

Stefano Baroni

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152
papers

29,986
citations

50
h-index

154
g-index

154
ext. papers

34,440
ext. citations

5.2
avg. IF

6.56
L-index

#	Paper	IF	Citations
152	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
151	Phonons and related crystal properties from density-functional perturbation theory. <i>Reviews of Modern Physics</i> , 2001 , 73, 515-562	40.5	5812
150	Green's-function approach to linear response in solids. <i>Physical Review Letters</i> , 1987 , 58, 1861-1864	7.4	1546
149	Ab initio calculation of phonon dispersions in semiconductors. <i>Physical Review B</i> , 1991 , 43, 7231-7242	3.3	1348
148	Band offsets in lattice-matched heterojunctions: A model and first-principles calculations for GaAs/AlAs. <i>Physical Review Letters</i> , 1988 , 61, 734-737	7.4	465
147	Ab initio calculation of the macroscopic dielectric constant in silicon. <i>Physical Review B</i> , 1986 , 33, 7017-7021	3.1	406
146	Taming multiple valency with density functionals: A case study of defective ceria. <i>Physical Review B</i> , 2005 , 71,	3.3	347
145	Electronic and atomistic structures of clean and reduced ceria surfaces. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 22860-7	3.4	314
144	Anharmonic Phonon Lifetimes in Semiconductors from Density-Functional Perturbation Theory. <i>Physical Review Letters</i> , 1995 , 75, 1819-1822	7.4	270
143	Quantum ESPRESSO toward the exascale. <i>Journal of Chemical Physics</i> , 2020 , 152, 154105	3.9	227
142	Turbo charging time-dependent density-functional theory with Lanczos chains. <i>Journal of Chemical Physics</i> , 2008 , 128, 154105	3.9	207
141	Ab initio calculation of phonon dispersions in II-VI semiconductors. <i>Physical Review B</i> , 1993 , 47, 3588-3593	3.3	196
140	Reptation Quantum Monte Carlo: A Method for Unbiased Ground-State Averages and Imaginary-Time Correlations. <i>Physical Review Letters</i> , 1999 , 82, 4745-4748	7.4	184
139	Efficient approach to time-dependent density-functional perturbation theory for optical spectroscopy. <i>Physical Review Letters</i> , 2006 , 96, 113001	7.4	166
138	Electronic structure of surface-supported bis(phthalocyaninato) terbium(III) single molecular magnets. <i>Nano Letters</i> , 2008 , 8, 3364-8	11.5	165
137	Reply to 'Comment on 'Taming multiple valency with density functionals: A case study of defective ceria'' <i>Physical Review B</i> , 2005 , 72,	3.3	161
136	Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. <i>Physical Review Letters</i> , 1989 , 62, 2853-2856	7.4	161

