Alfredo Pasquarello

List of Publications by Year in Descending Order

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	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
349	Atomic-Level Description of Thermal Fluctuations in Inorganic Lead Halide Perovskites.. *Journal of Physical Chemistry Letters*, **2022**, 3382-3391	6.4	2
348	Vertex function compliant with the Ward identity for quasiparticle self-consistent calculations beyond GW. *Physical Review B*, **2021**, 103,	3.3	3
347	Band gaps of liquid water and hexagonal ice through advanced electronic-structure calculations. *Physical Review Research*, **2021**, 3,	3.9	3
346	Electronic Structure of Water from Koopmans-Compliant Functionals. *Journal of Chemical Theory and Computation*, **2021**, 17, 3923-3930	6.4	0
345	High-performance NiOOH/FeOOH electrode for OER catalysis. *Journal of Chemical Physics*, **2021**, 154, 024706	3.9	1
344	Atomic-Scale Modelling of Electrochemical Interfaces through Constant Fermi Level Molecular Dynamics **2021**, 221-240		1
343	Band alignment at the CaF2/Si(111) interface through advanced electronic structure calculations. *Physical Review B*, **2020**, 101,	3.3	3
342	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	2.8	1
341	Oxygen evolution reaction: Bifunctional mechanism breaking the linear scaling relationship. *Journal of Chemical Physics*, **2020**, 152, 104712	3.9	8
340	On the Electronic and Optical Properties of Metal Organic Frameworks: Case Study of MIL-125 and MIL-125-NH2. *Journal of Physical Chemistry C*, **2020**, 124, 4065-4072	3.8	26
339	Accurate optical spectra through time-dependent density functional theory based on screening-dependent hybrid functionals. *Physical Review Research*, **2020**, 2,	3.9	11
338	Exploring Defects in Semiconductor Materials Through Constant Fermi Level Ab-Initio Molecular Dynamics. *Springer Series in Materials Science*, **2020**, 39-55	0.9	
337	Small Electron Polarons in CsPbBr3: Competition between Electron Localization and Delocalization. *Chemistry of Materials*, **2020**, 32, 8393-8400	9.6	6
336	Low-Frequency Dielectric Response of Tetragonal Perovskite CHNHPbI. *Journal of Physical Chemistry Letters*, **2020**, 11, 6279-6285	6.4	4
335	Finite-size corrections of defect energy levels involving ionic polarization. *Physical Review B*, **2020**, 102,	3.3	5
334	Evaluation of Photocatalysts for Water Splitting through Combined Analysis of Surface Coverage and Energy-Level Alignment. *ACS Catalysis*, **2020**, 10, 13186-13195	13.1	10

333	Unraveling the synergy between metal□organic frameworks and co-catalysts in photocatalytic water splitting. *Journal of Materials Chemistry A*, **2020**, 8, 20493-20502	13	5
332	Band alignment at □Ga2O3/III-N (III = Al, Ga) interfaces through hybrid functional calculations. *Applied Physics Letters*, **2020**, 117, 102103	3.4	10
331	Adjustable potential probes for band-gap predictions of extended systems through nonempirical hybrid functionals. *Physical Review B*, **2019**, 99,	3.3	12
330	Reaction pathway of oxygen evolution on Pt(1 1 1) revealed through constant Fermi level molecular dynamics. *Journal of Catalysis*, **2019**, 375, 135-139	7.3	7
329	Defect Formation Energies of Interstitial C, Si, and Ge Impurities in □Ga2O3. *Physica Status Solidi - Rapid Research Letters*, **2019**, 13, 1800633	2.5	7
328	Electron and Hole Polarons at the BiVO-Water Interface. *ACS Applied Materials & Interfaces*, **2019**, 11, 18423-18426	9.5	16
327	Extrinsic Defects in Amorphous Oxides: Hydrogen, Carbon, and Nitrogen Impurities in Alumina. *Physical Review Applied*, **2019**, 11,	4.3	4
326	Effect of the Solvent on the Oxygen Evolution Reaction at the TiO2□Water Interface. *Journal of Physical Chemistry C*, **2019**, 123, 18467-18474	3.8	17
