

Alfredo Pasquarello

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350 papers	29,608 citations	67 h-index	167 g-index
370 ext. papers	33,186 ext. citations	4.7 avg, IF	7.08 L-index

#	Paper	IF	Citations
350	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , 2009 , 21, 395502	1.8	13251
349	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. <i>Physical Review B</i> , 1993 , 47, 10142-10153	3.3	1181
348	Identification of Raman Defect Lines as Signatures of Ring Structures in Vitreous Silica. <i>Physical Review Letters</i> , 1998 , 80, 5145-5147	7.4	337
347	Accurate theory of excitons in GaAs-Ga _{1-x} Al _x As quantum wells. <i>Physical Review B</i> , 1990 , 42, 8928-8938	3.3	336
346	Ab initio molecular dynamics for d-electron systems: Liquid copper at 1500 K. <i>Physical Review Letters</i> , 1992 , 69, 1982-1985	7.4	333
345	First solvation shell of the Cu(II) aqua ion: evidence for fivefold coordination. <i>Science</i> , 2001 , 291, 856-9	33.3	314
344	Finite-size supercell correction schemes for charged defect calculations. <i>Physical Review B</i> , 2012 , 86,	3.3	295
343	Fully Unconstrained Approach to Noncollinear Magnetism: Application to Small Fe Clusters. <i>Physical Review Letters</i> , 1998 , 80, 3622-3625	7.4	291
342	sp ² /sp ³ hybridization ratio in amorphous carbon from C 1s core-level shifts: X-ray photoelectron spectroscopy and first-principles calculation. <i>Physical Review B</i> , 2001 , 65,	3.3	281
341	Ab initio molecular dynamics in a finite homogeneous electric field. <i>Physical Review Letters</i> , 2002 , 89, 157602	7.4	266
340	Structural and electronic properties of liquid and amorphous SiO ₂ : An ab initio molecular dynamics study. <i>Physical Review Letters</i> , 1995 , 74, 4682-4685	7.4	251
339	Organic Cathode for Aqueous Zn-Ion Batteries: Taming a Unique Phase Evolution toward Stable Electrochemical Cycling. <i>Chemistry of Materials</i> , 2018 , 30, 3874-3881	9.6	236
338	Defect energy levels in density functional calculations: alignment and band gap problem. <i>Physical Review Letters</i> , 2008 , 101, 046405	7.4	231
337	Defect levels through hybrid density functionals: Insights and applications. <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 775-789	1.3	228
336	Hole subbands in strained GaAs-Ga _{1-x} Al _x As quantum wells: Exact solution of the effective-mass equation. <i>Physical Review B</i> , 1987 , 36, 5887-5894	3.3	216
335	Interface structure between silicon and its oxide by first-principles molecular dynamics. <i>Nature</i> , 1998 , 396, 58-60	50.4	209
334	Band offsets at semiconductor-oxide interfaces from hybrid density-functional calculations. <i>Physical Review Letters</i> , 2008 , 101, 106802	7.4	207

333	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. <i>Physical Review B</i> , 1996 , 53, 1180-1185	3.3	204
332	Oxygen vacancy in monoclinic HfO ₂ : A consistent interpretation of trap assisted conduction, direct electron injection, and optical absorption experiments. <i>Applied Physics Letters</i> , 2006 , 89, 262904	3.4	200
331	Theory of Si 2p core-level shifts at the Si(001)-SiO ₂ interface. <i>Physical Review B</i> , 1996 , 53, 10942-10950	3.3	200
330	Structure and Hyperfine Parameters of E1' Centers in Quartz and in Vitreous SiO ₂ . <i>Physical Review Letters</i> , 1997 , 78, 887-890	7.4	194
329	Effect of metal elements in catalytic growth of carbon nanotubes. <i>Physical Review Letters</i> , 2008 , 100, 156102	7.4	176
328	Si 2p core-level shifts at the Si(001)-SiO ₂ interface: A first-principles study. <i>Physical Review Letters</i> , 1995 , 74, 1024-1027	7.4	174
327	Model of vitreous SiO ₂ generated by an ab initio molecular-dynamics quench from the melt. <i>Physical Review B</i> , 1995 , 52, 12690-12695	3.3	163
326	Si-O-Si bond-angle distribution in vitreous silica from first-principles ²⁹ Si NMR analysis. <i>Physical Review B</i> , 2000 , 62, R4786-R4789	3.3	145
325	Raman scattering intensities in Quartz: A first-principles investigation. <i>Physical Review B</i> , 2001 , 63,	3.3	143
324	Band offsets at the Si/SiO ₂ interface from many-body perturbation theory. <i>Physical Review Letters</i> , 2008 , 100, 186401	7.4	141
323	Dynamical Charge Tensors and Infrared Spectrum of Amorphous SiO ₂ . <i>Physical Review Letters</i> , 1997 , 79, 1766-1769	7.4	133
322	Defect levels of dangling bonds in silicon and germanium through hybrid functionals. <i>Physical Review B</i> , 2008 , 78,	3.3	133
321	First-principles investigation of high- ϵ dielectrics: Comparison between the silicates and oxides of hafnium and zirconium. <i>Physical Review B</i> , 2004 , 69,	3.3	124
320	Band-edge problem in the theoretical determination of defect energy levels: The O vacancy in ZnO as a benchmark case. <i>Physical Review B</i> , 2011 , 84,	3.3	122
319	Nitrogen Incorporation at Si(001)/SiO ₂ Interfaces: Relation between N 1s Core-Level Shifts and Microscopic Structure. <i>Physical Review Letters</i> , 1997 , 79, 5174-5177	7.4	122
318	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2005 , 220,	1	122
317	Ring currents in icosahedral c60. <i>Science</i> , 1992 , 257, 1660-1	33.3	122
316	Origin of the High-Frequency Doublet in the Vibrational Spectrum of Vitreous SiO ₂ . <i>Science</i> , 1997 , 275, 1925-7	33.3	121