135	GW quasiparticle spectra from occupied states only. <i>Physical Review B</i> , 2010 , 81,	3.3	155
134	Vibrational and dielectric properties of C60 from density-functional perturbation theory. <i>Journal of Chemical Physics</i> , 1994 , 100, 8537-8539	3.9	150
133	Structure and thermodynamics of SixGe1-x alloys from ab initio Monte Carlo simulations. <i>Physical Review Letters</i> , 1991 , 66, 2116-2119	7.4	144
132	turboTDDFT Γ code for the simulation of molecular spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , 2011 , 182, 1744-1754	4.2	133
131	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2005 , 220,	1	122
130	Templated growth of metal-organic coordination chains at surfaces. <i>Angewandte Chemie - International Edition</i> , 2005 , 44, 6142-5	16.4	118
129	Phonon spectra of ultrathin GaAs/AlAs superlattices: An ab initio calculation. <i>Physical Review B</i> , 1990 , 41, 3870-3873	3.3	110
128	First-principles calculation of the thermal properties of silver. <i>Physical Review B</i> , 1999 , 59, 965-969	3.3	109
127	Hydrogen and coordination bonding supramolecular structures of trimesic acid on Cu(110). <i>Journal of Physical Chemistry A</i> , 2007 , 111, 12589-603	2.8	107
126	Structure, rotational dynamics, and superfluidity of small OCS-doped He clusters. <i>Physical Review Letters</i> , 2003 , 90, 143401	7.4	104
125	Phonon dispersions in GaxAl1-xAs alloys. <i>Physical Review Letters</i> , 1990 , 65, 84-87	7.4	104
124	Tuning band offsets at semiconductor interfaces by intralayer deposition. <i>Physical Review B</i> , 1991 , 43, 7347-7350	3.3	98
123	Optimal representation of the polarization propagator for large-scale GW calculations. <i>Physical Review B</i> , 2009 , 79,	3.3	95
122	Effects of disorder on the Raman spectra of GaAs/AlAs superlattices. <i>Physical Review B</i> , 1992 , 45, 4280-4288	3.3	87
121	4-5 Phase transition in tin: A theoretical study based on density-functional perturbation theory. <i>Physical Review B</i> , 1998 , 57, 10421-10423	3.3	86
120	Magnons in real materials from density-functional theory. <i>Physical Review B</i> , 2000 , 61, R6459-R6462	3.3	85
119	Surface Precursors and Reaction Mechanisms for the Thermal Reduction of Graphene Basal Surfaces Oxidized by Atomic Oxygen. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 4730-4737	3.8	82
118	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. <i>Physical Review B</i> , 1994 , 49, 5323-5328	3.3	81

117	Dependence of the crystal lattice constant on isotopic composition: Theory and ab initio calculations for C, Si, and Ge. <i>Solid State Communications</i> , 1994 , 90, 295-297	1.6	81
116	Time-dependent density functional theory study of squaraine dye-sensitized solar cells. <i>Chemical Physics Letters</i> , 2009 , 475, 49-53	2.5	79
115	Interaction of hydrogen with cerium oxide surfaces: a quantum mechanical computational study. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 19380-5	3.4	77
114	Elastic constants of crystals from linear-response theory. <i>Physical Review Letters</i> , 1987 , 59, 2662-2665	7.4	73
113	Monitoring two-dimensional coordination reactions: directed assembly of co-terephthalate nanosystems on Au(111). <i>Journal of Physical Chemistry B</i> , 2006 , 110, 5627-32	3.4	72
112	High-pressure thermal expansion, bulk modulus, and phonon structure of diamond. <i>Physical Review B</i> , 1999 , 60, 9444-9449	3.3	70
111	Microscopic theory and quantum simulation of atomic heat transport. <i>Nature Physics</i> , 2016 , 12, 80-84	16.2	63
110	Engineering the reactivity of metal catalysts: a model study of methane dehydrogenation on Rh(111). <i>Journal of the American Chemical Society</i> , 2004 , 126, 16732-3	16.4	63
109	Oxygen dissociation by concerted action of di-iron centers in metal-organic coordination networks at surfaces: modeling non-heme iron enzymes. <i>Nano Letters</i> , 2011 , 11, 5414-20	11.5	60
108	Exact-exchange extension of the local-spin-density approximation in atoms: Calculation of total energies and electron affinities. <i>Journal of Chemical Physics</i> , 1983 , 79, 6140-6144	3.9	60
107	Computational spectroscopy of helium-solvated molecules: effective inertia, from small He clusters toward the nanodroplet regime. <i>Journal of Chemical Physics</i> , 2005 , 123, 114306	3.9	57
106	Oxygen self-diffusion in alpha-quartz. <i>Physical Review Letters</i> , 2001 , 86, 4564-7	7.4	56
105	Structure and phase stability of GaxIn1-xP solid solutions from computational alchemy. <i>Physical Review Letters</i> , 1994 , 72, 4001-4004	7.4	56
104	Temperature-dependent surface relaxations of Ag(111). <i>Physical Review B</i> , 1999 , 59, 970-974	3.3	53
103	Theory of the Anomalous Rayleigh Dispersion at H/W(110) Surfaces. <i>Physical Review Letters</i> , 1996 , 77, 2491-2494	7.4	50
102	First principles thermoelasticity of MgSiO3-perovskite: Consequences for the inferred properties of the lower mantle. <i>Geophysical Research Letters</i> , 2001 , 28, 2699-2702	4.9	49
101	Methane dehydrogenation on Rh@Cu(111): a first-principles study of a model catalyst. <i>Journal of the American Chemical Society</i> , 2006 , 128, 12448-54	16.4	48
100	Dielectric and thermal effects on the optical properties of natural dyes: a case study on solvated cyanin. <i>Journal of the American Chemical Society</i> , 2011 , 133, 15425-33	16.4	46

