Stefano Baroni

List of Publications by Year in descending order

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152 papers	39,229 citations	31949 53 h-index	9090 144 g-index
154 all docs	154 docs citations	154 times ranked	29086 citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	0.7	18,183
2	Phonons and related crystal properties from density-functional perturbation theory. Reviews of Modern Physics, 2001, 73, 515-562.	16.4	7,534
3	Greenâ€™s-function approach to linear response in solids. Physical Review Letters, 1987, 58, 1861-1864.	2.9	1,807
4	Ab initiocalculation of phonon dispersions in semiconductors. Physical Review B, 1991, 43, 7231-7242.	1.1	1,619
5	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	1.2	796
6	Band Offsets in Lattice-Matched Heterojunctions: A Model and First-Principles Calculations for GaAs/AlAs. Physical Review Letters, 1988, 61, 734-737.	2.9	507
7	Ab initiocalculation of the macroscopic dielectric constant in silicon. Physical Review B, 1986, 33, 7017-7021.	1.1	499
8	Taming multiple valency with density functionals:â€ƒA case study of defective ceria. Physical Review B, 2005, 71, .	1.1	383
9	Electronic and Atomistic Structures of Clean and Reduced Ceria Surfaces. Journal of Physical Chemistry B, 2005, 109, 22860-22867.	1.2	358
10	Anharmonic Phonon Lifetimes in Semiconductors from Density-Functional Perturbation Theory. Physical Review Letters, 1995, 75, 1819-1822.	2.9	325
11	Turbo charging time-dependent density-functional theory with Lanczos chains. Journal of Chemical Physics, 2008, 128, 154105.	1.2	234
12	Ab initiocalculation of phonon dispersions in II-VI semiconductors. Physical Review B, 1993, 47, 3588-3592.	1.1	229
13	Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. Physical Review Letters, 1989, 62, 2853-2856.	2.9	221
14	Efficient Approach to Time-Dependent Density-Functional Perturbation Theory for Optical Spectroscopy. Physical Review Letters, 2006, 96, 113001.	2.9	208
15	Reptation Quantum Monte Carlo: A Method for Unbiased Ground-State Averages and Imaginary-Time Correlations. Physical Review Letters, 1999, 82, 4745-4748.	2.9	197
16	Vibrational and dielectric properties of C60 from densityâ€functional perturbation theory. Journal of Chemical Physics, 1994, 100, 8537-8539.	1.2	184
17	Electronic Structure of Surface-supported Bis(phthalocyaninato) terbium(III) Single Molecular Magnets. Nano Letters, 2008, 8, 3364-3368.	4.5	183
18	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	177

#	Article	IF	Citations
19	Reply to â€œComment on â€˜Taming multiple valency with density functionals: A case study of defective ceria' â€• Physical Review B, 2005, 72, .	1.1	177
20	GW quasiparticle spectra from occupied states only. Physical Review B, 2010, 81, .	1.1	172
21	turboTDDFT â€“ A code for the simulation of molecular spectra using the Liouvilleâ€“Lanczos approach to time-dependent density-functional perturbation theory. Computer Physics Communications, 2011, 182, 1744-1754.	3.0	167
22	Structure and thermodynamics ofSixGe1âˆ’xalloys fromab initioMonte Carlo simulations. Physical Review Letters, 1991, 66, 2116-2119.	2.9	155
23	Templated Growth of Metal-Organic Coordination Chains at Surfaces. Angewandte Chemie - International Edition, 2005, 44, 6142-6145.	7.2	125
24	First-principles calculation of the thermal properties of silver. Physical Review B, 1999, 59, 965-969.	1.1	124
25	Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach. Nature Communications, 2019, 10, 3853.	5.8	122
26	Magnons in real materials from density-functional theory. Physical Review B, 2000, 61, R6459-R6462.	1.1	118