315	First-principles study of dynamical and dielectric properties of tetragonal zirconia. <i>Physical Review B</i> , 2001 , 64,	3.3	121
314	Concentration of small ring structures in vitreous silica from a first-principles analysis of the Raman spectrum. <i>Physical Review Letters</i> , 2003 , 90, 027401	7.4	116
313	Migration of oxygen vacancy in HfO ₂ and across the HfO ₂ /SiO ₂ interface: A first-principles investigation. <i>Applied Physics Letters</i> , 2007 , 91, 192905	3.4	114
312	Oxide versus Nonoxide Cathode Materials for Aqueous Zn Batteries: An Insight into the Charge Storage Mechanism and Consequences Thereof. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 674-682	9.5	114
311	Finite-size supercell correction for charged defects at surfaces and interfaces. <i>Physical Review Letters</i> , 2013 , 110, 095505	7.4	113
310	Alignment of defect levels and band edges through hybrid functionals: Effect of screening in the exchange term. <i>Physical Review B</i> , 2010 , 81,	3.3	112
309	Theory of atomic-scale dielectric permittivity at insulator interfaces. <i>Physical Review B</i> , 2005 , 71,	3.3	108
308	Structurally relaxed models of the Si(001)/SiO ₂ interface. <i>Applied Physics Letters</i> , 1996 , 68, 625-627	3.4	104
307	Magnetoresistive junctions based on epitaxial graphene and hexagonal boron nitride. <i>Physical Review B</i> , 2009 , 80,	3.3	98
306	Hybrid-functional calculations with plane-wave basis sets: Effect of singularity correction on total energies, energy eigenvalues, and defect energy levels. <i>Physical Review B</i> , 2009 , 80,	3.3	96
305	Ring currents in topologically complex molecules: Application to C ₆₀ , C ₇₀ , and their hexa-anions. <i>Physical Review A</i> , 1993 , 47, 1783-1789	2.6	96
304	Dangling bond defects at Si-SiO ₂ interfaces: atomic structure of the P(b1) center. <i>Physical Review Letters</i> , 2000 , 85, 2773-6	7.4	93
303	Nonempirical dielectric-dependent hybrid functional with range separation for semiconductors and insulators. <i>Physical Review Materials</i> , 2018 , 2,	3.2	93
302	A hybrid density functional study of lithium in ZnO: Stability, ionization levels, and diffusion. <i>Physical Review B</i> , 2009 , 80,	3.3	92
301	Dynamic structure factor of vitreous silica from first principles: Comparison to neutron-inelastic-scattering experiments. <i>Physical Review B</i> , 1998 , 57, 14133-14140	3.3	88
300	Structural and electronic properties of small copper clusters: a first principles study. <i>Chemical Physics Letters</i> , 1995 , 238, 215-221	2.5	87
299	Origin of low electron-hole recombination rate in metal halide perovskites. <i>Energy and Environmental Science</i> , 2018 , 11, 101-105	35.4	86
298	Oxygen diffusion through the disordered oxide network during silicon oxidation. <i>Physical Review Letters</i> , 2002 , 88, 125901	7.4	86

297	Self-compensation due to point defects in Mg-doped GaN. <i>Physical Review B</i> , 2016 , 93,	3.3	85
296	Pressure-induced structural changes in liquid SiO ₂ from Ab initio simulations. <i>Physical Review Letters</i> , 2002 , 89, 245504	7.4	83
295	Band offsets of lattice-matched semiconductor heterojunctions through hybrid functionals and G0W0. <i>Physical Review B</i> , 2014 , 89,	3.3	81
294	Multiscale modeling of oxygen diffusion through the oxide during silicon oxidation. <i>Physical Review B</i> , 2004 , 70,	3.3	81
293	First-principles study of structural, electronic, dynamical, and dielectric properties of zircon. <i>Physical Review B</i> , 2001 , 63,	3.3	80
292	Metal adatoms on graphene and hexagonal boron nitride: Towards rational design of self-assembly templates. <i>Physical Review B</i> , 2010 , 82,	3.3	78
291	Transition structure at the Si(100)-SiO ₂ interface. <i>Physical Review Letters</i> , 2003 , 90, 186101	7.4	77
290	Short- and intermediate-range structure of liquid GeSe ₂ . <i>Physical Review B</i> , 2001 , 64,	3.3	75
289	Structural and electronic properties of small Cu _n clusters using generalized-gradient approximations within density functional theory. <i>Journal of Chemical Physics</i> , 1998 , 109, 6626-6630	3.9	74
288	Effect of Subband Coupling on Exciton Binding Energies and Oscillator Strengths in GaAs-Ga 1- x Al x As Quantum Wells. <i>Europhysics Letters</i> , 1988 , 6, 259-264	1.6	74
287	Microscopic Structure of Liquid GeSe ₂ : The Problem of Concentration Fluctuations over Intermediate Range Distances. <i>Physical Review Letters</i> , 1998 , 80, 2342-2345	7.4	72
286	Dielectric discontinuity at interfaces in the atomic-scale limit: permittivity of ultrathin oxide films on silicon. <i>Physical Review Letters</i> , 2003 , 91, 267601	7.4	71
285	Assessing the accuracy of hybrid functionals in the determination of defect levels: Application to the As antisite in GaAs. <i>Physical Review B</i> , 2011 , 84,	3.3	69
284	Charge transition levels of carbon-, oxygen-, and hydrogen-related defects at the SiC/SiO ₂ interface through hybrid functionals. <i>Physical Review B</i> , 2011 , 84,	3.3	69
283	Atomistic structure of the Si(100)/SiO ₂ interface: A synthesis of experimental data. <i>Applied Physics Letters</i> , 2003 , 83, 1417-1419	3.4	65
282	Reaction of the oxygen molecule at the Si(100)-SiO ₂ interface during silicon oxidation. <i>Physical Review Letters</i> , 2004 , 93, 086102	7.4	64
281	Predictive Determination of Band Gaps of Inorganic Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 5507-5512	6.4	63
280	Density-functional perturbation theory for lattice dynamics with ultrasoft pseudopotentials. <i>Physical Review B</i> , 1997 , 56, R11369-R11372	3.3	63

279	Dielectric constants of Zr silicates: a first-principles study. <i>Physical Review Letters</i> , 2002 , 89, 117601	7.4	63
278	Band-edge levels in semiconductors and insulators: Hybrid density functional theory versus many-body perturbation theory. <i>Physical Review B</i> , 2012 , 86,	3.3	62
277	Band offsets at the Ge/GeO ₂ interface through hybrid density functionals. <i>Applied Physics Letters</i> , 2009 , 94, 141911	3.4	61
276	Band alignments and defect levels in Si/HfO ₂ gate stacks: Oxygen vacancy and Fermi-level pinning. <i>Applied Physics Letters</i> , 2008 , 92, 132911	3.4	61
275	First principles study of photoelectron spectra of Cu _n - clusters. <i>Physical Review Letters</i> , 1995 , 75, 2104-2107	7.4	61
274	Origin of the first sharp diffraction peak in the structure factor of disordered network-forming systems: Layers or voids?. <i>Journal of Chemical Physics</i> , 2001 , 114, 7976-7979	3.9	60
273	Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions. <i>Journal of Chemical Physics</i> , 2015 , 142, 034501	3.9	57
272	Band-edge positions in GW: Effects of starting point and self-consistency. <i>Physical Review B</i> , 2014 , 90,	3.3	57
271	Fraction of boroxol rings in vitreous boron oxide from a first-principles analysis of Raman and NMR spectra. <i>Physical Review Letters</i> , 2005 , 95, 137401	7.4	57
270	Intermediate Range Order and Bonding Character in Disordered Network-Forming Systems. <i>Journal of the American Chemical Society</i> , 1999 , 121, 2943-2944	16.4	57
269	Correspondence of defect energy levels in hybrid density functional theory and many-body perturbation theory. <i>Physical Review B</i> , 2013 , 88,	3.3	56
268	Alignment of Redox Levels at Semiconductor/Water Interfaces. <i>Chemistry of Materials</i> , 2018 , 30, 94-111	9.6	56
267	Atomic structure of the two intermediate phase glasses SiSe ₄ and GeSe ₄ . <i>Physical Review B</i> , 2009 , 79,	3.3	55
266	Structural and electronic properties of an abrupt 4H-SiC(0001)/SiO ₂ interface model: Classical molecular dynamics simulations and density functional calculations. <i>Physical Review B</i> , 2007 , 76,	3.3	55
265	Vibrational spectra of vitreous germania from first-principles. <i>Physical Review B</i> , 2006 , 74,	3.3	55
264	Accurate band gaps of extended systems via efficient vertex corrections in GW. <i>Physical Review B</i> , 2015 , 92,	3.3	54
263	Short and intermediate range order in amorphous GeSe ₂ . <i>Physical Review B</i> , 2008 , 77,	3.3	54
262	Proton diffusion mechanism in amorphous SiO ₂ . <i>Physical Review Letters</i> , 2006 , 97, 155901	7.4	54

