Atomistic model structure of the Ge(100)â€“GeO2 interface. Microelectronic Engineering, 2009, 86, 1589-1591.	2.4	13
227	Vibrational properties of vitreous GeSe2with the Beckeâ€“Leeâ€“Yangâ€“Parr density functional. Journal of Physics Condensed Matter, 2011, 23, 295401.	1.8	13
228	Amphoteric defects in GaAs leading to Fermi-level pinning: A hybrid functional study. Microelectronic Engineering, 2013, 109, 50-53.	2.4	13
229	First principles study of As 2p core-level shifts at GaAs/Al2O3 interfaces. Applied Physics Letters, 2013, 102, .	3.3	13
230	Arsenic related defect states resonant with the semiconductor conduction band at the In0.53Ga0.47As/oxide interface: A density functional study. Microelectronic Engineering, 2015, 147, 260-263.	2.4	13
231	Giant apparent lattice distortions in STM images of corrugated sp²-hybridised monolayers. New Journal of Physics, 2016, 18, 103027.	2.9	13
232	Atomic-Level Description of Thermal Fluctuations in Inorganic Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2022, 13, 3382-3391.	4.6	13
233	Atomistic model structure of the Si(100)â€“SiO2 interface from a synthesis of experimental data. Applied Surface Science, 2004, 234, 190-196.	6.1	12
234	Density functional theory with finite electric field. International Journal of Quantum Chemistry, 2005, 101, 666-670.	2.0	12

#	Article	IF	Citations
235	Atomically controlled interfaces for future nanoelectronics. Journal of Physics Condensed Matter, 2005, 17, V1-V5.	1.8	12
236	Formation energy of threefold coordinated oxygen in SiO2 systems. Applied Surface Science, 2000, 166, 451-454.	6.1	11
237	O2 oxidation reaction at the Si(100)-SiO2 interface: A first-principles investigation. Journal of Materials Science, 2005, 40, 3047-3050.	3.7	11
238	Modelling of paramagnetic trivalent silicon defect centres in amorphous silica and at Siâ€“SiO2 interfaces. Journal of Physics Condensed Matter, 2005, 17, S2099-S2113.	1.8	11
239	Umari and Pasquarello Reply:. Physical Review Letters, 2006, 96, .	7.8	11
240	Li-related defects in ZnO: Hybrid functional calculations. Physica B: Condensed Matter, 2009, 404, 4797-4799.	2.7	11
241	First-principles investigation of the relation between structural and NMR parameters in vitreous GeO2. Journal of Physics Condensed Matter, 2010, 22, 145501.	1.8	11
242	Charge trapping in substoichiometric germanium oxide. Microelectronic Engineering, 2011, 88, 1428-1431.	2.4	11
243	Electron density of states at Ge/oxide interfaces due to formation. Microelectronic Engineering, 2011, 88, 391-394.	2.4	11
244	Low-strain interface models for epitaxial graphene on SiC(0001). Diamond and Related Materials, 2012, 23, 178-183.	3.9	11
245	Accurate determination of charge transition levels of the As-As dimer defect at GaAs/oxide interfaces through hybrid functionals. Applied Physics Letters, 2013, 103, .	3.3	11
246	Minimum energy path and atomistic mechanism of the elementary step in oxygen diffusion in silicon: A density-functional study. Physical Review B, 2014, 89, .	3.2	11
247	Oxygen defects in GaAs: A hybrid functional study. Physical Review B, 2016, 93, .	3.2	11
248	Migration of Mg and other interstitial metal dopants in GaN. Physica Status Solidi - Rapid Research Letters, 2017, 11, 1700081.	2.4	11
249	Defect Formation Energies of Interstitial C, Si, and Ge Impurities in Î² â€Ga 2 O 3. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800633.	2.4	11
250	High-performance NiOOH/FeOOH electrode for OER catalysis. Journal of Chemical Physics, 2021, 154, 024706.	3.0	11
251	Atomic structure at the Si(001)â€“SiO2 interface: from the interpretation of Si 2p core-level shifts to a model structure. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2002, 96, 102-106.	3.5	10