27	Hydrogen and Coordination Bonding Supramolecular Structures of Trimesic Acid on Cu(110). Journal of Physical Chemistry A, 2007, 111, 12589-12603.	1.1	118
28	Phonon spectra of ultrathin GaAs/AlAs superlattices: Anab initiocalculation. Physical Review B, 1990, 41, 3870-3873.	1.1	116
29	Structure, Rotational Dynamics, and Superfluidity of Small OCS-Doped He Clusters. Physical Review Letters, 2003, 90, 143401.	2.9	111
30	Phonon dispersions inGaxAl1âˆ’xAs alloys. Physical Review Letters, 1990, 65, 84-87.	2.9	108
31	Î±â†”Î² phase transition in tin: A theoretical study based on density-functional perturbation theory. Physical Review B, 1998, 57, 10421-10423.	1.1	106
32	Tuning band offsets at semiconductor interfaces by intralayer deposition. Physical Review B, 1991, 43, 7347-7350.	1.1	103
33	Optimal representation of the polarization propagator for large-scale<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations. Physical Review B, 2009, 79, .	1.1	103
34	Surface Precursors and Reaction Mechanisms for the Thermal Reduction of Graphene Basal Surfaces Oxidized by Atomic Oxygen. Journal of Physical Chemistry C, 2011, 115, 4730-4737.	1.5	101
35	Dependence of the crystal lattice constant on isotopic composition: Theory and ab initio calculations for C, Si, and Ge. Solid State Communications, 1994, 90, 295-297.	0.9	94
36	Microscopic theory and quantum simulation of atomic heat transport. Nature Physics, 2016, 12, 80-84.	6.5	93

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37	Effects of disorder on the Raman spectra of GaAs/AlAs superlattices. Physical Review B, 1992, 45, 4280-4288.	1.1	88
38	Elastic Constants of Crystals from Linear-Response Theory. Physical Review Letters, 1987, 59, 2662-2665.	2.9	87
39	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. Physical Review B, 1994, 49, 5323-5328.	1.1	87
40	Interaction of Hydrogen with Cerium Oxide Surfaces:â€‰ a Quantum Mechanical Computational Study. Journal of Physical Chemistry B, 2006, 110, 19380-19385.	1.2	85
41	High-pressure thermal expansion, bulk modulus, and phonon structure of diamond. Physical Review B, 1999, 60, 9444-9449.	1.1	84
42	Time-dependent density functional theory study of squaraine dye-sensitized solar cells. Chemical Physics Letters, 2009, 475, 49-53.	1.2	82
43	Engineering the Reactivity of Metal Catalysts:Â A Model Study of Methane Dehydrogenation on Rh(111). Journal of the American Chemical Society, 2004, 126, 16732-16733.	6.6	80
44	Monitoring Two-Dimensional Coordination Reactions:Â Directed Assembly of Coâ^'Terephthalate Nanosystems on Au(111). Journal of Physical Chemistry B, 2006, 110, 5627-5632.	1.2	74
45	Oxygen Dissociation by Concerted Action of Di-Iron Centers in Metalâ€“Organic Coordination Networks at Surfaces: Modeling Non-Heme Iron Enzymes. Nano Letters, 2011, 11, 5414-5420.	4.5	66
46	Exactâ€exchange extension of the localâ€spinâ€density approximation in atoms: Calculation of total energies and electron affinities. Journal of Chemical Physics, 1983, 79, 6140-6144.	1.2	63
47	Structure and phase stability ofGaxIn1â^'xP solid solutions from computational alchemy. Physical Review Letters, 1994, 72, 4001-4004.	2.9	61
48	Methane Dehydrogenation on Rh@Cu(111):Â A First-Principles Study of a Model Catalyst. Journal of the American Chemical Society, 2006, 128, 12448-12454.	6.6	60
49	Temperature-dependent surface relaxations of Ag(111). Physical Review B, 1999, 59, 970-974.	1.1	58
50	Oxygen Self-Diffusion inÎ±-Quartz. Physical Review Letters, 2001, 86, 4564-4567.	2.9	57