261	Validity of the bond-energy picture for the energetics at Si/SiO ₂ interfaces. <i>Physical Review B</i> , 2000 , 62, R16326-R16329	3.3	54
260	Nitrogen bonding configurations at nitrated Si(001) surfaces and Si(001)/SiO ₂ interfaces: A first-principles study of core-level shifts. <i>Physical Review B</i> , 2001 , 63,	3.3	54
259	Diffusion mechanism of Cu adatoms on a Cu(001) surface. <i>Surface Science</i> , 1994 , 306, L575-L578	1.8	54
258	Medium-range structural properties of vitreous germania obtained through first-principles analysis of vibrational spectra. <i>Physical Review Letters</i> , 2005 , 95, 075505	7.4	52
257	Binding energies of excited shallow acceptor states in GaAs/Ga _{1-x} Al _x As quantum wells. <i>Physical Review B</i> , 1989 , 40, 5602-5612	3.3	52
256	Medium-range structure of vitreous SiO ₂ obtained through first-principles investigation of vibrational spectra. <i>Physical Review B</i> , 2009 , 79,	3.3	51
255	Magnetism of carbon clusters. <i>Physical Review B</i> , 1994 , 50, 16459-16463	3.3	51
254	Ab Initio Electronic Structure of Liquid Water. <i>Physical Review Letters</i> , 2016 , 117, 186401	7.4	50
253	Role of Polarons in Water Splitting: The Case of BiVO ₄ . <i>ACS Energy Letters</i> , 2018 , 3, 1693-1697	20.1	50
252	Origin of fine structure in Si photoelectron spectra at silicon surfaces and interfaces. <i>Physical Review Letters</i> , 2006 , 96, 157601	7.4	50
251	Nonempirical hybrid functionals for band gaps and polaronic distortions in solids. <i>Physical Review B</i> , 2018 , 97,	3.3	49
250	Atomic-Scale Simulation of Electrochemical Processes at Electrode/Water Interfaces under Referenced Bias Potential. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 1880-1884	6.4	48
249	Infrared spectra at surfaces and interfaces from first principles: evolution of the spectra across the Si(100)-SiO ₂ interface. <i>Physical Review Letters</i> , 2005 , 95, 187402	7.4	48
248	Infrared spectra of jennite and tobermorite from first-principles. <i>Cement and Concrete Research</i> , 2014 , 60, 11-23	10.3	47
247	Redox levels in aqueous solution: Effect of van der Waals interactions and hybrid functionals. <i>Journal of Chemical Physics</i> , 2015 , 143, 244508	3.9	46
246	Electronic Levels of Excess Electrons in Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 20556-20559	6.4	45
245	First principles investigation of defects at interfaces between silicon and amorphous high- κ oxides. <i>Microelectronic Engineering</i> , 2007 , 84, 2022-2027	2.5	44
244	First-principles modeling of paramagnetic Si dangling-bond defects in amorphous SiO ₂ . <i>Physical Review B</i> , 2002 , 66,	3.3	44

243	Comparison of structurally relaxed models of the Si(001)-SiO ₂ interface based on different crystalline oxide forms. <i>Applied Surface Science</i> , 1996 , 104-105, 317-322	6.7	44
242	Structural, Dynamical, and Electronic Properties of Liquid Water: A Hybrid Functional Study. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 7456-70	3.4	43
241	Band gaps and dielectric constants of amorphous hafnium silicates: A first-principles investigation. <i>Applied Physics Letters</i> , 2007 , 90, 082907	3.4	43
240	Supported Fe nanoclusters: evolution of magnetic properties with cluster size. <i>Physical Review Letters</i> , 2003 , 90, 247202	7.4	42
239	Atomistic models of the Si(100)/SiO ₂ interface: structural, electronic and dielectric properties. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, S2065-S2074	1.8	41
238	First-principles study of NH ₃ exposed Si(001)/SiO ₂ : Relation between N 1s core-level shifts and atomic structure. <i>Applied Physics Letters</i> , 2000 , 76, 553-555	3.4	41
237	First principles molecular dynamics calculation of the structure and acidity of a bulk zeolite. <i>Chemical Physics Letters</i> , 1994 , 226, 245-250	2.5	41
236	Intrinsic defects in GaAs and InGaAs through hybrid functional calculations. <i>Physica B: Condensed Matter</i> , 2012 , 407, 2833-2837	2.8	40
235	First-principles investigation of the structural and vibrational properties of vitreous GeSe ₂ . <i>Physical Review B</i> , 2007 , 75,	3.3	40
234	Gauge-invariant two-photon transitions in quantum wells. <i>Physical Review B</i> , 1988 , 38, 6206-6210	3.3	40
233	Infrared and Raman spectra of disordered materials from first principles. <i>Diamond and Related Materials</i> , 2005 , 14, 1255-1261	3.5	39
232	First-principles determination of defect energy levels through hybrid density functionals and GW. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 133202	1.8	38
231	Structural assignments of NMR chemical shifts in Ge _x Se _{1-x} glasses via first-principles calculations for GeSe ₂ , Ge ₄ Se ₉ , and GeSe crystals. <i>Physical Review B</i> , 2010 , 82,	3.3	38
230	First principles investigation of defect energy levels at semiconductor-oxide interfaces: Oxygen vacancies and hydrogen interstitials in the Si/SiO ₂ /HfO ₂ stack. <i>Journal of Applied Physics</i> , 2009 , 105, 061603	2.5	38
229	Charge fluctuations and concentration fluctuations at intermediate-range distances in the disordered network-forming materials SiO ₂ , SiSe ₂ , and GeSe ₂ . <i>Physical Review B</i> , 2004 , 70,	3.3	38
228	Electronic and dielectric properties of a suboxide interlayer at the silicon/silica interface in MOS devices. <i>Surface Science</i> , 2005 , 586, 183-191	1.8	38
227	Spherosiloxane H ₈ Si ₈ O ₁₂ clusters on Si(001): First-principles calculation of Si 2p core-level shifts. <i>Physical Review B</i> , 1996 , 54, R2339-R2342	3.3	38
226	Comparison of vacancy and antisite defects in GaAs and InGaAs through hybrid functionals. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 045801	1.8	37