325	Picture of the wet electron: a localized transient state in liquid water. *Chemical Science*, **2019**, 10, 7442-7448	9.4	22
324	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. *Npj Computational Materials*, **2019**, 5,	10.9	33
323	Nonempirical hybrid functionals for band gaps of inorganic metal-halide perovskites. *Physical Review Materials*, **2019**, 3,	3.2	12
322	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	9.5	114
321	pH-Dependent Catalytic Reaction Pathway for Water Splitting at the BiVO4□Water Interface from the Band Alignment. *ACS Energy Letters*, **2018**, 3, 829-834	20.1	34
320	pH-Dependent Surface Chemistry from First Principles: Application to the BiVO(010)-Water Interface. *ACS Applied Materials & Interfaces*, **2018**, 10, 10011-10021	9.5	32
319	Comment on "Fundamental Resolution of Difficulties in the Theory of Charged Point Defects in Semiconductors". *Physical Review Letters*, **2018**, 120, 039603	7.4	3
318	Origin of low electron□hole recombination rate in metal halide perovskites. *Energy and Environmental Science*, **2018**, 11, 101-105	35.4	86
317	Nonempirical hybrid functionals for band gaps and polaronic distortions in solids. *Physical Review B*, **2018**, 97,	3.3	49
316	Atomic-Scale Simulation of Electrochemical Processes at Electrode/Water Interfaces under Referenced Bias Potential. *Journal of Physical Chemistry Letters*, **2018**, 9, 1880-1884	6.4	48

315	Role of Polarons in Water Splitting: The Case of BiVO4. *ACS Energy Letters*, **2018**, 3, 1693-1697	20.1	50
314	Organic Cathode for Aqueous Zn-Ion Batteries: Taming a Unique Phase Evolution toward Stable Electrochemical Cycling. *Chemistry of Materials*, **2018**, 30, 3874-3881	9.6	236
313	Mechanism suppressing charge recombination at iodine defects in CH3NH3PbI3 by polaron formation. *Journal of Materials Chemistry A*, **2018**, 6, 16863-16867	13	23
312	Partial vibrational density of states for amorphous solids from inelastic neutron scattering. *Physical Review B*, **2018**, 98,	3.3	2
311	Nonempirical dielectric-dependent hybrid functional with range separation for semiconductors and insulators. *Physical Review Materials*, **2018**, 2,	3.2	93
310	Alignment of Redox Levels at Semiconductor–Water Interfaces. *Chemistry of Materials*, **2018**, 30, 94-111	9.6	56
309	Reactivity and energy level of a localized hole in liquid water. *Physical Chemistry Chemical Physics*, **2018**, 20, 30281-30289	3.6	4
308	Sizable Excitonic Effects Undermining the Photocatalytic Efficiency of BiCuVO. *Journal of Physical Chemistry Letters*, **2018**, 9, 5698-5703	6.4	18
307	Absolute Energy Levels of Liquid Water. *Journal of Physical Chemistry Letters*, **2018**, 9, 3212-3216	6.4	35
306	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
305	Surface Polarons Reducing Overpotentials in the Oxygen Evolution Reaction. *ACS Catalysis*, **2018**, 8, 5847-5851	13	127
304	Oxygen DX center in In0.17Al0.83N: Nonradiative recombination and persistent photoconductivity. *Applied Physics Letters*, **2017**, 110, 072101	3.4	2
303	Electronic Levels of Excess Electrons in Liquid Water. *Journal of Physical Chemistry Letters*, **2017**, 8, 2055-2059	6.4	45
302	Nature of electron trap states under inversion at In0.53Ga0.47As/Al2O3 interfaces. *Applied Physics Letters*, **2017**, 110, 111602	3.4	2
301	Redox Levels through Constant Fermi-Level ab Initio Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 1769-1777	6.4	13
300	Electronic and structural characterization of barrier-type amorphous aluminium oxide. *Electrochimica Acta*, **2017**, 224, 503-516	6.7	17
299	Predictive Determination of Band Gaps of Inorganic Halide Perovskites. *Journal of Physical Chemistry Letters*, **2017**, 8, 5507-5512	6.4	63