252	Structural properties of amorphous GeSe₂. Journal of Physics Condensed Matter, 2007, 19, 415111.	1.8	10

#	Article	IF	Citations
253	Defect energy levels of the Asâ€“As dimer at InGaAs/oxide interfaces: A first principles study. Microelectronic Engineering, 2013, 109, 60-63.	2.4	10
254	The OAs defect in GaAs: A hybrid density functional study. Applied Surface Science, 2014, 291, 6-10.	6.1	10
255	Intercalation of H at the graphene/SiC(0001) interface: Structure and stability from first principles. Applied Surface Science, 2014, 291, 64-68.	6.1	10
256	Interfacial Ga-As suboxide: Structural and electronic properties. Applied Physics Letters, 2015, 107, .	3.3	10
257	Reactivity and energy level of a localized hole in liquid water. Physical Chemistry Chemical Physics, 2018, 20, 30281-30289.	2.8	10
258	One-Shot Approach for Enforcing Piecewise Linearity on Hybrid Functionals: Application to Band Gap Predictions. Journal of Physical Chemistry Letters, 2022, 13, 3066-3071.	4.6	10
259	Interpretation of three-photon spectra in alkali halides. Physical Review B, 1990, 41, 12230-12235.	3.2	9
260	Effect of continuum states on two-photon absorption in quantum wells. Physical Review B, 1990, 41, 12728-12734.	3.2	9
261	Magnetic properties of theS-like bound hole states in GaAs/AlxGa1â^'xAs quantum wells. Physical Review B, 1994, 49, 10794-10797.	3.2	9
262	Dependence of the O2diffusion rate on oxide thickness during silicon oxidation. Journal of Physics Condensed Matter, 2003, 15, S1553-S1560.	1.8	9
263	Stability and charge transfer at the interface between SiC(0001) and epitaxial graphene. Microelectronic Engineering, 2011, 88, 1478-1481.	2.4	9
264	One-dimensional random potentials allowing for extended states. Journal of Physics Condensed Matter, 1989, 1, 9509-9512.	1.8	8
265	Excitonic effects on the two-photon transition rate in quantum wells. Superlattices and Microstructures, 1991, 9, 157-160.	3.1	8
266	Assignment of Fermi-level pinning and optical transitions to the (AsGa)2-OAs center in oxygen-doped GaAs. Applied Physics Letters, 2013, 103, 142108.	3.3	8
267	Unraveling the synergy between metalâ€“organic frameworks and co-catalysts in photocatalytic water splitting. Journal of Materials Chemistry A, 2020, 8, 20493-20502.	10.3	8
268	Infrared-absorption spectra of acceptors confined in GaAs/AlxGa1â^'xAs quantum wells in the presence of an external magnetic field. Physical Review B, 1994, 50, 10953-10957.	3.2	7
269	A first principles study of small Cun clusters based on local-density and generalized-gradient approximations to density functional theory. Computational Materials Science, 1998, 10, 463-467.	3.0	7
270	Infrared properties of ultrathin oxides on Si(100). Microelectronic Engineering, 2005, 80, 420-423.	2.4	7

#	Article	IF	Citations
271	(Invited) Electronic and Structural Properties at Ge/GeO₂ Interfaces: A Density-Functional Investigation. ECS Transactions, 2010, 33, 123-132.	0.5	7
272	Overcoming Bipolar Doping Difficulty in Wide Gap Semiconductors. , 2011, , 213-239.		7
273	Partial Molar Volumes of Aqua Ions from First Principles. Journal of Chemical Theory and Computation, 2017, 13, 3427-3431.	5.3	7
274	Extrinsic Defects in Amorphous Oxides: Hydrogen, Carbon, and Nitrogen Impurities in Alumina. Physical Review Applied, 2019, 11, .	3.8	7
275	Low-Frequency Dielectric Response of Tetragonal Perovskite CH₃NH₃PbI₃. Journal of Physical Chemistry Letters, 2020, 11, 6279-6285.	4.6	7
276	Band alignment at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CaF</mml:mi><mml:mn>2</mml:mn></mml	3.2	7
	interface through advanced electronic structure calculations. Physical Review B, 2020, 101, .		