99	Rotational dynamics of CO solvated in small He clusters: a quantum Monte Carlo study. <i>Journal of Chemical Physics</i> , 2004 , 120, 9071-6	3.9	45
98	Energy-level alignment in organic dye-sensitized TiO ₂ from GW calculations. <i>Journal of Chemical Physics</i> , 2013 , 139, 014709	3.9	43
97	turboTDDFT 2.0: Hybrid functionals and new algorithms within time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , 2014 , 185, 2080-2089	4.2	43
96	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 9839-9846	3.4	43
95	Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. <i>Surface Science</i> , 2002 , 501, 182-190	1.8	42
94	Nonlinear piezoelectricity in CdTe. <i>Physical Review B</i> , 1993 , 47, 16252-16256	3.3	41
93	Third-order density-functional perturbation theory: A practical implementation with applications to anharmonic couplings in Si. <i>Solid State Communications</i> , 1994 , 91, 813-816	1.6	41
92	Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach. <i>Nature Communications</i> , 2019 , 10, 3853	17.4	39
91	Effects of disorder on the vibrational properties of SiGe alloys: Failure of mean-field approximations. <i>Physical Review Letters</i> , 1992 , 69, 1959-1962	7.4	38
90	Electronic structure of InP/Ga _{0.47} In _{0.53} As interfaces. <i>Physical Review B</i> , 1990 , 41, 12106-12110	3.3	38
89	The reconstruction of nickel and rhodium (001) surfaces upon carbon, nitrogen or oxygen adsorptions. <i>Surface Science</i> , 1999 , 437, 18-28	1.8	36
88	Anomalous pressure-induced transition(s) in ice XI. <i>Physical Review Letters</i> , 2004 , 92, 105502	7.4	35
87	Ab initio calculation of the band offset at strained GaAs/InAs (001) heterojunctions. <i>Physical Review B</i> , 1993 , 48, 17607-17610	3.3	35
86	The surface chemistry of metal-oxygen interactions: a first-principles study of O:Rh(110). <i>Surface Science</i> , 1997 , 370, 166-178	1.8	33
85	Adsorption of chlorine on Ag(111): No subsurface Cl at low coverage. <i>Physical Review B</i> , 2008 , 78,	3.3	33
84	Order-disorder phase boundary between ice VII and VIII obtained by first principles. <i>Chemical Physics Letters</i> , 2010 , 499, 236-240	2.5	30
83	Computer simulation of quantum melting in hydrogen clusters. <i>ChemPhysChem</i> , 2005 , 6, 1884-8	3.2	30
82	The phonon spectra of LiH and LiD from density-functional perturbation theory. <i>Solid State Communications</i> , 1996 , 98, 203-207	1.6	30