298	Identification of Semiconductor Defects through Constant-Fermi-Level Ab Initio Molecular Dynamics: Application to GaAs. *Physical Review Applied*, **2017**, 8,	4.3	4

297	Migration of Mg and other interstitial metal dopants in GaN. *Physica Status Solidi - Rapid Research Letters*, **2017**, 11, 1700081	2.5	9
296	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	
295	Electron trap states at InGaAs/oxide interfaces under inversion through constant Fermi-level ab initio molecular dynamics. *Journal of Physics Condensed Matter*, **2017**, 29, 505702	1.8	3
294	Partial Molar Volumes of Aqua Ions from First Principles. *Journal of Chemical Theory and Computation*, **2017**, 13, 3427-3431	6.4	5
293	Accuracy of GW for calculating defect energy levels in solids. *Physical Review B*, **2017**, 96,	3.3	17
292	Note: Assessment of the SCAN+rVV10 functional for the structure of liquid water. *Journal of Chemical Physics*, **2017**, 147, 216101	3.9	23
291	Comprehensive modeling of the band gap and absorption spectrum of BiVO4. *Physical Review Materials*, **2017**, 1,	3.2	31
290	Self-compensation due to point defects in Mg-doped GaN. *Physical Review B*, **2016**, 93,	3.3	85
289	Structural, Dynamical, and Electronic Properties of Liquid Water: A Hybrid Functional Study. *Journal of Physical Chemistry B*, **2016**, 120, 7456-70	3.4	43
288	Oxygen defects in GaAs: A hybrid functional study. *Physical Review B*, **2016**, 93,	3.3	8
287	Diffusion of interstitial oxygen in silicon and germanium: a hybrid functional study. *Journal of Physics Condensed Matter*, **2016**, 28, 495801	1.8	4
286	Ab initio Electronic Structure of Liquid Water. *Physical Review Letters*, **2016**, 117, 186401	7.4	50
285	Giant apparent lattice distortions in STM images of corrugated sp2-hybridised monolayers. *New Journal of Physics*, **2016**, 18, 103027	2.9	10
284	Absolute deformation potentials of two-dimensional materials. *Physical Review B*, **2016**, 94,	3.3	27
283	Oxygen defects in amorphous Al2O3: A hybrid functional study. *Applied Physics Letters*, **2016**, 109, 062903	3.4	30
282	Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets. *Journal of Chemical Theory and Computation*, **2016**, 12, 3456-62	6.4	19
281	Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions. *Journal of Chemical Physics*, **2015**, 142, 034501	3.9	57
280	First-principles determination of defect energy levels through hybrid density functionals and GW. *Journal of Physics Condensed Matter*, **2015**, 27, 133202	1.8	38

279	Energetics of native point defects in GaN: A density-functional study. *Microelectronic Engineering*, **2015**, 147, 51-54	2.5	33
278	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	2.5	13
277	Accurate band gaps of extended systems via efficient vertex corrections in GW. *Physical Review B*, **2015**, 92,	3.3	54
276	Fermi-level pinning through defects at GaAs/oxide interfaces: A density functional study. *Physical Review B*, **2015**, 92,	3.3	26
275	Redox levels in aqueous solution: Effect of van der Waals interactions and hybrid functionals. *Journal of Chemical Physics*, **2015**, 143, 244508	3.9	46
274	Band alignment and chemical bonding at the GaAs/Al2O3 interface: A hybrid functional study. *Applied Physics Letters*, **2015**, 107, 211601	3.4	16
273	Interfacial Ga-As suboxide: Structural and electronic properties. *Applied Physics Letters*, **2015**, 107, 031605	3.4	10
272	Band offsets of lattice-matched semiconductor heterojunctions through hybrid functionals and G0W0. *Physical Review B*, **2014**, 89,	3.3	81
271	Minimum energy path and atomistic mechanism of the elementary step in oxygen diffusion in silicon: A density-functional study. *Physical Review B*, **2014**, 89,	3.3	11