277	Hole subbands in quantum wells: Comparison between theory and hot-electron-acceptor-luminescence experiments. Physical Review B, 1992, 46, 2625-2627.	3.2	6
278	Oxygen species in SiO2: a first-principles investigation. Microelectronic Engineering, 2001, 59, 167-172.	2.4	6
279	Evidence of concentration fluctuations in disordered network-forming systems: the case of GeSe4and SiSe2. Journal of Physics Condensed Matter, 2003, 15, S1537-S1546.	1.8	6
280	Electronic Structure at Realistic Si(100)-SiO2Interfaces. Japanese Journal of Applied Physics, 2004, 43, 7895-7898.	1.5	6
281	Comment on â€œStructural Analysis of theSiO2/Si(100)Interface by Means of Photoelectron Diffractionâ€• Physical Review Letters, 2005, 94, 189601; discussion 189602.	7.8	6
282	Ab initio molecular dynamics of liquid hydrogen chloride. Journal of Chemical Physics, 2005, 122, 114512.	3.0	6
283	Hyper-Raman Spectrum of Vitreous Silica from First Principles. Physical Review Letters, 2007, 98, .	7.8	6
284	Band gap opening at the 6Hâ€“SiC(0001) surface passivated by an epitaxial silicon oxynitride layer: A first-principles investigation. Surface Science, 2008, 602, 2989-2993.	1.9	6
285	First-principles theory of infrared absorption spectra at surfaces and interfaces: Application to theSi(100):H2Osurface. Physical Review B, 2008, 78, .	3.2	6
286	Electronic Structure of Water from Koopmans-Compliant Functionals. Journal of Chemical Theory and Computation, 2021, 17, 3923-3930.	5.3	6
287	Core-Level Shifts in Si(001)-SiO2 Systems: The Value of First-Principle Investigations. , 1998, , 89-102.		5
288	Energetics of oxygen species in crystalline and amorphous SiO2: a first-principles investigation. Solid-State Electronics, 2002, 46, 1873-1878.	1.4	5

#	Article	IF	Citations
289	Silicon crystal distortions at the Si(100)â€“SiO2 interface from analysis of ion-scattering. Microelectronic Engineering, 2004, 72, 197-200.	2.4	5
290	Supported nanoclusters: Preadsorbates tuning catalytic activity. Physical Review B, 2005, 71, .	3.2	5
291	Alignment of Defect Energy Levels at Si-SiO[sub 2] Interface from Hybrid Density Functional Calculations. , 2010, , .		5
292	First principles study of electronic and structural properties of the Ge/GeO2 interface. Physica B: Condensed Matter, 2012, 407, 2926-2931.	2.7	5
293	Defect levels at GaAs/Al2O3 interfaces: Asâ€“As dimer vs. Ga dangling bond. Applied Surface Science, 2014, 291, 16-19.	6.1	5
294	Comment on â€œFundamental Resolution of Difficulties in the Theory of Charged Point Defects in Semiconductorsâ€• Physical Review Letters, 2018, 120, 039603.	7.8	5
295	Comment on â€˜â€˜Effect of biaxial strain on acceptor-level energies inInyGa1âˆ’yAs/AlxGa1âˆ’xAs (on GaAs) quantum wellsâ€™â€™. Physical Review B, 1990, 42, 7641-7642.	3.2	4
296	High exciton binding energies in GaAs/GaAlAs quantum wells. Superlattices and Microstructures, 1991, 9, 1-4.	3.1	4
297	Effective-State Approach to Second-Order Perturbation Theory. Europhysics Letters, 1992, 17, 387-392.	2.0	4
298	Application of variational techniques to time-dependent perturbation theory. Physical Review B, 1993, 48, 5090-5094.	3.2	4
299	Infrared absorption frequencies and oscillator strengths of acceptors confined in GaAs/AlGaAs quantum wells. Applied Physics Letters, 1994, 65, 3365-3367.	3.3	4
300	Network transformation processes during oxidation of silicon. Microelectronic Engineering, 1999, 48, 89-94.	2.4	4
301	An Electronegativity-Induced Spin Repulsion Effect. Journal of Physical Chemistry A, 2005, 109, 8385-8390.	2.5	4
302	Charge transition levels of the Ge dangling bond defect at Ge/insulator interfaces. Materials Science in Semiconductor Processing, 2008, 11, 226-229.	4.0	4
303	Stability of valence alternation pairs across the substoichiometric region at Ge/GeO2 interfaces. Physica B: Condensed Matter, 2012, 407, 2939-2942.	2.7	4
304	First-principles study of H adsorption on graphene/SiC(0001). Physica Status Solidi (B): Basic Research, 2013, 250, 2523-2528.	1.5	4
305	Diffusion of interstitial oxygen in silicon and germanium: a hybrid functional study. Journal of Physics Condensed Matter, 2016, 28, 495801.	1.8	4
306	Oxygen DX center in In0.17Al0.83N: Nonradiative recombination and persistent photoconductivity. Applied Physics Letters, 2017, 110, 072101.	3.3	4

#	Article	IF	Citations
307	Identification of Semiconductor Defects through Constant-Fermi-Level AbÂInitio Molecular Dynamics: Application to GaAs. Physical Review Applied, 2017, 8, .	3.8	4
