

PHYSICAL REVIEW B

For editorial and subscription correspondence,
please see inside front cover
(ISSN: 0163-1829)

PERIODICALS
Postmaster send address changes to:
American Institute of Physics
500 Sunnyside Boulevard
Woodbury, NY 11797-2999

THIRD SERIES, VOLUME 59, NUMBER 3

CONTENTS

15 JANUARY 1999-I

Subject Matter Categories for Physical Review B	iii
Editorial Policies and Practices of Physical Review B	iv
General Information for Contributors	vii
Guidelines for Estimating Length for Physical Review B	xi

BRIEF REPORTS

Electronic structure: wide-band, narrow-band, and strongly correlated systems

Interband transitions in photonic crystals	1551
Joshua N. Winn, Shanhui Fan, John D. Joannopoulos, and Erich P. Ippen	
Electronic band structure of CuInSe_2 : Bulk and (112) surface	1555
J. A. Rodríguez, L. Quiroga, A. Camacho, and R. Baquero	
Spin gap and paired wave function for the frustrated antiferromagnetic spin- $\frac{1}{2}$ zigzag ladder	1559
Z. N. C. Ha	

Semiconductors I: bulk

Bragg diffraction from indium phosphide infilled fcc silica colloidal crystals	1563
H. Míguez, A. Blanco, F. Meseguer, C. López, H. M. Yates, M. E. Pemble, V. Fornés, and A. Mifsud	
Segregation effects at vacancies in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and $\text{Si}_x\text{Ge}_{1-x}$ alloys	1567
P. Bogusławski and J. Bernholc	
Electronic structure study of liquid germanium based on x-ray-absorption near-edge structure spectroscopy	1571
Chenxi Li, Kunquan Lu, Yuren Wang, Kozaburo Tamura, Shinya Hosokawa, and Masanori Inui	
Direct experimental evidence for the role of oxygen in the luminescent properties of GaN	1575
M. Toth, K. Fleischer, and M. R. Phillips	
Reversible photoinduced changes of electronic transport in narrow-gap amorphous Sb_2Se_3	1579
T. Aoki, H. Shimada, N. Hirao, N. Yoshida, K. Shimakawa, and S. R. Elliott	
Birefringence in ordered $\text{Ga}_{0.47}\text{In}_{0.53}\text{As/InP}$	1582
R. Wirth, J. Porsche, F. Scholz, and A. Hangleiter	
Time-resolved far-infrared reflectance of n -type GaAs	1586
Niels A. van Dantzig and Paul C. M. Planken	
Temperature dependence of the lifetime of 4.3-eV photoluminescence in oxygen-deficient amorphous SiO_2	1590
Kwang Soo Seol, Makoto Fujimaki, Yoshimichi Ohki, and Hiroyuki Nishikawa	