81	Accurate and inexpensive prediction of the color optical properties of anthocyanins in solution. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 3816-22	2.8	28
80	Accurate thermal conductivities from optimally short molecular dynamics simulations. <i>Scientific Reports</i> , 2017 , 7, 15835	4.9	28
79	Auxiliary-field quantum Monte Carlo calculations for systems with long-range repulsive interactions. <i>Physical Review Letters</i> , 1993 , 71, 1148-1151	7.4	28
78	Energetically driven reorganization of a modified catalytic surface under reaction conditions. <i>Journal of the American Chemical Society</i> , 2005 , 127, 2351-7	16.4	27
77	Phonon softening and high-pressure low-symmetry phases of cesium iodide. <i>Physical Review Letters</i> , 1992 , 69, 1069-1072	7.4	27
76	Computational spectroscopy of carbon monoxide isotopomers in helium clusters. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 7640-5	2.8	26
75	Spin-flop ordering from frustrated ferro- and antiferromagnetic interactions: a combined theoretical and experimental study of a Mn/Fe(100) monolayer. <i>Physical Review Letters</i> , 2005 , 95, 117201	7.4	26
74	Structural and electronic properties of spinel semiconductors: An ab initio pseudopotential study of MgIn ₂ S ₅ . <i>Physical Review B</i> , 1988 , 38, 8258-8263	3.3	26
73	Exact-exchange extension of the local-spin-density approximation in atoms. II. The iron series. <i>Journal of Chemical Physics</i> , 1984 , 80, 5703-5708	3.9	26
72	Atomic intermixing in short period GaAs/AlAs superlattices. <i>Surface Science</i> , 1992 , 267, 171-175	1.8	24
71	turboEELS code for the simulation of the electron energy loss and inelastic X-ray scattering spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , 2015 , 196, 460-469	4.2	23
70	Theoretical study of cubic versus tetragonal structures of defect zinc-blende semiconductors: CdIn ₂ Se ₄ . <i>Physical Review B</i> , 1989 , 40, 1725-1731	3.3	23
69	High-pressure low-symmetry phases of cesium halides. <i>Physical Review B</i> , 1995 , 51, 8060-8068	3.3	22
68	Bulk and interfacial strain in Si/Ge heterostructures. <i>Physical Review B</i> , 1994 , 49, 7490-7498	3.3	22
67	Itinerant ferromagnetic phase of the Hubbard model. <i>Physical Review B</i> , 2011 , 83,	3.3	21
66	Theory of band offsets at semiconductor heterojunctions: An ab-initio linear response approach. <i>Superlattices and Microstructures</i> , 1989 , 6, 31-37	2.8	21
65	Gauge Invariance of Thermal Transport Coefficients. <i>Journal of Low Temperature Physics</i> , 2016 , 185, 79-86	3	19
64	Electron energy loss and inelastic x-ray scattering cross sections from time-dependent density-functional perturbation theory. <i>Physical Review B</i> , 2013 , 88,	3.3	19

63	Vibrational broadening of x-ray emission spectra: A first-principles study on diamond. <i>Physical Review B</i> , 1997 , 55, 9649-9658	3.3	19
62	Can We Tune the Band Offset at Semiconductor Heterojunctions?. <i>NATO ASI Series Series B: Physics</i> , 1989 , 251-271		19
61	Molecular design of photoactive acenes for organic photovoltaics. <i>Journal of Chemical Physics</i> , 2009 , 130, 194701	3.9	18
60	DFT study of a weakly pi-bonded C ₂ H ₄ on oxygen-covered Ag(100). <i>Journal of Physical Chemistry B</i> , 2006 , 110, 367-76	3.4	18
59	Computational spectroscopy of doped He clusters. <i>Computer Physics Communications</i> , 2005 , 169, 404-407.	4.2	18
58	Effects of isotopic disorder on the Raman spectra of crystals: Theory and ab initio calculations for diamond and germanium. <i>Physical Review B</i> , 2000 , 61, 9387-9392	3.3	18
57	Activated Adsorption of Ethylene on Atomic-Oxygen-Covered Ag(100) and Ag(210): Formation of an Oxametallacycle. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 1019-1027	3.8	17
56	Fast hybrid density-functional computations using plane-wave basis sets. <i>Electronic Structure</i> , 2019 , 1, 015009	2.6	16
55	Dynamical-charge neutrality at a crystal surface. <i>Physical Review B</i> , 1998 , 57, 5742-5745	3.3	16
54	Adsorption of ethylene on stepped Ag() surfaces. <i>Surface Science</i> , 2004 , 566-568, 1018-1023	1.8	15
53	Thermodynamic properties and lattice dynamics of silver at high pressure: A first-principles study. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1999 , 79, 911-919		15
52	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. <i>Journal of Chemical Physics</i> , 2015 , 142, 034111	3.9	14
51	Sampling Molecular Conformers in Solution with Quantum Mechanical Accuracy at a Nearly Molecular-Mechanics Cost. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4385-9	6.4	14
50	Topological quantization and gauge invariance of charge transport in liquid insulators. <i>Nature Physics</i> , 2019 , 15, 967-972	16.2	14
49	Harnessing molecular excited states with Lanczos chains. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 074204	1.8	14
48	SixC1 \times O ₂ alloys: A possible route to stabilize carbon-based silica-like solids?. <i>Solid State Communications</i> , 2007 , 144, 273-276	1.6	14
47	Co-adsorption of ethylene and oxygen on the Ag(001) surface. <i>Surface Science</i> , 2003 , 532-535, 191-197	1.8	14
46	Theory and Numerical Simulation of Heat Transport in Multicomponent Systems. <i>Physical Review Letters</i> , 2019 , 122, 255901	7.4	13