225	Defect levels of carbon-related defects at the SiC/SiO ₂ interface from hybrid functionals. <i>Physical Review B</i> , 2011 , 83,	3.3	36
224	Structural Composition of First-Neighbor Shells in GeSe ₂ and GeSe ₄ Glasses from a First-Principles Analysis of NMR Chemical Shifts. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 7755-7759	3.8	36
223	Absolute Energy Levels of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 3212-3216	6.4	35
222	pH-Dependent Catalytic Reaction Pathway for Water Splitting at the BiVO ₄ /Water Interface from the Band Alignment. <i>ACS Energy Letters</i> , 2018 , 3, 829-834	20.1	34
221	Energetics of native point defects in GaN: A density-functional study. <i>Microelectronic Engineering</i> , 2015 , 147, 51-54	2.5	33
220	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	33
219	Dynamical monopoles and dipoles in a condensed molecular system: The case of liquid water. <i>Physical Review B</i> , 2003 , 68,	3.3	33
218	pH-Dependent Surface Chemistry from First Principles: Application to the BiVO ₄ (010)-Water Interface. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 10011-10021	9.5	32
217	Identification of defect levels at As/oxide interfaces through hybrid functionals. <i>Microelectronic Engineering</i> , 2011 , 88, 1436-1439	2.5	32
216	Dynamics of structural relaxation upon Rydberg excitation of an impurity in an Ar crystal. <i>Chemical Physics</i> , 1998 , 233, 343-352	2.3	32
215	Comprehensive modeling of the band gap and absorption spectrum of BiVO ₄ . <i>Physical Review Materials</i> , 2017 , 1,	3.2	31
214	Polarizability and dielectric constant in density-functional supercell calculations with discrete k-point samplings. <i>Physical Review B</i> , 2003 , 68,	3.3	30
213	Oxygen defects in amorphous Al ₂ O ₃ : A hybrid functional study. <i>Applied Physics Letters</i> , 2016 , 109, 062903	3.4	30
212	Electron trapping in substoichiometric germanium oxide. <i>Applied Physics Letters</i> , 2010 , 97, 092903	3.4	29
211	Carbon rehybridization at the graphene/SiC(0001) interface: Effect on stability and atomic-scale corrugation. <i>Physical Review B</i> , 2012 , 85,	3.3	29
210	Breakdown of intermediate-range order in liquid GeSe ₂ at high temperatures. <i>Journal of Physics Condensed Matter</i> , 2000 , 12, L697-L704	1.8	29
209	Effect of improved band-gap description in density functional theory on defect energy levels in α-quartz. <i>Physica B: Condensed Matter</i> , 2007 , 401-402, 670-673	2.8	27
208	Microscopic origin of concentration fluctuations over intermediate range distances in network-forming disordered systems. <i>Physical Review B</i> , 2007 , 75,	3.3	27

207	Absolute deformation potentials of two-dimensional materials. <i>Physical Review B</i> , 2016 , 94,	3.3	27
206	Surface Polarons Reducing Overpotentials in the Oxygen Evolution Reaction. <i>ACS Catalysis</i> , 2018 , 8, 5847-5851	2.7	27
205	On the Electronic and Optical Properties of Metal-Organic Frameworks: Case Study of MIL-125 and MIL-125-NH ₂ . <i>Journal of Physical Chemistry C</i> , 2020 , 124, 4065-4072	3.8	26
204	Fermi-level pinning through defects at GaAs/oxide interfaces: A density functional study. <i>Physical Review B</i> , 2015 , 92,	3.3	26
203	Binding energies of ground and excited states of shallow acceptors in GaAs/Ga _{1-x} Al _x As quantum wells. <i>Physical Review B</i> , 1990 , 42, 5349-5352	3.3	26
202	Dangling bond charge transition levels in AlAs, GaAs, and InAs. <i>Applied Physics Letters</i> , 2010 , 97, 191901	3.4	25
201	Noncollinear magnetism in liquid oxygen: A first-principles molecular dynamics study. <i>Physical Review B</i> , 2004 , 70,	3.3	25
200	Modeling of the Raman spectrum of vitreous silica: concentration of small ring structures. <i>Physica B: Condensed Matter</i> , 2002 , 316-317, 572-574	2.8	25
199	First-principles electronic structure study of Ti-PTCDA contacts. <i>Physical Review B</i> , 2002 , 65,	3.3	25
198	Interpretation of photoelectron spectra in Cu _n - clusters including thermal and final-state effects: The case of Cu ₇ ⁺ . <i>Physical Review B</i> , 1996 , 54, 8913-8918	3.3	25
197	Alignment of hydrogen-related defect levels at the Si/SiO ₂ interface. <i>Physica B: Condensed Matter</i> , 2007 , 401-402, 546-549	2.8	24
196	Dielectric effect of a thin SiO ₂ interlayer at the interface between silicon and high-k oxides. <i>Microelectronic Engineering</i> , 2004 , 72, 299-303	2.5	24
195	Mechanism suppressing charge recombination at iodine defects in CH ₃ NH ₃ PbI ₃ by polaron formation. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 16863-16867	1.3	23
194	Note: Assessment of the SCAN+rVV10 functional for the structure of liquid water. <i>Journal of Chemical Physics</i> , 2017 , 147, 216101	3.9	23
193	Absence of charge-charge correlations at intermediate-range distances in disordered network-forming materials. <i>Physical Review B</i> , 2003 , 68,	3.3	23
192	Picture of the wet electron: a localized transient state in liquid water. <i>Chemical Science</i> , 2019 , 10, 7442-7448	3.4	22
191	Density-functional perturbational theory for dielectric tensors in the ultrasoft pseudopotential scheme. <i>Physical Review B</i> , 2004 , 69,	3.3	22
190	Theory of excitons in GaAs/Ga _{1-x} Al _x As quantum wells including valence band mixing. <i>Superlattices and Microstructures</i> , 1989 , 5, 59-63	2.8	22

189	Vibrational spectra of vitreous SiO and vitreous GeO from first principles. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 415112	1.8	21
188	Hydrogen in Si(100)SiO ₂ HfO ₂ gate stacks: Relevant charge states and their location. <i>Applied Physics Letters</i> , 2007 , 91, 262901	3.4	21
187	Equivalent oxide thickness of a thin oxide interlayer in gate insulator stacks on silicon. <i>Applied Physics Letters</i> , 2005 , 86, 192901	3.4	21
186	Structure of liquid GexSe1-x at the stiffness threshold composition. <i>Physical Review B</i> , 1998 , 58, R14661-R14664	3.5	21
185	Proton-induced fixed positive charge at the Si(100)-SiO ₂ interface. <i>Physical Review Letters</i> , 2007 , 99, 126102	7.4	20
184	Ab initio study of charged states of H in amorphous SiO ₂ . <i>Microelectronic Engineering</i> , 2005 , 80, 288-291	2.5	20
183	Abrupt model interface for the 4H(1000)SiC-SiO ₂ interface. <i>Microelectronic Engineering</i> , 2005 , 80, 38-41	2.5	20
182	Vibrational amplitudes in vitreous silica. <i>Physical Review B</i> , 2000 , 61, 3951-3959	3.3	20
181	Infrared transitions between shallow acceptor states in GaAs-Ga _{1-x} Al _x As quantum wells. <i>Physical Review B</i> , 1991 , 44, 1118-1127	3.3	20
180	Nitrogen 1s core-level shifts at the NH ₃ saturated Si(100)-2x1 surface: a first-principles study. <i>Surface Science</i> , 2001 , 490, L614-L618	1.8	19
179	Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3456-62	6.4	19
178	Comparison between various finite-size supercell correction schemes for charged defect calculations. <i>Physica B: Condensed Matter</i> , 2012 , 407, 3063-3067	2.8	18
177	First-principles study of Si 2p core-level shifts at water and hydrogen covered Si(001)2x1 surfaces. <i>Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena</i> , 1996 , 14, 2809		18
176	First-principles analysis of the Raman spectrum of vitreous silica: comparison with the vibrational density of states. <i>Journal of Physics Condensed Matter</i> , 2003 , 15, S1547-S1552	1.8	18
175	Titanium oxides and silicates as high-dielectrics: A first-principles investigation. <i>International Journal of Quantum Chemistry</i> , 2005 , 101, 793-801	2.1	18
174	Atomic-scale modelling of kinetic processes occurring during silicon oxidation. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, S2051-S2063	1.8	18
173	Sizable Excitonic Effects Undermining the Photocatalytic Efficiency of ECuVO. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 5698-5703	6.4	18
172	Electronic and structural characterization of barrier-type amorphous aluminium oxide. <i>Electrochimica Acta</i> , 2017 , 224, 503-516	6.7	17