Semiconductors II: surfaces, interfaces, microstructures, and related topics

Mechanisms for the stability of Al and B adatoms on the Si(111) $\sqrt{3} \times \sqrt{3} R30^\circ$ surface	1594
Sanwu Wang, M. W. Radny, and P. V. Smith	
Piecewise diffusion of the silicon dimer	1598
Brian Borovsky, Michael Krueger, and Eric Ganz	
Chemical equilibrium between excitons, electrons, and negatively charged excitons in semiconductor quantum wells	1602
J. Siviniant, D. Scalbert, A. V. Kavokin, D. Coquillat, and J-P. Lascaray	
Infrared transitions between hydrogenic states in cylindrical GaAs quantum-well wires under applied magnetic fields	1605
Pablo Villamil, N. Porras-Montenegro, and J. C. Granada	
Surface states and Fermi-level pinning at clean and Al covered GaN surfaces	1609
S. Picozzi, A. Continenza, and A. J. Freeman	
End states due to a spin-Peierls transition in quantum wires	1613
S. M. Reimann, M. Koskinen, and M. Manninen	
Two-electron artificial molecule	1617
B. Partoens, A. Matulis, and F. M. Peeters	
Interface and longitudinal optical phonon modes in cylindrical quantum dots	1621
Clément Kanyinda-Malu and Rosa María de la Cruz	
Photoluminescence kinetics of indirect excitons in GaAs/Al _x Ga _{1-x} As coupled quantum wells	1625
L. V. Butov, A. Imamoglu, A. V. Mintsev, K. L. Campman, and A. C. Gossard	
Effect of cross capacitance in three-junction single-electron transistors	1629
Jinhee Kim, Sangchul Oh, Jong Wan Park, Jeong-O Lee, Hyuk Chan Kwon, Se Il Park, Kyu Tae Kim, Kyung Hwa Yoo, and Ju-Jin Kim	
Rehybridization of electronic structure in compressed two-dimensional quantum dot superlattices	1633
G. Medeiros-Ribeiro, D. A. A. Ohlberg, R. Stanley Williams, and James R. Heath	
Andreev tunneling in quantum dots: A slave-boson approach	1637
P. Schwab and R. Raimondi	
Magnetoluminescence oscillations of a doped (Al,Ga)As/GaAs single heterojunction	1641
Yongmin Kim, C. H. Perry, Kyu-Seok Lee, and D. G. Rickel	
Raman spectral study of silicon nanowires	1645
Bibo Li, Dapeng Yu, and Shu-Lin Zhang	
Finely resolved transmission spectra and band structure of two-dimensional photonic crystals using emission from InAs quantum dots	1649
D. Labilloy, H. Benisty, C. Weisbuch, C. J. M. Smith, T. F. Krauss, R. Houdré, and U. Oesterle	

Surface physics, low-dimensional systems, and related topics

Ground-state energy of confined charged bosons in two dimensions	1653
A. Gonzalez, B. Partoens, A. Matulis, and F. M. Peeters	
Convergent N^2 -scaling iterative method of photoelectron diffraction and low-energy electron diffraction for ordered or disordered systems	1657
Huasheng Wu and S. Y. Tong	
Imaging of sub-unit-cell structures in the contact mode of the scanning force microscope	1661
H. Hölscher, W. Raberg, U. D. Schwarz, A. Hasbach, K. Wandelt, and R. Wiesendanger	
Structural studies of multiwall carbon nanotubes by neutron diffraction	1665
A. Burian, J. C. Dore, H. E. Fischer, and J. Sloan	
Effect of surface-height derivative processes on ion-bombardment-induced ripple formation	1669
G. Carter	

Multilayer-relaxed structure of the (1×2) Pt(110) surface	1673
J. I. Lee, W. Mannstadt, and A. J. Freeman	
Oscillatory lattice relaxation at metal surfaces	1677
Jun-Hyung Cho, Ismail, Zhenyu Zhang, and E. W. Plummer	
Imperfect magnetic nanostructures on a Ag(001) surface	1681
V. S. Stepanyuk, W. Hergert, P. Rennert, K. Wildberger, R. Zeller, and P. H. Dederichs	
Far-infrared absorption in small metal particles	1685
A. V. Plyukhin, A. K. Sarychev, and A. M. Dykhne	
Scaling behavior of the critical terrace width for step-flow growth	1689
Ivan Markov	
Attempt to deposit carbon nitride films by electrodeposition from an organic liquid	1693
Qiang Fu, Jin-Ting Jiu, Kai Cai, Hao Wang, Chuan-Bao Cao, and He-Sun Zhu	