51	Computational spectroscopy of helium-solvated molecules: Effective inertia, from small He clusters toward the nanodroplet regime. Journal of Chemical Physics, 2005, 123, 114306.	1.2	57
52	First principles thermoelasticity of MgSiO3-perovskite: Consequences for the inferred properties of the lower mantle. Geophysical Research Letters, 2001, 28, 2699-2702.	1.5	55
53	turboTDDFT 2.0â€"Hybrid functionals and new algorithms within time-dependent density-functional perturbation theory. Computer Physics Communications, 2014, 185, 2080-2089.	3.0	55
54	Energy-level alignment in organic dye-sensitized TiO2 from GW calculations. Journal of Chemical Physics, 2013, 139, 014709.	1.2	53

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55	Theory of the Anomalous Rayleigh Dispersion at H/W(110) Surfaces. Physical Review Letters, 1996, 77, 2491-2494.	2.9	51
56	Theoretical study of cubic versus tetragonal structures of defect zinc-blende semiconductors:CdIn2Se4. Physical Review B, 1989, 40, 1725-1731.	1.1	50
57	Dielectric and Thermal Effects on the Optical Properties of Natural Dyes: A Case Study on Solvated Cyanin. Journal of the American Chemical Society, 2011, 133, 15425-15433.	6.6	50
58	Effects of disorder on the vibrational properties of SiGe alloys: Failure of mean-field approximations. Physical Review Letters, 1992, 69, 1959-1962.	2.9	49
59	Accurate thermal conductivities from optimally short molecular dynamics simulations. Scientific Reports, 2017, 7, 15835.	1.6	49
60	Nonlinear piezoelectricity in CdTe. Physical Review B, 1993, 47, 16252-16256.	1.1	48
61	Third-order density-functional perturbation theory: A practical implementation with applications to anharmonic couplings in Si. Solid State Communications, 1994, 91, 813-816.	0.9	48
62	Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. Surface Science, 2002, 501, 182-190.	0.8	47
63	Rotational dynamics of CO solvated in small He clusters: A quantum Monte Carlo study. Journal of Chemical Physics, 2004, 120, 9071-9076.	1.2	46
64	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. Journal of Physical Chemistry B, 2002, 106, 9839-9846.	1.2	45
65	Structural and electronic properties of spinel semiconductors: Anab initiopseudopotential study ofMgIn2S4. Physical Review B, 1988, 38, 8258-8263.	1.1	41
66	turboEELSâ€"A code for the simulation of the electron energy loss and inelastic X-ray scattering spectra using the Liouvilleâ€"Lanczos approach to time-dependent density-functional perturbation theory. Computer Physics Communications, 2015, 196, 460-469.	3.0	41
67	Electronic structure of InP/Ga0.47In0.53As interfaces. Physical Review B, 1990, 41, 12106-12110.	1.1	40
68	Orderâ€"disorder phase boundary between ice VII and VIII obtained by first principles. Chemical Physics Letters, 2010, 499, 236-240.	1.2	40
69	Ab initiocalculation of the band offset at strained GaAs/InAs (001) heterojunctions. Physical Review B, 1993, 48, 17607-17610.	1.1	37
70	Anomalous Pressure-Induced Transition(s) in Ice XI. Physical Review Letters, 2004, 92, 105502.	2.9	37
71	Energetically Driven Reorganization of a Modified Catalytic Surface under Reaction Conditions. Journal of the American Chemical Society, 2005, 127, 2351-2357.	6.6	37
72	Adsorption of chlorine on Ag(111): No subsurface Cl at low coverage. Physical Review B, 2008, 78, .	1.1	37

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73	The reconstruction of nickel and rhodium (001) surfaces upon carbon, nitrogen or oxygen adsorptions. Surface Science, 1999, 437, 18-28.	0.8	36