171	Effect of the Solvent on the Oxygen Evolution Reaction at the TiO ₂ /Water Interface. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 18467-18474	3.8	17
170	Accuracy of GW for calculating defect energy levels in solids. <i>Physical Review B</i> , 2017 , 96,	3.3	17
169	Charge transition levels of nitrogen dangling bonds at Si/SiO ₂ interfaces: A first-principles study. <i>Physical Review B</i> , 2010 , 81,	3.3	17
168	A hybrid functional scheme for defect levels and band alignments at semiconductor/oxide interfaces. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2010 , 207, 270-276	1.6	17
167	Si 2p core-level shifts in small molecules: a first principles study. <i>Physica Scripta</i> , 1996 , T66, 118-120	2.6	17
166	Mixed Wannier-Bloch functions for electrons and phonons in periodic systems. <i>Physical Review Letters</i> , 2006 , 96, 216403	7.4	17
165	Modeling phase separation in nonstoichiometric silica. <i>Physical Review Letters</i> , 2004 , 93, 135501	7.4	17
164	Ab initio molecular dynamics investigation of the structure and the noncollinear magnetism in liquid oxygen: occurrence of O ₄ molecular units. <i>Physical Review Letters</i> , 2002 , 89, 197204	7.4	17
163	Modeling of Si 2p core-level shifts at Si/(ZrO ₂) _x (SiO ₂) _{1-x} interfaces. <i>Applied Physics Letters</i> , 2002 , 81, 4233-4235	3.4	17
162	Number of independent partial structure factors for a disordered n-component system. <i>Physical Review B</i> , 1999 , 59, 5-7	3.3	17
161	Two-photon transitions to excitons in quantum wells. <i>Physical Review B</i> , 1990 , 42, 9073-9079	3.3	17
160	Electron and Hole Polarons at the BiVO ₃ -Water Interface. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 18423-18426	9.5	16
159	Band alignment and chemical bonding at the GaAs/Al ₂ O ₃ interface: A hybrid functional study. <i>Applied Physics Letters</i> , 2015 , 107, 211601	3.4	16
158	Germanium core-level shifts at Ge/GeO ₂ interfaces through hybrid functionals. <i>Physical Review B</i> , 2012 , 85,	3.3	16
157	Amorphous hafnium silicates: structural, electronic and dielectric properties. <i>Microelectronic Engineering</i> , 2007 , 84, 2416-2419	2.5	16
156	Electronic properties of an epitaxial silicon oxynitride layer on a 6H-SiC(0001) surface: A first-principles investigation. <i>Applied Physics Letters</i> , 2007 , 91, 061930	3.4	16
155	First-principle study of C 1s core-level shifts in amorphous carbon. <i>Computational Materials Science</i> , 2001 , 22, 67-72	3.2	16
154	Theoretical calculations of shallow acceptor states in GaAs/Al _x Ga _{1-x} As quantum wells in the presence of an external magnetic field. <i>Physical Review B</i> , 1994 , 50, 2393-2398	3.3	16

- 153 Origin of Fermi-level pinning at GaAs surfaces and interfaces. *Journal of Physics Condensed Matter*, **2014**, 26, 492202 1.8 15
- 152 First principles study of substoichiometric germanium oxides. *Microelectronic Engineering*, **2009**, 86, 1760-1762 15
- 151 Dielectric susceptibility of dipolar molecular liquids by ab initio molecular dynamics: application to liquid HCl. *Chemical Physics Letters*, **2004**, 390, 193-198 2.5 15
- 150 Chemisorption pathways and Si 2p 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 3.4 15
- 149 Cu⁺⁺ and Li⁺ interaction with polyethylene oxide by ab initio molecular dynamics. *Journal of Chemical Physics*, **1998**, 108, 9933-9936 3.9 15
- 148 Polarization dependence of multiphoton transitions. *Physical Review B*, **1991**, 43, 3837-3846 3.3 15
- 147 Charge state of the O₂ molecule during silicon oxidation through hybrid functional calculations. *Physical Review B*, **2008**, 78, 3.3 14
- 146 Semiconductor defects at the 4H-SiC(0001)/SiO₂ interface. *Physica B: Condensed Matter*, **2007**, 401-402, 556-559 2.8 14
- 145 Carbon diffusion in CVD growth of carbon nanotubes on metal nanoparticles. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 2185-2188 1.3 14
- 144 Concentration fluctuations on intermediate range distances in liquid GeSe₂: the critical role of ionicity. *Computational Materials Science*, **2000**, 17, 115-121 3.2 14
- 143 Variational calculation of Fano linewidth: Application to excitons in quantum wells. *Physical Review B*, **1991**, 44, 3162-3167 3.3 14
- 142 Hole diffusion across leaky amorphous TiO₂ coating layers for catalytic water splitting at photoanodes. *Journal of Materials Chemistry A*, **2018**, 6, 11804-11810 13 14
- 141 Redox Levels through Constant Fermi-Level ab Initio Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 1769-1777 6.4 13
- 140 Arsenic related defect states resonant with the semiconductor conduction band at the In_{0.53}Ga_{0.47}As/oxide interface: A density functional study. *Microelectronic Engineering*, **2015**, 147, 260-263 2.5 13
- 139 Amphoteric defects in GaAs leading to Fermi-level pinning: A hybrid functional study. *Microelectronic Engineering*, **2013**, 109, 50-53 2.5 13
- 138 First principles study of As 2p core-level shifts at GaAs/Al₂O₃ interfaces. *Applied Physics Letters*, **2013**, 102, 201607 3.4 13
- 137 Formation of substoichiometric GeO_x at the Ge/HfO₂ interface. *Applied Physics Letters*, **2010**, 97, 202908 3.4 13
- 136 Vibrational properties of vitreous GeSe₂ with the Becke-Lee-Yang-Parr density functional. *Journal of Physics Condensed Matter*, **2011**, 23, 295401 1.8 13