45	Oxygen vibrations in OAg(0 0 1). <i>Surface Science</i> , 2003 , 530, 26-36	1.8	13
44	Characterization of Si-doped GaAs cross-sectional surfaces via ab initio simulations. <i>Physical Review B</i> , 2005 , 72,	3.3	13
43	Effects of disorder on the optical gap of (Zn,Mg)(S,Se). <i>Applied Physics Letters</i> , 1999 , 75, 2746-2748	3.4	13
42	InAs/GaSb(001) valence-band offset: Independence of interface composition and strain. <i>Applied Physics Letters</i> , 1996 , 69, 3218-3220	3.4	12
41	Pressure-induced structural instability of cesium halides from ab initio pseudopotential techniques. <i>Physical Review B</i> , 1987 , 35, 765-769	3.3	12
40	Reptation quantum Monte Carlo algorithm for lattice Hamiltonians with a directed-update scheme. <i>Physical Review E</i> , 2010 , 82, 046710	2.4	11
39	Unraveling the molecular mechanisms of color expression in anthocyanins. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 8757-8766	3.6	10
38	Multimodel Approach to the Optical Properties of Molecular Dyes in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4423-9	6.4	10
37	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. <i>Surface Science</i> , 2005 , 587, 50-54	1.8	10
36	Ab initio simulation of photoemission spectroscopy in solids: Plane-wave pseudopotential approach with applications to normal-emission spectra of Cu(001) and Cu(111). <i>Physical Review B</i> , 2008 , 77,	3.3	9
35	Density-Functional Perturbation Theory 2005 , 195-214		9
34	Heat Transport in Insulators from Ab Initio Green-Kubo Theory 2018 , 1-36		9
33	Zero-temperature dynamics of solid H4e from quantum Monte Carlo simulations. <i>Physical Review B</i> , 2009 , 80,	3.3	8
32	Absolute transition rates for rare events from dynamical decoupling of reaction variables. <i>Physical Review Letters</i> , 2012 , 109, 150601	7.4	8
31	The structure and phase stability of CO adsorbates on Rh(110). <i>Surface Science</i> , 1997 , 382, L666-L671	1.8	8
30	Reptation Quantum Monte Carlo 1999 , 313-341		8
29	Heat and charge transport in HO at ice-giant conditions from ab initio molecular dynamics simulations. <i>Nature Communications</i> , 2020 , 11, 3605	17.4	8
28	Discovery of a natural cyan blue: A unique food-sourced anthocyanin could replace synthetic brilliant blue. <i>Science Advances</i> , 2021 , 7,	14.3	8