74	Accurate and Inexpensive Prediction of the Color Optical Properties of Anthocyanins in Solution. Journal of Physical Chemistry A, 2015, 119, 3816-3822.	1.1	36
75	The surface chemistry of metal-oxygen interactions: a first-principles study of O:Rh(110). Surface Science, 1997, 370, 166-178.	0.8	35
76	Discovery of a natural cyan blue: A unique food-sourced anthocyanin could replace synthetic brilliant blue. Science Advances, 2021, 7, .	4.7	34
77	Auxiliary-field quantum Monte Carlo calculations for systems with long-range repulsive interactions. Physical Review Letters, 1993, 71, 1148-1151.	2.9	32
78	The phonon spectra of LiH and LiD from density-functional perturbation theory. Solid State Communications, 1996, 98, 203-207.	0.9	32
79	Gauge Invariance of Thermal Transport Coefficients. Journal of Low Temperature Physics, 2016, 185, 79-86.	0.6	31
80	Computer Simulation of Quantum Melting in Hydrogen Clusters. ChemPhysChem, 2005, 6, 1884-1888.	1.0	30
81	Electron energy loss and inelastic x-ray scattering cross sections from time-dependent density-functional perturbation theory. Physical Review B, 2013, 88, .	1.1	29
82	Fast hybrid density-functional computations using plane-wave basis sets. Electronic Structure, 2019, 1, 015009.	1.0	29
83	Heat transport in liquid water from first-principles and deep neural network simulations. Physical Review B, 2021, 104, .	1.1	29
84	Exactâ€exchange extension of the localâ€spinâ€density approximation in atoms. II. The iron series. Journal of Chemical Physics, 1984, 80, 5703-5708.	1.2	27
85	Phonon softening and high-pressure low-symmetry phases of cesium iodide. Physical Review Letters, 1992, 69, 1069-1072.	2.9	27
86	Spin-Flop Ordering from Frustrated Ferro- and Antiferromagnetic Interactions: A Combined Theoretical and Experimental Study of aMn/Fe(100)Monolayer. Physical Review Letters, 2005, 95, 117201.	2.9	27
87	Computational Spectroscopy of Carbon Monoxide Isotopomers in Helium Clusters. Journal of Physical Chemistry A, 2007, 111, 7640-7645.	1.1	26
88	Itinerant ferromagnetic phase of the Hubbard model. Physical Review B, 2011, 83, .	1.1	26
89	Atomic intermixing in short period GaAs/AlAs superlattices. Surface Science, 1992, 267, 171-175.	0.8	25
90	Theory and Numerical Simulation of Heat Transport in Multicomponent Systems. Physical Review Letters, 2019, 122, 255901.	2.9	25

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91	Topological quantization and gauge invariance of charge transport in liquid insulators. Nature Physics, 2019, 15, 967-972.	6.5	25
92	High-pressure low-symmetry phases of cesium halides. Physical Review B, 1995, 51, 8060-8068.	1.1	23
93	Viscosity in water from first-principles and deep-neural-network simulations. Npj Computational Materials, 2022, 8, .	3.5	23
94	Theory of band offsets at semiconductor heterojunctions: An ab-initio linear response approach. Superlattices and Microstructures, 1989, 6, 31-37.	1.4	22
95	Bulk and interfacial strain in Si/Ge heterostructures. Physical Review B, 1994, 49, 7490-7498.	1.1	22
96	Density-Functional Perturbation Theory. , 2005, , 195-214.		22
97	Vibrational broadening of x-ray emission spectra: A first-principles study on diamond. Physical Review B, 1997, 55, 9649-9658.	1.1	21
98	Activated Adsorption of Ethylene on Atomic-Oxygen-Covered Ag(100) and Ag(210):â€‰ Formation of an Oxametallacycle. Journal of Physical Chemistry C, 2008, 112, 1019-1027.	1.5	21
99	Can We Tune the Band Offset at Semiconductor Heterojunctions?. NATO ASI Series Series B: Physics, 1989, , 251-271.	0.2	21
100	Thermodynamic properties and lattice dynamics of silver at high pressure: A first-principles study. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1999, 79, 911-919.	0.6	20