ARTICLES

Electronic structure: wide-band, narrow-band, and strongly correlated systems

Effect of nonadiabaticity and disorder on nonlinear optical susceptibilities	1697
W. Z. Wang, Z. Shuai, A. Saxena, A. R. Bishop, and J. L. Brédas	
Thermal expansion of single-crystalline $\text{La}_{0.83}\text{Sr}_{0.17}\text{MnO}_3$: The importance of temperature-induced strain for the electrical resistivity	1701
J. J. Neumeier, K. Andres, and K. J. McClellan	
Correlated wave functions and the absence of long-range order in numerical studies of the Hubbard model	1706
M. Guerrero, G. Ortiz, and J. E. Gubernatis	
Dyson equation approach to many-body Green's functions and self-consistent RPA: Application to the Hubbard model	1712
Steffen Schäfer and Peter Schuck	
Form factors in the half-filled Hubbard model	1734
Fabian H. L. Eßler and Vladimir E. Korepin	
Metal-insulator transition in a degenerate Hubbard model	1739
Priya Mahadevan and D. D. Sarma	
Full-potential nonorthogonal local-orbital minimum-basis band-structure scheme	1743
Klaus Koepnick and Helmut Eschrig	
From ultrasoft pseudopotentials to the projector augmented-wave method	1758
G. Kresse and D. Joubert	
Electronic structure, chemical bonding, and optical properties of ferroelectric and antiferroelectric NaNO_2	1776
P. Ravindran, A. Delin, B. Johansson, O. Eriksson, and J. M. Wills	
Bulk and surface electronic structures of the semimetal Bi studied by angle-resolved photoemission spectroscopy	1786
Akinori Tanaka, Masayuki Hatano, Kazutoshi Takahashi, Hiroyuki Sasaki, Shoji Suzuki, and Shigeru Sato	
Competition between initial- and final-state effects in valence- and core-level x-ray photoemission of Sb-doped SnO_2	1792
R. G. Egdell, J. Rebane, T. J. Walker, and D. S. L. Law	
Magnetotransport in the doped Mott insulator	1800
Ekkehard Lange and Gabriel Kotliar	
Low-energy electrodynamics of SmB_6	1808
B. Gorshunov, N. Sluchanko, A. Volkov, M. Dressel, G. Knebel, A. Loidl, and S. Kunii	
Electronic structure of $\text{Ce}_{1-x}\text{Sr}_x\text{TiO}_3$: Comparison between substitutional and vacancy doping	1815
T. Yokoya, T. Sato, H. Fujisawa, T. Takahashi, A. Chainani, and M. Onoda	

Evidence of dynamic Jahn-Teller distortions in two-dimensional crystalline molecular films	1819
Jaewu Choi, P. A. Dowben, C. N. Borca, Shireen Adenwalla, A. V. Bune, Stephen Ducharme, V. M. Fridkin, S. P. Palto, and N. Petukhova	
Transport properties of one-dimensional Hubbard models	1825
S. Kirchner, H. G. Evertz, and W. Hanke	
Heterovalent and A-atom effects in $A(B'B'')O_3$ perovskite alloys	1834
L. Bellaiche, J. Padilla, and David Vanderbilt	
Effect of magnetic frustration on the single-hole spectral function in the t - t' - t'' - J model	1840
Y. Shibata, T. Tohyama, and S. Maekawa	
Dielectric function of hexagonal AlN films determined by spectroscopic ellipsometry in the vacuum-uv spectral range	1845
T. Wethkamp, K. Wilmers, C. Cobet, N. Esser, W. Richter, O. Ambacher, M. Stutzmann, and M. Cardona	
Selectively excited luminescence and magnetic circular dichroism of Cr^{4+} -doped YAG and YGG	1850
M. J. Riley, E. R. Krausz, N. B. Manson, and B. Henderson	
Excitonic effects in linear and nonlinear optical properties of C_{60}	1857
F. Bechstedt, M. Fiedler, and L. J. Sham	
Multiple-histogram method for quantum Monte Carlo simulations	1870
C. L. Martin	
Order- N photonic band structures for metals and other dispersive materials	1874
J. Arriaga, A. J. Ward, and J. B. Pendry	
Optical properties and electronic structures of $B2$ and $B19'$ phases of equiatomic Ni-Ti alloys	1878
Joo Yull Rhee, B. N. Harmon, and D. W. Lynch	
<i>Ab initio</i> and semiempirical calculations of H^- centers in MgO crystals	1885
M. M. Kukulja, E. V. Stefanovich, E. A. Kotomin, A. I. Popov, R. González, and Y. Chen	
Charge-density waves and surface Mott insulators for adlayer structures on semiconductors: Extended Hubbard modeling	1891
Giuseppe Santoro, Sandro Scandolo, and Erio Tosatti	
Orbital Kondo effect in $Ce_xLa_{1-x}B_6$: Scaling analysis	1902
H. Kusunose and Y. Kuramoto	