308	Electron trap states at InGaAs/oxide interfaces under inversion through constant Fermi-levelab initiomolecular dynamics. Journal of Physics Condensed Matter, 2017, 29, 505702.	1.8	4
309	Partial vibrational density of states for amorphous solids from inelastic neutron scattering. Physical Review B, 2018, 98, .	3.2	4
310	Car-Parrinello Molecular Dynamics in a Finite Homogeneous Electric Field. AIP Conference Proceedings, 2003, , .	0.4	3
311	Protons at the Si-SiO2 interface: a first principle investigation. Microelectronic Engineering, 2007, 84, 2035-2038.	2.4	3
312	Hydrogen Bonding of Ammonia with (H,OH)-Si(001) Revealed by Experimental and Ab Initio Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 5378-5388.	2.5	3
313	Magneto-optical studies of acceptors confined in GaAs/AlxGa1â^'xAs quantum wells. Physical Review B, 1994, 50, 4901-4904.	3.2	2
314	Structural and magnetic correlations in liquid oxygen: anab initiomolecular dynamics study. Journal of Physics Condensed Matter, 2003, 15, S89-S94.	1.8	2
315	Nitrogen adsorption on a supported iron nanocluster. Vacuum, 2004, 74, 173-177.	3.5	2
316	Finite electric field in density functional calculations with periodic boundary conditions. Computational Materials Science, 2004, 30, 116-119.	3.0	2
317	Ion scattering simulations of theSi(100)â^'SiO2interface. Physical Review B, 2006, 74, .	3.2	2
318	Proton Diffusion in Amorphous SiO2 and Hafnium Silicate by Ab Initio Molecular Dynamics. AIP Conference Proceedings, 2007, , .	0.4	2
319	Nitrogen fixation at passivated Fe nanoclusters supported by an oxide surface: Identification of viable reaction routes using density functional calculations. Physical Review B, 2009, 80, .	3.2	2
320	Advanced Calculations for Defects in Solids â€“ Electronic Structure Methods. Physica Status Solidi (B): Basic Research, 2011, 248, 17-18.	1.5	2
321	Nature of electron trap states under inversion at In0.53Ga0.47As/Al2O3 interfaces. Applied Physics Letters, 2017, 110, 111602.	3.3	2
322	Polarization dependence of two-photon transitions in quantum wells. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1991, 13, 337-342.	0.4	1
323	Complex Pattern of Impurity States in Shallow Semiconductor Quantum Wells. Europhysics Letters, 1991, 15, 447-451.	2.0	1
324	Shallow Impurities in GaAs-Ga1-xAlxAs Quantum Wells. Physica Scripta, 1991, T39, 182-187.	2.5	1

#	Article	IF	Citations
325	Ab initio molecular dynamics: application to liquid copper. Computational Materials Science, 1993, 1, 419-427.	3.0	1
326	FIRST-PRINCIPLES STUDIES OF Cu CLUSTERS. Surface Review and Letters, 1996, 03, 287-291.	1.1	1
327	Modelling of dielectric constants of amorphous Zr silicates. Journal of Physics Condensed Matter, 2005, 17, S2089-S2098.	1.8	1
328	Structural and Electronic Properties of Oxygen Vacancies in Monoclinic HfO2. Materials Research Society Symposia Proceedings, 2007, 996, 1.	0.1	1
329	Atomistic model of the 4H(0001)SiC-SiO2 interface: structural and electronic properties. AIP Conference Proceedings, 2007, , .	0.4	1
330	Core-Level Photoelectron Spectroscopy Probing Local Strain at Silicon Surfaces and Interfaces. AIP Conference Proceedings, 2007, , .	0.4	1
331	Defect Levels of the Ge Dangling Bond Defect. , 2010, , .		1
332	A Generalization of the Effective-Charge Concept: Dynamical Multipoles in Molecular Solids and Liquids. AIP Conference Proceedings, 2002, , .	0.4	0
333	Atomic-scale investigation of the dielectric screening at the interface between silicon and its oxide. Materials Research Society Symposia Proceedings, 2003, 786, 511.	0.1	0
334	Ã‰tude de propriÃ©tÃ©s structurales et dynamiques par dynamique molÃ©culaire ab initio : application aux verres et aux liquides vitreux. European Physical Journal Special Topics, 2003, 111, 373-393.	0.2	0
335	Atomic-Scale Modelling of the Si(100)-SiO2 Interface. AIP Conference Proceedings, 2005, , .	0.4	0
336	Metal catalyst in CVD growth of carbon nanotubes: role of chemical composition. , 2010, , .		0
337	Medium range structure of tetrahedrally-bonded glasses through the first principles investigation of Raman spectra. , 2012, , .		0
338	Migration of Mg and other interstitial metal dopants in GaN (Phys. Status Solidi RRL 7/2017). Physica Status Solidi - Rapid Research Letters, 2017, 11, 1770337.	2.4	0
339	Exploring Defects in Semiconductor Materials Through Constant Fermi Level Ab-Initio Molecular Dynamics. Springer Series in Materials Science, 2020, , 39-55.	0.6	0