135	Band offsets at Ge/GeO ₂ interfaces: Effect of different interfacial bonding patterns. <i>Microelectronic Engineering</i> , 2011 , 88, 1467-1470	2.5	13
134	Energy levels of candidate defects at SiC/SiO ₂ interfaces 2010 ,		13
133	Adjustable potential probes for band-gap predictions of extended systems through nonempirical hybrid functionals. <i>Physical Review B</i> , 2019 , 99,	3.3	12
132	First-principles simulation of vitreous systems. <i>Current Opinion in Solid State and Materials Science</i> , 2001 , 5, 503-508	12	12
131	Nonempirical hybrid functionals for band gaps of inorganic metal-halide perovskites. <i>Physical Review Materials</i> , 2019 , 3,	3.2	12
130	Minimum energy path and atomistic mechanism of the elementary step in oxygen diffusion in silicon: A density-functional study. <i>Physical Review B</i> , 2014 , 89,	3.3	11
129	Low-strain interface models for epitaxial graphene on SiC(0001). <i>Diamond and Related Materials</i> , 2012 , 23, 178-183	3.5	11
128	Accurate determination of charge transition levels of the As-As dimer defect at GaAs/oxide interfaces through hybrid functionals. <i>Applied Physics Letters</i> , 2013 , 103, 041602	3.4	11
127	First-principles investigation of the relation between structural and NMR parameters in vitreous GeO ₂ . <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 145501	1.8	11
126	Atomistic model structure of the Ge(100)/GeO ₂ interface. <i>Microelectronic Engineering</i> , 2009 , 86, 1589-1591	2.5	11
125	Li-related defects in ZnO: Hybrid functional calculations. <i>Physica B: Condensed Matter</i> , 2009 , 404, 4797-4799	2.5	11
124	Charge trapping in substoichiometric germanium oxide. <i>Microelectronic Engineering</i> , 2011 , 88, 1428-1431	2.5	11
123	Electron density of states at Ge/oxide interfaces due to formation. <i>Microelectronic Engineering</i> , 2011 , 88, 391-394	2.5	11
122	Atomistic model structure of the Si(100)/SiO ₂ interface from a synthesis of experimental data. <i>Applied Surface Science</i> , 2004 , 234, 190-196	6.7	11
121	Formation energy of threefold coordinated oxygen in SiO ₂ systems. <i>Applied Surface Science</i> , 2000 , 166, 451-454	6.7	11
120	Accurate optical spectra through time-dependent density functional theory based on screening-dependent hybrid functionals. <i>Physical Review Research</i> , 2020 , 2,	3.9	11
119	Giant apparent lattice distortions in STM images of corrugated sp ² -hybridised monolayers. <i>New Journal of Physics</i> , 2016 , 18, 103027	2.9	10
118	Defect energy levels of the As ₂ As dimer at InGaAs/oxide interfaces: A first principles study. <i>Microelectronic Engineering</i> , 2013 , 109, 60-63	2.5	10

117	Interfacial Ga-As suboxide: Structural and electronic properties. <i>Applied Physics Letters</i> , 2015 , 107, 031605	5.4	10
116	The OAs defect in GaAs: A hybrid density functional study. <i>Applied Surface Science</i> , 2014 , 291, 6-10	6.7	10
115	Umari and Pasquarello Reply.. <i>Physical Review Letters</i> , 2006 , 96,	7.4	10
114	Atomic structure at the Si(001)/SiO ₂ interface: from the interpretation of Si 2p core-level shifts to a model structure. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2002 , 96, 102-106	3.1	10
113	Density functional theory with finite electric field. <i>International Journal of Quantum Chemistry</i> , 2005 , 101, 666-670	2.1	10
112	Atomically controlled interfaces for future nanoelectronics. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, V1-V5	1.8	10
111	Evaluation of Photocatalysts for Water Splitting through Combined Analysis of Surface Coverage and Energy-Level Alignment. <i>ACS Catalysis</i> , 2020 , 10, 13186-13195	13.1	10
110	Band alignment at EGa ₂ O ₃ /III-N (III = Al, Ga) interfaces through hybrid functional calculations. <i>Applied Physics Letters</i> , 2020 , 117, 102103	3.4	10
109	Intercalation of H at the graphene/SiC(0001) interface: Structure and stability from first principles. <i>Applied Surface Science</i> , 2014 , 291, 64-68	6.7	9
108	Migration of Mg and other interstitial metal dopants in GaN. <i>Physica Status Solidi - Rapid Research Letters</i> , 2017 , 11, 1700081	2.5	9
107	Stability and charge transfer at the interface between SiC(0001) and epitaxial graphene. <i>Microelectronic Engineering</i> , 2011 , 88, 1478-1481	2.5	9
106	Structural properties of amorphous GeSe. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 415111	1.8	9
105	Dependence of the O ₂ diffusion rate on oxide thickness during silicon oxidation. <i>Journal of Physics Condensed Matter</i> , 2003 , 15, S1553-S1560	1.8	9
104	O ₂ oxidation reaction at the Si(100)-SiO ₂ interface: A first-principles investigation. <i>Journal of Materials Science</i> , 2005 , 40, 3047-3050	4.3	9
103	Modelling of paramagnetic trivalent silicon defect centres in amorphous silica and at Si/SiO ₂ interfaces. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, S2099-S2113	1.8	9
102	Magnetic properties of the S-like bound hole states in GaAs/Al _x Ga _{1-x} As quantum wells. <i>Physical Review B</i> , 1994 , 49, 10794-10797	3.3	9
101	Interpretation of three-photon spectra in alkali halides. <i>Physical Review B</i> , 1990 , 41, 12230-12235	3.3	9
100	Effect of continuum states on two-photon absorption in quantum wells. <i>Physical Review B</i> , 1990 , 41, 12728-12734	3.3	9