101	DFT Study of a Weakly Ï€-Bonded C2H4on Oxygen-Covered Ag(100). Journal of Physical Chemistry B, 2006, 110, 367-376.	1.2	20
102	Unraveling the molecular mechanisms of color expression in anthocyanins. Physical Chemistry Chemical Physics, 2019, 21, 8757-8766.	1.3	20
103	Heat and charge transport in H2O at ice-giant conditions from ab initio molecular dynamics simulations. Nature Communications, 2020, 11, 3605.	5.8	20
104	Effects of isotopic disorder on the Raman spectra of crystals: Theory andab initiocalculations for diamond and germanium. Physical Review B, 2000, 61, 9387-9392.	1.1	19
105	Molecular design of photoactive acenes for organic photovoltaics. Journal of Chemical Physics, 2009, 130, 194701.	1.2	19
106	Invariance principles in the theory and computation of transport coefficients. European Physical Journal B, 2021, 94, 160.	0.6	19
107	Computational spectroscopy of doped He clusters. Computer Physics Communications, 2005, 169, 404-407.	3.0	18
108	Oxygen vibrations in Oâ€“Ag(001). Surface Science, 2003, 530, 26-36.	0.8	17

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109	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. Journal of Chemical Physics, 2015, 142, 034111.	1.2	17
110	Spin dynamics from time-dependent density functional perturbation theory. European Physical Journal B, 2018, 91, 1.	0.6	17
111	Dynamical-charge neutrality at a crystal surface. Physical Review B, 1998, 57, 5742-5745.	1.1	16
112	Adsorption of ethylene on stepped Ag() surfaces. Surface Science, 2004, 566-568, 1018-1023.	0.8	16
113	SixC1â^'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	0.9	16
114	Temperature- and vacancy-concentration-dependence of heat transport in Li3ClO from multi-method numerical simulations. Npj Computational Materials, 2022, 8, .	3.5	16
115	Harnessing molecular excited states with Lanczos chains. Journal of Physics Condensed Matter, 2010, 22, 074204.	0.7	15
116	Sampling Molecular Conformers in Solution with Quantum Mechanical Accuracy at a Nearly Molecular-Mechanics Cost. Journal of Chemical Theory and Computation, 2016, 12, 4385-4389.	2.3	15
117	Effects of disorder on the optical gap of (Zn,Mg)(S,Se). Applied Physics Letters, 1999, 75, 2746-2748.	1.5	14
118	Co-adsorption of ethylene and oxygen on the Ag(001) surface. Surface Science, 2003, 532-535, 191-197.	0.8	14
119	Characterization of Si-doped GaAs cross-sectional surfaces viaab initiosimulations. Physical Review B, 2005, 72, .	1.1	14
120	Gauge Fixing for Heat-Transport Simulations. Journal of Chemical Theory and Computation, 2020, 16, 3352-3362.	2.3	14
121	InAs/GaSb(001) valenceâ€band offset: Independence of interface composition and strain. Applied Physics Letters, 1996, 69, 3218-3220.	1.5	13
122	Reptation quantum Monte Carlo algorithm for lattice Hamiltonians with a directed-update scheme. Physical Review E, 2010, 82, 046710.	0.8	13
123	Multimodel Approach to the Optical Properties of Molecular Dyes in Solution. Journal of Chemical Theory and Computation, 2016, 12, 4423-4429.	2.3	13
124	Pressure-induced structural instability of cesium halides fromab initiopseudopotential techniques. Physical Review B, 1987, 35, 765-769.	1.1	12
125	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. Surface Science, 2005, 587, 50-54.	0.8	12
126	Thermal and Tidal Evolution of Uranus with a Growing Frozen Core. Planetary Science Journal, 2021, 2, 222.	1.5	12

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127	Heat Transport in Insulators from Ab Initio Green-Kubo Theory. , 2018, , 1-36.		11