27	3. Density-Functional Perturbation Theory for Quasi-Harmonic Calculations 2010 , 39-58		7
26	Effects of isotopic disorder on the Raman spectra of crystals: theory and ab initio calculations for diamond and germanium. <i>Computational Materials Science</i> , 2000 , 17, 395-399	3.2	7
25	Hartree-Fock energy bands in molecular crystals: Solid hydrogen in the cubic phase. <i>Physical Review B</i> , 1984 , 30, 7187-7193	3.3	7
24	Spin dynamics from time-dependent density functional perturbation theory. <i>European Physical Journal B</i> , 2018 , 91, 1	1.2	7
23	Gauge Fixing for Heat-Transport Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3352-3362	6.4	6
22	The Liouville-Lanczos Approach to Time-Dependent Density-Functional (Perturbation) Theory. <i>Lecture Notes in Physics</i> , 2012 , 375-390	0.8	6
21	Approximate treatment of semicore states in GW calculations with application to Au clusters. <i>Journal of Chemical Physics</i> , 2014 , 140, 124101	3.9	5
20	Characterizing In and N impurities in GaAs from ab initio computer simulation of (110) cross-sectional STM images. <i>Physical Review B</i> , 2007 , 75,	3.3	5
19	Thermal and Tidal Evolution of Uranus with a Growing Frozen Core. <i>Planetary Science Journal</i> , 2021 , 2, 222	2.9	5
18	Ab initio study of electron energy loss spectra of bulk bismuth up to 100 eV. <i>Physical Review B</i> , 2017 , 95,	3.3	4
17	Metallization of the C60/Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations. <i>Journal of Chemical Physics</i> , 2010 , 132, 234710	3.9	4
16	Unraveling excited states of doped helium clusters. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 12749-53	2.8	4
15	Heat transport in liquid water from first-principles and deep neural network simulations. <i>Physical Review B</i> , 2021 , 104,	3.3	4
14	Optical properties of anthocyanins in the gas phase. <i>Chemical Physics Letters</i> , 2015 , 618, 24-29	2.5	3
13	Cross-sectional imaging of sharp Si interlayers embedded in gallium arsenide. <i>Applied Physics Letters</i> , 2006 , 88, 022115	3.4	3
12	Oxidation States, Thouless Pumps, and Nontrivial Ionic Transport in Nonstoichiometric Electrolytes. <i>Physical Review X</i> , 2020 , 10,	9.1	3
11	Invariance principles in the theory and computation of transport coefficients. <i>European Physical Journal B</i> , 2021 , 94, 160	1.2	3
10	QEHeat: An open-source energy flux calculator for the computation of heat-transport coefficients from first principles. <i>Computer Physics Communications</i> , 2021 , 269, 108090	4.2	3

9	Ab initio studies of structural and electronic properties 2008 , 17-54		2
8	High Pressure Lattice Instabilities and Structural Phase Transformations in Solids from Ab-Initio Lattice Dynamics. <i>Materials Research Society Symposia Proceedings</i> , 1997 , 499, 233		1
7	Temperature- and vacancy-concentration-dependence of heat transport in Li ₃ ClO from multi-method numerical simulations. <i>Npj Computational Materials</i> , 2022 , 8,	10.9	1
6	Heat Transport in Insulators from Ab Initio Green-Kubo Theory 2020 , 809-844		1
5	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. <i>Physical Review B</i> , 2020 , 102,	3.3	1
4	Structure and Thermodynamics of SiGe Alloys from Computational Alchemy 1992 , 133-149		0
3	Accelerating GW Calculations with Optimal Polarizability Basis 2011 , 61-78		
2	Vibrational properties of isolated ALAs monolayers embedded in GaAs: a theoretical study of the effects of disorder. <i>Applied Surface Science</i> , 1992 , 56-58, 617-621	6.7	
1	Band Offsets at Semiconductor Heterojunctions: Bulk or Interface Properties?. <i>NATO ASI Series Series B: Physics</i> , 1989 , 51-60		