99	Oxygen evolution reaction: Bifunctional mechanism breaking the linear scaling relationship. <i>Journal of Chemical Physics</i> , 2020 , 152, 104712	3.9	8
98	Oxygen defects in GaAs: A hybrid functional study. <i>Physical Review B</i> , 2016 , 93,	3.3	8
97	Assignment of Fermi-level pinning and optical transitions to the (AsGa) ₂ -OAs center in oxygen-doped GaAs. <i>Applied Physics Letters</i> , 2013 , 103, 142108	3.4	8
96	Excitonic effects on the two-photon transition rate in quantum wells. <i>Superlattices and Microstructures</i> , 1991 , 9, 157-160	2.8	8
95	Reaction pathway of oxygen evolution on Pt(1 1 1) revealed through constant Fermi level molecular dynamics. <i>Journal of Catalysis</i> , 2019 , 375, 135-139	7.3	7
94	Defect Formation Energies of Interstitial C, Si, and Ge Impurities in β -Ga ₂ O ₃ . <i>Physica Status Solidi - Rapid Research Letters</i> , 2019 , 13, 1800633	2.5	7
93	(Invited) Electronic and Structural Properties at Ge/GeO ₂ Interfaces: A Density-Functional Investigation. <i>ECS Transactions</i> , 2010 , 33, 123-132	1	7
92	A first principles study of small Cun clusters based on local-density and generalized-gradient approximations to density functional theory. <i>Computational Materials Science</i> , 1998 , 10, 463-467	3.2	7
91	Infrared properties of ultrathin oxides on Si(100). <i>Microelectronic Engineering</i> , 2005 , 80, 420-423	2.5	7
90	Infrared-absorption spectra of acceptors confined in GaAs/Al _x Ga _{1-x} As quantum wells in the presence of an external magnetic field. <i>Physical Review B</i> , 1994 , 50, 10953-10957	3.3	7
89	One-dimensional random potentials allowing for extended states. <i>Journal of Physics Condensed Matter</i> , 1989 , 1, 9509-9512	1.8	7
88	Overcoming Bipolar Doping Difficulty in Wide Gap Semiconductors 2011 , 213-239		6
87	First-principles theory of infrared absorption spectra at surfaces and interfaces: Application to the Si(100):H ₂ O surface. <i>Physical Review B</i> , 2008 , 78,	3.3	6
86	Band gap opening at the 6H-SiC(0 0 0 1) surface passivated by an epitaxial silicon oxynitride layer: A first-principles investigation. <i>Surface Science</i> , 2008 , 602, 2989-2993	1.8	6
85	Hyper-Raman Spectrum of Vitreous Silica from First Principles. <i>Physical Review Letters</i> , 2007 , 98,	7.4	6
84	Evidence of concentration fluctuations in disordered network-forming systems: the case of GeSe ₄ and SiSe ₂ . <i>Journal of Physics Condensed Matter</i> , 2003 , 15, S1537-S1546	1.8	6
83	Electronic Structure at Realistic Si(100)-SiO ₂ Interfaces. <i>Japanese Journal of Applied Physics</i> , 2004 , 43, 7895-7898	1.4	6
82	Comment on "Structural analysis of the SiO ₂ /Si(100) interface by means of photoelectron diffraction". <i>Physical Review Letters</i> , 2005 , 94, 189601; discussion 189602	7.4	6

81	Ab initio molecular dynamics of liquid hydrogen chloride. <i>Journal of Chemical Physics</i> , 2005 , 122, 114512	3.9	6
80	Oxygen species in SiO ₂ : a first-principles investigation. <i>Microelectronic Engineering</i> , 2001 , 59, 167-172	2.5	6
79	Hole subbands in quantum wells: Comparison between theory and hot-electron-acceptor-luminescence experiments. <i>Physical Review B</i> , 1992 , 46, 2625-2627	3.3	6
78	Small Electron Polarons in CsPbBr ₃ : Competition between Electron Localization and Delocalization. <i>Chemistry of Materials</i> , 2020 , 32, 8393-8400	9.6	6
77	Defect levels at GaAs/Al ₂ O ₃ interfaces: As ₂ As dimer vs. Ga dangling bond. <i>Applied Surface Science</i> , 2014 , 291, 16-19	6.7	5
76	Partial Molar Volumes of Aqua Ions from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3427-3431	6.4	5
75	First principles study of electronic and structural properties of the Ge/GeO ₂ interface. <i>Physica B: Condensed Matter</i> , 2012 , 407, 2926-2931	2.8	5
74	Alignment of Defect Energy Levels at Si-SiO ₂ Interface from Hybrid Density Functional Calculations 2010 ,		5
73	Silicon crystal distortions at the Si(1 0 0)/SiO ₂ interface from analysis of ion-scattering. <i>Microelectronic Engineering</i> , 2004 , 72, 197-200	2.5	5
72	Energetics of oxygen species in crystalline and amorphous SiO ₂ : a first-principles investigation. <i>Solid-State Electronics</i> , 2002 , 46, 1873-1878	1.7	5
71	Supported nanoclusters: Preadsorbates tuning catalytic activity. <i>Physical Review B</i> , 2005 , 71,	3.3	5
70	Core-Level Shifts in Si(001)-SiO ₂ Systems: The Value of First-Principle Investigations 1998 , 89-102		5
69	Finite-size corrections of defect energy levels involving ionic polarization. <i>Physical Review B</i> , 2020 , 102,	3.3	5
68	Unraveling the synergy between metal-organic frameworks and co-catalysts in photocatalytic water splitting. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 20493-20502	13	5
67	Extrinsic Defects in Amorphous Oxides: Hydrogen, Carbon, and Nitrogen Impurities in Alumina. <i>Physical Review Applied</i> , 2019 , 11,	4.3	4
66	Diffusion of interstitial oxygen in silicon and germanium: a hybrid functional study. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 495801	1.8	4
65	Identification of Semiconductor Defects through Constant-Fermi-Level Ab Initio Molecular Dynamics: Application to GaAs. <i>Physical Review Applied</i> , 2017 , 8,	4.3	4
64	Stability of valence alternation pairs across the substoichiometric region at Ge/GeO ₂ interfaces. <i>Physica B: Condensed Matter</i> , 2012 , 407, 2939-2942	2.8	4

63	Network transformation processes during oxidation of silicon. <i>Microelectronic Engineering</i> , 1999 , 48, 89-94	2.5	4
62	Application of variational techniques to time-dependent perturbation theory. <i>Physical Review B</i> , 1993 , 48, 5090-5094	3.3	4
61	High exciton binding energies in GaAs/GaAlAs quantum wells. <i>Superlattices and Microstructures</i> , 1991 , 9, 1-4	2.8	4
60	Effective-State Approach to Second-Order Perturbation Theory. <i>Europhysics Letters</i> , 1992 , 17, 387-392	1.6	4
59	Comment on "Effect of biaxial strain on acceptor-level energies in In _y Ga _{1-y} As/Al _x Ga _{1-x} As (on GaAs) quantum wells". <i>Physical Review B</i> , 1990 , 42, 7641-7642	3.3	4
58	Low-Frequency Dielectric Response of Tetragonal Perovskite CH ₃ NH ₃ PbI ₃ . <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 6279-6285	6.4	4
57	Reactivity and energy level of a localized hole in liquid water. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 30281-30289	3.6	4
56	Band alignment at the CaF ₂ /Si(111) interface through advanced electronic structure calculations. <i>Physical Review B</i> , 2020 , 101,	3.3	3
55	Comment on "Fundamental Resolution of Difficulties in the Theory of Charged Point Defects in Semiconductors". <i>Physical Review Letters</i> , 2018 , 120, 039603	7.4	3
54	Electron trap states at InGaAs/oxide interfaces under inversion through constant Fermi-level ab initio molecular dynamics. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 505702	1.8	3
53	First-principles study of H adsorption on graphene/SiC(0001). <i>Physica Status Solidi (B): Basic Research</i> , 2013 , 250, 2523-2528	1.3	3
52	Advances in Electronic Structure Methods for Defects and Impurities in Solids 2011 , 1-16		3
51	Protons at the Si-SiO ₂ interface: a first principle investigation. <i>Microelectronic Engineering</i> , 2007 , 84, 2035-2038	2.5	3
50	Charge transition levels of the Ge dangling bond defect at Ge/insulator interfaces. <i>Materials Science in Semiconductor Processing</i> , 2008 , 11, 226-229	4.3	3
49	An electronegativity-induced spin repulsion effect. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 8385-90	2.8	3
48	Infrared absorption frequencies and oscillator strengths of acceptors confined in GaAs/AlGaAs quantum wells. <i>Applied Physics Letters</i> , 1994 , 65, 3365-3367	3.4	3
47	Vertex function compliant with the Ward identity for quasiparticle self-consistent calculations beyond GW. <i>Physical Review B</i> , 2021 , 103,	3.3	3
46	Band gaps of liquid water and hexagonal ice through advanced electronic-structure calculations. <i>Physical Review Research</i> , 2021 , 3,	3.9	3