270	Intercalation of H at the graphene/SiC(0001) interface: Structure and stability from first principles. *Applied Surface Science*, **2014**, 291, 64-68	6.7	9
269	Defect levels at GaAs/Al2O3 interfaces: As$_2$As dimer vs. Ga dangling bond. *Applied Surface Science*, **2014**, 291, 16-19	6.7	5
268	Origin of Fermi-level pinning at GaAs surfaces and interfaces. *Journal of Physics Condensed Matter*, **2014**, 26, 492202	1.8	15
267	Band-edge positions in GW: Effects of starting point and self-consistency. *Physical Review B*, **2014**, 90,	3.3	57
266	Infrared spectra of jennite and tobermorite from first-principles. *Cement and Concrete Research*, **2014**, 60, 11-23	10.3	47
265	The OAs defect in GaAs: A hybrid density functional study. *Applied Surface Science*, **2014**, 291, 6-10	6.7	10
264	Defect energy levels of the As$_2$As dimer at InGaAs/oxide interfaces: A first principles study. *Microelectronic Engineering*, **2013**, 109, 60-63	2.5	10
263	Correspondence of defect energy levels in hybrid density functional theory and many-body perturbation theory. *Physical Review B*, **2013**, 88,	3.3	56
262	Amphoteric defects in GaAs leading to Fermi-level pinning: A hybrid functional study. *Microelectronic Engineering*, **2013**, 109, 50-53	2.5	13

261	Finite-size supercell correction for charged defects at surfaces and interfaces. *Physical Review Letters*, **2013**, 110, 095505	7.4	113
260	Accurate determination of charge transition levels of the As-As dimer defect at GaAs/oxide interfaces through hybrid functionals. *Applied Physics Letters*, **2013**, 103, 041602	3.4	11
259	Assignment of Fermi-level pinning and optical transitions to the (AsGa)2-OAs center in oxygen-doped GaAs. *Applied Physics Letters*, **2013**, 103, 142108	3.4	8
258	First principles study of As 2p core-level shifts at GaAs/Al2O3 interfaces. *Applied Physics Letters*, **2013**, 102, 201607	3.4	13
257	First-principles study of H adsorption on graphene/SiC(0001). *Physica Status Solidi (B): Basic Research*, **2013**, 250, 2523-2528	1.3	3
256	Germanium core-level shifts at Ge/GeO2 interfaces through hybrid functionals. *Physical Review B*, **2012**, 85,	3.3	16
255	Comparison of vacancy and antisite defects in GaAs and InGaAs through hybrid functionals. *Journal of Physics Condensed Matter*, **2012**, 24, 045801	1.8	37
254	Comparison between various finite-size supercell correction schemes for charged defect calculations. *Physica B: Condensed Matter*, **2012**, 407, 3063-3067	2.8	18
253	Intrinsic defects in GaAs and InGaAs through hybrid functional calculations. *Physica B: Condensed Matter*, **2012**, 407, 2833-2837	2.8	40
252	First principles study of electronic and structural properties of the Ge/GeO2 interface. *Physica B: Condensed Matter*, **2012**, 407, 2926-2931	2.8	5
251	Stability of valence alternation pairs across the substoichiometric region at Ge/GeO2 interfaces. *Physica B: Condensed Matter*, **2012**, 407, 2939-2942	2.8	4
250	Low-strain interface models for epitaxial graphene on SiC(0001). *Diamond and Related Materials*, **2012**, 23, 178-183	3.5	11
249	Finite-size supercell correction schemes for charged defect calculations. *Physical Review B*, **2012**, 86,	3.3	295
248	Carbon rehybridization at the graphene/SiC(0001) interface: Effect on stability and atomic-scale corrugation. *Physical Review B*, **2012**, 85,	3.3	29
247	Band-edge levels in semiconductors and insulators: Hybrid density functional theory versus many-body perturbation theory. *Physical Review B*, **2012**, 86,	3.3	62
246	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,	3.3	122
245	Assessing the accuracy of hybrid functionals in the determination of defect levels: Application to the As antisite in GaAs. *Physical Review B*, **2011**, 84,	3.3	69