Semiconductors I: bulk

Modeling hydrogen in $CuInSe_2$ and $CuInS_2$ solar cell materials using implanted muons	1912
J. M. Gil, P. J. Mendes, L. P. Ferreira, H. V. Alberto, R. C. Vilão, N. Ayres de Campos, A. Weidinger, Y. Tomm, Ch. Niedermayer, M. V. Yakushev, R. D. Tomlinson, S. P. Cottrell, and S. F. J. Cox	
Finite-size errors in quantum many-body simulations of extended systems	1917
P. R. C. Kent, Randolph Q. Hood, A. J. Williamson, R. J. Needs, W. M. C. Foulkes, and G. Rajagopal	
Electronic structure and energetics of pressure-induced two-dimensional C_{60} polymers	1930
Susumu Okada and Susumu Saito	
Optically detected electron paramagnetic resonance of AlN single crystals	1937
P. M. Mason, H. Przybylinska, G. D. Watkins, W. J. Choyke, and G. A. Slack	
Positron affinity in semiconductors: Theoretical and experimental studies	1948
J. Kuriplach, M. Šob, G. Brauer, W. Anwand, E.-M. Nicht, P. G. Coleman, and N. Wagner	
Properties of the D_1 bound exciton in $4H$ -SiC	1956
T. Egilsson, J. P. Bergman, I. G. Ivanov, A. Henry, and E. Janzén	
Efficient bulk photogeneration of charge carriers and photoconductivity gain in arylamino-PPV polymer sandwich cells	1964
T. K. Däubler, D. Neher, H. Rost, and H. H. Hörhold	
Exciton-impurity interactions in high-purity InP	1973
R. Benzaquen, R. Leonelli, and S. Charbonneau	

Optically pumped NMR in CdS single crystals	1986
Tanja Pietraß and Marco Tomaselli	
Semiconductors II: surfaces, interfaces, microstructures, and related topics	
Evolution of coherent islands in $\text{Si}_{1-x}\text{Ge}_x/\text{Si}(001)$	1990
J. A. Floro, E. Chason, L. B. Freund, R. D. Twisten, R. Q. Hwang, and G. A. Lucadamo	
Acoustic waves in finite superlattices: Influence of buffer layers	1999
M. Hammouchi, E. H. El Boudouti, A. Nougouai, B. Djafari-Rouhani, M. L. H. Lahlaoui, A. Akjouj, and L. Dobrzynski	
Asymptotic derivation of the glued-wetting-layer model and contact-angle condition for Stranski-Krastanow islands	2011
B. J. Spencer	
Ni/Si(111) system: Formation and evolution of two- and three-dimensional phases studied by spectromicroscopy	2018
L. Gregoratti, S. Günther, J. Kovač, M. Marsi, R. J. Phaneuf, and M. Kiskinova	
Photoionization of silicon particles in SiO_2	2025
V. V. Afanas'ev and A. Stesmans	
Electron standing waves on the $\text{Si}(111)-\sqrt{3}\times\sqrt{3}\text{-Ag}$ surface	2035
Norio Sato, Sakura Takeda, Tadaaki Nagao, and Shuji Hasegawa	
Scaling of exciton binding energy and virial theorem in semiconductor quantum wells and wires	2040
Yong Zhang and A. Mascarenhas	
Size effect on chalcogen deep levels in Si quantum dots	2045
Jian Song, Shang Yuan Ren, and John D. Dow	
Mn spin domains in highly photoexcited $(\text{Cd,Mn})\text{Te}/(\text{Cd,Mg})\text{Te}$ quantum wells	2050
M. G. Tyazhlov, V. D. Kulakovskii, A. I. Filin, D. R. Yakovlev, A. Waag, and G. Landwehr	
Longitudinal effective mass and band structure of quasiperiodic Fibonacci superlattices	2057
A. Bruno-Alfonso, F. J. Ribeiro, A. Latgé, and L. E. Oliveira	
Repulsion of single-well fundamental edge magnetoplasmons in double quantum wells	2063
O. G. Balev and P. Vasilopoulos	
Coupled quantum dots as quantum gates	2070
Guido Burkard, Daniel Loss, and David P. DiVincenzo	
Thomas–Fermi–Dirac–von Weizsäcker hydrodynamics in laterally modulated electronic systems	2079
B. P. van Zyl and E. Zaremba	
Angle-resolved Raman spectroscopy of the collective modes in an electron bilayer	2095
D. S. Kainth, D. Richards, A. S. Bhatti, H. P. Hughes, M. Y. Simmons, E. H. Linfield, and D. A. Ritchie	
Berry phase and adiabaticity of a spin diffusing in a nonuniform magnetic field	2102
S. A. van Langen, H. P. A. Knops, J. C. J. Paasschens, and C. W. J. Beenakker	
Time-dependent study of bistability in resonant-tunneling structures	2111
E. Keçecioglu and M. Cemal Yalabik	
Individual scatterers as microscopic origin of equilibration between spin-polarized edge channels in the quantum Hall regime	2116
Y. Acremann, T. Heinzel, K. Ensslin, E. Gini, H. Melchior, and M. Holland	
Electromagnetic response of a pinned Wigner crystal	2120
H. A. Fertig	
Numerical study of current distribution in finite planar Hall samples with disorder	2142
K. Shizuya	
Spin-dependent recombination of photoinduced carriers in phthalocyanine/ C_{60} heterojunctions	2151
Ichiro Hiromitsu, Yoshiaki Kaimori, Mayuko Kitano, and Takashi Ito	