128	Ab initiostudy of electron energy loss spectra of bulk bismuth up to 100 eV. Physical Review B, 2017, 95, .	1.1	10
129	Ab initiosimulation of photoemission spectroscopy in solids: Plane-wave pseudopotential approach with applications to normal-emission spectra of Cu(001) and Cu(111). Physical Review B, 2008, 77, .	1.1	9
130	Absolute Transition Rates for Rare Events from Dynamical Decoupling of Reaction Variables. Physical Review Letters, 2012, 109, 150601.	2.9	9
131	Oxidation States, Thoulessâ€™ Pumps, and Nontrivial Ionic Transport in Nonstoichiometric Electrolytes. Physical Review X, 2020, 10, .	2.8	9
132	The structure and phase stability of CO adsorbates on Rh(110). Surface Science, 1997, 382, L666-L671.	0.8	8
133	Effects of isotopic disorder on the Raman spectra of crystals: theory and ab initio calculations for diamond and germanium. Computational Materials Science, 2000, 17, 395-399.	1.4	8
134	Zero-temperature dynamics of solid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mmultiscripts><mml:mtext>H</mml:mtext><mml:mprescripts /><mml:none /><mml:mn>4</mml:mn></mml:mmultiscripts><mml:mtext>e</mml:mtext></mml:mrow></mml:math>from quantum Monte Carlo simulations. Physical Review B, 2009, 80, .	1.1	8
135	3. Density-Functional Perturbation Theory for Quasi-Harmonic Calculations. , 2010, , 39-58.		8
136	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. Physical Review B, 2020, 102, .	1.1	8
137	Reptation Quantum Monte Carlo. , 1999, , 313-341.		8
138	Hartree-Fock energy bands in molecular crystals: Solid hydrogen in the cubic phase. Physical Review B, 1984, 30, 7187-7193.	1.1	7
139	QEHeat: An open-source energy flux calculator for the computation of heat-transport coefficients from first principles. Computer Physics Communications, 2021, 269, 108090.	3.0	7
140	The Liouville-Lanczos Approach to Time-Dependent Density-Functional (Perturbation) Theory. Lecture Notes in Physics, 2012, , 375-390.	0.3	7
141	Characterizing In and N impurities in GaAs fromab initiocomputer simulation of (110) cross-sectional STM images. Physical Review B, 2007, 75, .	1.1	6
142	Metallization of the C60/Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2010, 132, 234710.	1.2	5
143	Approximate treatment of semicore states in GW calculations with application to Au clusters. Journal of Chemical Physics, 2014, 140, 124101.	1.2	5
144	Cross-sectional imaging of sharp Si interlayers embedded in gallium arsenide. Applied Physics Letters, 2006, 88, 022115.	1.5	4

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145	Unraveling Excited States of Doped Helium Clusters. Journal of Physical Chemistry A, 2007, 111, 12749-12753.	1.1	4
146	Optical properties of anthocyanins in the gas phase. Chemical Physics Letters, 2015, 618, 24-29.	1.2	4
147	Heat Transport in Insulators from Ab Initio Green-Kubo Theory. , 2020, , 809-844.		4
148	High Pressure Lattice Instabilities and Structural Phase Transformations in Solids from Ab-Initio Lattice Dynamics. Materials Research Society Symposia Proceedings, 1997, 499, 233.	0.1	2
149	Ab initio studies of structural and electronic properties. , 2008, , 17-54.		2
150	Structure and Thermodynamics of SiGe Alloys from Computational Alchemy. , 1992, , 133-149.		1
151	Vibrational properties of isolated AlAs monolayers embedded in GaAs: a theoretical study of the effects of disorder. Applied Surface Science, 1992, 56-58, 617-621.	3.1	0
152	Band Offsets at Semiconductor Heterojunctions: Bulk or Interface Properties?. NATO ASI Series Series B: Physics, 1989, , 51-60.	0.2	0