45	Oxygen DX center in In _{0.17} Al _{0.83} N: Nonradiative recombination and persistent photoconductivity. <i>Applied Physics Letters</i> , 2017 , 110, 072101	3.4	2
44	Nature of electron trap states under inversion at In _{0.53} Ga _{0.47} As/Al ₂ O ₃ interfaces. <i>Applied Physics Letters</i> , 2017 , 110, 111602	3.4	2
43	Partial vibrational density of states for amorphous solids from inelastic neutron scattering. <i>Physical Review B</i> , 2018 , 98,	3.3	2
42	Advanced Calculations for Defects in Solids I Electronic Structure Methods. <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 17-18	1.3	2
41	Nitrogen fixation at passivated Fe nanoclusters supported by an oxide surface: Identification of viable reaction routes using density functional calculations. <i>Physical Review B</i> , 2009 , 80,	3.3	2
40	Proton Diffusion in Amorphous SiO ₂ and Hafnium Silicate by Ab Initio Molecular Dynamics. <i>AIP Conference Proceedings</i> , 2007 ,	0	2
39	Ion scattering simulations of the Si(100)/BiO ₂ interface. <i>Physical Review B</i> , 2006 , 74,	3.3	2
38	Car-Parrinello Molecular Dynamics in a Finite Homogeneous Electric Field. <i>AIP Conference Proceedings</i> , 2003 ,	0	2
37	Structural and magnetic correlations in liquid oxygen: an ab initio molecular dynamics study. <i>Journal of Physics Condensed Matter</i> , 2003 , 15, S89-S94	1.8	2
36	Nitrogen adsorption on a supported iron nanocluster. <i>Vacuum</i> , 2004 , 74, 173-177	3.7	2
35	Magneto-optical studies of acceptors confined in GaAs/Al _x Ga _{1-x} As quantum wells. <i>Physical Review B</i> , 1994 , 50, 4901-4904	3.3	2
34	Atomic-Level Description of Thermal Fluctuations in Inorganic Lead Halide Perovskites.. <i>Journal of Physical Chemistry Letters</i> , 2022 , 3382-3391	6.4	2
33	Hydrogen Bonding of Ammonia with (H,OH)-Si(001) Revealed by Experimental and Ab Initio Photoelectron Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 5378-5388	2.8	1
32	Predicting Polaronic Defect States by Means of Generalized Koopmans Density Functional Calculations 2011 , 183-199		1
31	LDA + U and Hybrid Functional Calculations for Defects in ZnO, SnO ₂ , and TiO ₂ 2011 , 155-164		1
30	Defect Levels Through Hybrid Density Functionals: Insights and Applications 2011 , 111-137		1
29	Structural and Electronic Properties of Oxygen Vacancies in Monoclinic HfO ₂ . <i>Materials Research Society Symposia Proceedings</i> , 2007 , 996, 1		1
28	Finite electric field in density functional calculations with periodic boundary conditions. <i>Computational Materials Science</i> , 2004 , 30, 116-119	3.2	1

- 27 Modelling of dielectric constants of amorphous Zr silicates. *Journal of Physics Condensed Matter*, **2005**, 17, S2089-S2098 1.8 1
- 26 FIRST-PRINCIPLES STUDIES OF Cu CLUSTERS. *Surface Review and Letters*, **1996**, 03, 287-291 1.1 1
- 25 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 1
- 24 Complex Pattern of Impurity States in Shallow Semiconductor Quantum Wells. *Europhysics Letters*, **1991**, 15, 447-451 1.6 1
- 23 Shallow Impurities in GaAs-Ga_{1-x}Al_xAs Quantum Wells. *Physica Scripta*, **1991**, T39, 182-187 2.6 1
- 22 High-performance NiOOH/FeOOH electrode for OER catalysis. *Journal of Chemical Physics*, **2021**, 154, 024706 3.9 1
- 21 Atomic-Scale Modelling of Electrochemical Interfaces through Constant Fermi Level Molecular Dynamics **2021**, 221-240 1
- 20 Electronic Structure of Water from Koopmans-Compliant Functionals. *Journal of Chemical Theory and Computation*, **2021**, 17, 3923-3930 6.4 0
- 19 One-Shot Approach for Enforcing Piecewise Linearity on Hybrid Functionals: Application to Band Gap Predictions.. *Journal of Physical Chemistry Letters*, **2022**, 3066-3071 6.4 0
- 18 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 2.5
- 17 Time-Dependent Density Functional Study on the Excitation Spectrum of Point Defects in Semiconductors **2011**, 341-358
- 16 SiO₂ in Density Functional Theory and Beyond **2011**, 201-211
- 15 Electrostatic Interactions between Charged Defects in Supercells **2011**, 241-258
- 14 Ab Initio Green's Function Calculation of Hyperfine Interactions for Shallow Defects in Semiconductors **2011**, 305-339
- 13 Accurate Gap Levels and Their Role in the Reliability of Other Calculated Defect Properties **2011**, 139-154
- 12 Critical Evaluation of the LDA + U Approach for Band Gap Corrections in Point Defect Calculations: The Oxygen Vacancy in ZnO Case Study **2011**, 165-181
- 11 Accurate Kohn-Sham DFT With the Speed of Tight Binding: Current Techniques and Future Directions in Materials Modelling **2011**, 285-303
- 10 Which Electronic Structure Method for The Study of Defects: A Commentary **2011**, 359-379

- 9 Formation Energies of Point Defects at Finite Temperatures **2011**, 259-284
- 8 Accurate Treatment of Solids with the HSE Screened Hybrid **2011**, 97-110
- 7 Calculation of Semiconductor Band Structures and Defects by the Screened Exchange Density Functional **2011**, 79-96
- 6 Accelerating GW Calculations with Optimal Polarizability Basis **2011**, 61-78
- 5 Electronic Properties of Interfaces and Defects from Many-Body Perturbation Theory: Recent Developments and Applications **2011**, 33-60
- 4 Accuracy of Quantum Monte Carlo Methods for Point Defects in Solids **2011**, 17-31
- 3 Atomic-scale investigation of the dielectric screening at the interface between silicon and its oxide. *Materials Research Society Symposia Proceedings*, **2003**, 786, 511
- 2 Ab initio molecular dynamics: application to liquid copper. *Computational Materials Science*, **1993**, 1, 419-427
- 1 Exploring Defects in Semiconductor Materials Through Constant Fermi Level Ab-Initio Molecular Dynamics. *Springer Series in Materials Science*, **2020**, 39-55 0.9