244	Defect levels of carbon-related defects at the SiC/SiO2 interface from hybrid functionals. *Physical Review B*, **2011**, 83,	3.3	36

243	Charge transition levels of carbon-, oxygen-, and hydrogen-related defects at the SiC/SiO2 interface through hybrid functionals. *Physical Review B*, **2011**, 84,	3.3	69
242	Time-Dependent Density Functional Study on the Excitation Spectrum of Point Defects in Semiconductors **2011**, 341-358		
241	SiO2 in Density Functional Theory and Beyond **2011**, 201-211		
240	Electrostatic Interactions between Charged Defects in Supercells **2011**, 241-258		
239	Overcoming Bipolar Doping Difficulty in Wide Gap Semiconductors **2011**, 213-239		6
238	Ab Initio Green Function Calculation of Hyperfine Interactions for Shallow Defects in Semiconductors **2011**, 305-339		
237	Accurate Gap Levels and Their Role in the Reliability of Other Calculated Defect Properties **2011**, 139-154		
236	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		
235	Accurate Kohn Sham DFT With the Speed of Tight Binding: Current Techniques and Future Directions in Materials Modelling **2011**, 285-303		
234	Which Electronic Structure Method for The Study of Defects: A Commentary **2011**, 359-379		
233	Formation Energies of Point Defects at Finite Temperatures **2011**, 259-284		
232	Defect levels through hybrid density functionals: Insights and applications. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 775-789	1.3	228
231	Advanced Calculations for Defects in Solids Electronic Structure Methods. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 17-18	1.3	2
230	Vibrational properties of vitreous GeSe2 with the Becke-Lee-Yang-Parr density functional. *Journal of Physics Condensed Matter*, **2011**, 23, 295401	1.8	13
229	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	3.8	36
228	Identification of defect levels at As/oxide interfaces through hybrid functionals. *Microelectronic Engineering*, **2011**, 88, 1436-1439	2.5	32
227	Charge trapping in substoichiometric germanium oxide. *Microelectronic Engineering*, **2011**, 88, 1428-1431	2.5	11
226	Stability and charge transfer at the interface between SiC(0001) and epitaxial graphene. *Microelectronic Engineering*, **2011**, 88, 1478-1481	2.5	9

225	Electron density of states at Ge/oxide interfaces due to formation. *Microelectronic Engineering*, **2011**, 88, 391-394	2.5	11
224	Band offsets at Ge/GeO2 interfaces: Effect of different interfacial bonding patterns. *Microelectronic Engineering*, **2011**, 88, 1467-1470	2.5	13
223	Predicting Polaronic Defect States by Means of Generalized Koopmans Density Functional Calculations **2011**, 183-199		1
222	LDA + U and Hybrid Functional Calculations for Defects in ZnO, SnO2, and TiO2 **2011**, 155-164		1
221	Defect Levels Through Hybrid Density Functionals: Insights and Applications **2011**, 111-137		1
220	Accurate Treatment of Solids with the HSE Screened Hybrid **2011**, 97-110		
219	Calculation of Semiconductor Band Structures and Defects by the Screened Exchange Density Functional **2011**, 79-96		
218	Accelerating GW Calculations with Optimal Polarizability Basis **2011**, 61-78		
217	Electronic Properties of Interfaces and Defects from Many-Body Perturbation Theory: Recent Developments and Applications **2011**, 33-60		
216	Accuracy of Quantum Monte Carlo Methods for Point Defects in Solids **2011**, 17-31		
215	Advances in Electronic Structure Methods for Defects and Impurities in Solids **2011**, 1-16		3
214	Dangling bond charge transition levels in AlAs, GaAs, and InAs. *Applied Physics Letters*, **2010**, 97, 191901	3.4	25
213	Charge transition levels of nitrogen dangling bonds at Si/SiO2 interfaces: A first-principles study. *Physical Review B*, **2010**, 81,	3.3	17