Multiphoton photoemission and electric-field-induced optical second-harmonic generation as probes of charge transfer across the Si/SiO ₂ interface	2164
J. G. Mihaychuk, N. Shamir, and H. M. van Driel	
Persistent photoconductivity in semimetallic Al _x Ga _{1-x} Sb/InAs quantum wells	2174
L. C. Tsai, J. C. Fan, Y. F. Chen, and Ikai Lo	
Strong-field magnetotransport of conducting composites with a columnar microstructure	2180
David J. Bergman and Yakov M. Strel'nik	
Hydrodynamic balance-equation analysis of spatiotemporal domains and negative differential conductance in a voltage-biased GaAs superlattice	2199
J. C. Cao and X. L. Lei	
Folded acoustic and confined optical phonons in a (Si ₁₅ Ge ₄) ₅₀ atomic-layer superlattice	2207
R. W. G. Syme, D. J. Lockwood, and J.-M. Baribeau	
Well-width dependence of exciton-phonon scattering in In _x Ga _{1-x} As/GaAs single quantum wells	2215
P. Borri, W. Langbein, J. M. Hvam, and F. Martelli	
Angle dependence of the spontaneous emission from confined optical modes in photonic dots	2223
T. Gutbrod, M. Bayer, A. Forchel, P. A. Knipp, T. L. Reinecke, A. Tartakovskii, V. D. Kulakovskii, N. A. Gippius, and S. G. Tikhodeev	
Band-gap renormalization in modulation-doped In _{1-x} Ga _x As/GaAs V-shaped quantum wires	2230
R. Rinaldi, G. Coli', A. Passaseo, and R. Cingolani	
Structural fingerprints in the reflectance anisotropy spectra of InP(001)(2×4) surfaces	2234
W. G. Schmidt, E. L. Briggs, J. Bernholc, and F. Bechstedt	
Strong emission from As monolayers in AlSb	2240
E. R. Glaser, T. A. Kennedy, B. R. Bennett, and B. V. Shanabrook	
Near-field second-harmonic generation of semiconductor quantum dots	2245
Ansheng Liu and Garnett W. Bryant	
Excitonic absorption of GaN epilayers on sapphire: Dynamics, intensity, and temperature dependence	2254
H. Haag, P. Gilliot, R. Lévy, B. Hönerlage, O. Briot, S. Ruffenach-Clur, and R. L. Aulombard	
Two-dimensional magnetoplasma/Bernstein modes coupled with bulk and surface optical phonons	2261
Norman J. M. Horing and Godfrey Gumbs	
<i>Ab initio</i> pseudopotential method for the calculation of conductance in quantum wires	2267
Hyoung Joon Choi and Jisoon Ihm	
Bound polaron in a polar semiconductor heterojunction	2276
S. L. Ban and J. E. Hasbun	
Quantum transport by means of O(N) real-space methods	2284
Stephan Roche	