212	Metal adatoms on graphene and hexagonal boron nitride: Towards rational design of self-assembly templates. *Physical Review B*, **2010**, 82,	3.3	78
211	Structural assignments of NMR chemical shifts in GexSe1□ glasses via first-principles calculations for GeSe2, Ge4Se9, and GeSe crystals. *Physical Review B*, **2010**, 82,	3.3	38
210	Alignment of defect levels and band edges through hybrid functionals: Effect of screening in the exchange term. *Physical Review B*, **2010**, 81,	3.3	112
209	(Invited) Electronic and Structural Properties at Ge/GeO2 Interfaces: A Density-Functional Investigation. *ECS Transactions*, **2010**, 33, 123-132	1	7
208	Electron trapping in substoichiometric germanium oxide. *Applied Physics Letters*, **2010**, 97, 092903	3.4	29

207	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
206	Formation of substoichiometric GeOx at the Ge□HfO2 interface. *Applied Physics Letters*, **2010**, 97, 202908	3.4	13
205	Energy levels of candidate defects at SiC/SiO2 interfaces **2010**,		13
204	Alignment of Defect Energy Levels at Si-SiO2 Interface from Hybrid Density Functional Calculations **2010**,		5
203	A hybrid functional scheme for defect levels and band alignments at semiconductor□oxide interfaces. *Physica Status Solidi (A) Applications and Materials Science*, **2010**, 207, 270-276	1.6	17
202	Medium-range structure of vitreous SiO2 obtained through first-principles investigation of vibrational spectra. *Physical Review B*, **2009**, 79,	3.3	51
201	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,	3.3	2
200	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,	3.3	96
199	First principles investigation of defect energy levels at semiconductor-oxide interfaces: Oxygen vacancies and hydrogen interstitials in the Si□SiO2□HfO2 stack. *Journal of Applied Physics*, **2009**, 105, 061603	2.5	38
198	Atomistic model structure of the Ge(100)□GeO2 interface. *Microelectronic Engineering*, **2009**, 86, 1589-1591	2.5	11
197	First principles study of substoichiometric germanium oxides. *Microelectronic Engineering*, **2009**, 86, 1760-1762	2.5	15
196	Li-related defects in ZnO: Hybrid functional calculations. *Physica B: Condensed Matter*, **2009**, 404, 4797-4799	2.8	11
195	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, **2009**, 21, 395502	1.8	13251
194	Magnetoresistive junctions based on epitaxial graphene and hexagonal boron nitride. *Physical Review B*, **2009**, 80,	3.3	98
193	Atomic structure of the two intermediate phase glasses SiSe4 and GeSe4. *Physical Review B*, **2009**, 79,	3.3	55
192	Band offsets at the Ge/GeO2 interface through hybrid density functionals. *Applied Physics Letters*, **2009**, 94, 141911	3.4	61
191	A hybrid density functional study of lithium in ZnO: Stability, ionization levels, and diffusion. *Physical Review B*, **2009**, 80,	3.3	92
190	Effect of metal elements in catalytic growth of carbon nanotubes. *Physical Review Letters*, **2008**, 100, 156102	7.4	176

189	Band alignments and defect levels in Si□HfO2 gate stacks: Oxygen vacancy and Fermi-level pinning. *Applied Physics Letters*, **2008**, 92, 132911	3.4	61
188	Defect energy levels in density functional calculations: alignment and band gap problem. *Physical Review Letters*, **2008**, 101, 046405	7.4	231
187	Band offsets at semiconductor-oxide interfaces from hybrid density-functional calculations. *Physical Review Letters*, **2008**, 101, 106802	7.4	207
186	Defect levels of dangling bonds in silicon and germanium through hybrid functionals. *Physical Review B*, **2008**, 78,	3.3	133
185	First-principles theory of infrared absorption spectra at surfaces and interfaces: Application to the Si(100):H2O surface. *Physical Review B*, **2008**, 78,	3.3	6