Surface physics, low-dimensional systems, and related topics

Structural transitions and global minima of sodium chloride clusters	2292
Jonathan P. K. Doye and David J. Wales	
NMR study of localized electrons in conductive Langmuir-Blodgett films	2301
Hiroshi Tsukada	
Oxygen K-edge x-ray-absorption fine-structure study of surface methoxy species on Cu(111) and Ni(111)	2307
K. Amemiya, Y. Kitajima, Y. Yonamoto, S. Terada, H. Tsukabayashi, T. Yokoyama, and T. Ohta	
Photoelectron diffraction study of ultrathin Fe films on Cu{111}	2313
A. Theobald, O. Schaff, C. J. Hirschmugl, V. Fernandez, K.-M. Schindler, M. Polcik, A. M. Bradshaw, and D. P. Woodruff	
Effects of exchange, correlation, and numerical approximations on the computed properties of the rutile TiO ₂ (100) surface	2320
J. Muscat, N. M. Harrison, and G. Thornton	

Interpretation of O binding-site preferences on close-packed group-VIII metal surfaces	2327
Peter J. Feibelman	
Adsorption of atomic and molecular oxygen and desorption of silicon monoxide on Si(111) surfaces	2332
T. Hoshino	
Surface-morphology evolution during unstable homoepitaxial growth of GaAs(110)	2341
P. Tejedor, P. Šmilauer, C. Roberts, and B. A. Joyce	
Structural transformations in the Stranski-Krastanov growth of Mg on Mo(001)	2346
M. C. Gallagher, M. S. Fyfield, and S. A. Joyce	
Electronic structure of face-centered-tetragonal iron in ferromagnetic iron-copper multilayers	2352
S. J. Lloyd and R. E. Dunin-Borkowski	
Gold-induced faceting on a Si(001) vicinal surface: Spot-profile-analyzing LEED and reflection-electron-microscopy study	2363
H. Minoda, K. Yagi, F.-J. Meyer zu Heringdorf, A. Meier, D. Kähler, and M. Horn von Hoegen	
Positive magnetoresistance and hole-hole scattering in GaAs/Al _{0.5} Ga _{0.5} As heterostructures under uniaxial compression	2376
V. Kravchenko, N. Minina, A. Savin, O. P. Hansen, C. B. Sorensen, and W. Kraak	
Magnetoconductivity of ultrathin epitaxial Ag films on Si(111) 7×7 at low temperatures	2383
M. Henzler, T. Lüer, and J. Heitmann	
Finite-size effect on the Raman spectra of carbon nanotubes	2388
R. Saito, T. Takeya, T. Kimura, G. Dresselhaus, and M. S. Dresselhaus	
Angular correlation functions of light scattered from weakly rough metal surfaces	2393
C. S. West and K. A. O'Donnell	
Growth kinetics of a nanoprotuberance under the action of an oscillating nanotip	2407
J. P. Aimé, D. Michel, R. Boisgard, and L. Nony	
Spectroscopy of low-coordinated surface sites: Theoretical study of MgO	2417
Alexander L. Shluger, Peter V. Sushko, and Lev N. Kantorovich	
Co/Pt(110) interface: An x-ray-diffraction study	2431
E. Lundgren, J. Alvarez, X. Torrelles, K. F. Peters, H. Isern, and S. Ferrer	
Model of noncontact scanning force microscopy on ionic surfaces	2436
Alexander I. Livshits, Alexander L. Shluger, Andrew L. Rohl, and Adam S. Foster	
Theoretical determination of the adsorption geometry of Na on the Si(001) surface	2449
P. Gravila and P. F. Meier	
Near-field optical microscopy of two-dimensional photonic and plasmonic crystals	2454
Igor I. Smolyaninov, Walid Atia, and Christopher C. Davis	
Errata	
Erratum: Occupied and unoccupied electronic band structure of WSe ₂ [Phys. Rev. B 55 , 10 400 (1997)]	2461
Th. Finteis, M. Hengsberger, Th. Straub, K. Fauth, R. Claessen, P. Auer, P. Steiner, S. Hüfner, P. Blaha, M. Vögt, M. Lux-Steiner, and E. Bucher	
Erratum: Piezo-optics of InP in the visible-ultraviolet range [Phys. Rev. B 57 , 4432 (1998)]	2462
D. Rönnow, P. Santos, M. Cardona, E. Anastassakis, and M. Kuball	
Cumulative Author Index	2463