184	Band offsets at the Si/SiO2 interface from many-body perturbation theory. *Physical Review Letters*, **2008**, 100, 186401	7.4	141
183	Charge state of the O2 molecule during silicon oxidation through hybrid functional calculations. *Physical Review B*, **2008**, 78,	3.3	14
182	Carbon diffusion in CVD growth of carbon nanotubes on metal nanoparticles. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 2185-2188	1.3	14
181	Band gap opening at the 6H□SiC(0 0 0 1) surface passivated by an epitaxial silicon oxynitride layer: A first-principles investigation. *Surface Science*, **2008**, 602, 2989-2993	1.8	6
180	Charge transition levels of the Ge dangling bond defect at Ge/insulator interfaces. *Materials Science in Semiconductor Processing*, **2008**, 11, 226-229	4.3	3
179	Short and intermediate range order in amorphous GeSe2. *Physical Review B*, **2008**, 77,	3.3	54
178	Migration of oxygen vacancy in HfO2□SiO2 interface: A first-principles investigation. *Applied Physics Letters*, **2007**, 91, 192905	3.4	114
177	Proton Diffusion in Amorphous SiO2 and Hafnium Silicate by Ab Initio Molecular Dynamics. *AIP Conference Proceedings*, **2007**,	0	2
176	Amorphous hafnium silicates: structural, electronic and dielectric properties. *Microelectronic Engineering*, **2007**, 84, 2416-2419	2.5	16
175	Alignment of hydrogen-related defect levels at the Si□SiO2 interface. *Physica B: Condensed Matter*, **2007**, 401-402, 546-549	2.8	24
174	Semiconductor defects at the 4H-SiC(0001)/SiO2 interface. *Physica B: Condensed Matter*, **2007**, 401-402, 556-559	2.8	14
173	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	2.8	27
172	First principles investigation of defects at interfaces between silicon and amorphous high-□oxides. *Microelectronic Engineering*, **2007**, 84, 2022-2027	2.5	44

171	Protons at the Si-SiO2 interface: a first principle investigation. *Microelectronic Engineering*, **2007**, 84, 2035-2038	2.5	3
170	Vibrational spectra of vitreous SiO and vitreous GeO from first principles. *Journal of Physics Condensed Matter*, **2007**, 19, 415112	1.8	21
169	Structural properties of amorphous GeSe. *Journal of Physics Condensed Matter*, **2007**, 19, 415111	1.8	9
168	Electronic properties of an epitaxial silicon oxynitride layer on a 6H-SiC(0001) surface: A first-principles investigation. *Applied Physics Letters*, **2007**, 91, 061930	3.4	16
167	Band gaps and dielectric constants of amorphous hafnium silicates: A first-principles investigation. *Applied Physics Letters*, **2007**, 90, 082907	3.4	43
166	Structural and electronic properties of an abrupt 4H□SiC(0001)□SiO2 interface model: Classical molecular dynamics simulations and density functional calculations. *Physical Review B*, **2007**, 76,	3.3	55
165	First-principles investigation of the structural and vibrational properties of vitreous GeSe2. *Physical Review B*, **2007**, 75,	3.3	40
164	Hydrogen in Si(100)□SiO2□HfO2 gate stacks: Relevant charge states and their location. *Applied Physics Letters*, **2007**, 91, 262901	3.4	21
163	Hyper-Raman Spectrum of Vitreous Silica from First Principles. *Physical Review Letters*, **2007**, 98,	7.4	6
162	Proton-induced fixed positive charge at the Si(100)-SiO2 interface. *Physical Review Letters*, **2007**, 99, 126102	7.4	20
161	Microscopic origin of concentration fluctuations over intermediate range distances in network-forming disordered systems. *Physical Review B*, **2007**, 75,	3.3	27
160	Structural and Electronic Properties of Oxygen Vacancies in Monoclinic HfO2. *Materials Research Society Symposia Proceedings*, **2007**, 996, 1		1
159	Umari and Pasquarello Reply:. *Physical Review Letters*, **2006**, 96,	7.4	10
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