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 55, NUMBER 3 ***CONTENTS*** **15 JANUARY 1997-I**

Volume Page ..... (i)–(ii)
Subject Matter Categories for Physical Review B iii
Editorial Policies and Practices of Physical Review B ..... iv–vi
General Information for Contributors ..... vii–x
Guidelines for Estimating Length for Physical Review B xi

BRIEF REPORTS

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

Thermoelectric properties of $R_xCe_{1-x}Pd_3$ (R=Y, $La_{0.5}Y_{0.5}$, Nd) 1283
Y. Ijiri and F. J. DiSalvo
α-γ transition in Ce from temperature-dependent band-structure calculations 1288
T. Jarlborg, E. G. Moroni, and G. Grimvall
Photorefractive properties of manganese-modified potassium sodium strontium barium niobate crystals 1292
H. R. Xia, C. J. Wang, H. C. Chen, and X. L. Lu
Correction to Slater exchange potential to yield exact Kohn-Sham potential generating the Hartree-Fock density 1295
A. Holas and N. H. March
Ground state of $(TMTSF)_2ClO_4$ in high magnetic fields: The creation of Su-Schrieffer-Heeger solitons 1299
A. G. Lebed
Unification of the metal-insulator transitions driven by the impurity concentration and by the magnetic field in arsenic-doped germanium 1303
I. Shlimak, M. Kaveh, R. Ussyshkin, V. Ginodman, and L. Resnick

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

Quinquethiophene light-emitting diodes with molecular dimensions 1306
A. J. Pal, T. Östergård, J. Paloheimo, and H. Stubb
Structures and electrical conductance of the Si(111)-$\sqrt{3}\times\sqrt{3}$-Ag surface with additional Ag adsorption at low temperatures 1310
Xiao Tong, Shuji Hasegawa, and Shozo Ino
Magnetotransport properties of Fibonacci semiconductor superlattices 1314
J. Q. You, Lide Zhang, and Q. B. Yang
Negatively charged excitons in coupled double quantum wells 1318
A. J. Shields, J. L. Osborne, D. M. Whittaker, M. Y. Simmons, M. Pepper, and D. A. Ritchie
Kinetics of Si monomer trapping at steps and islands on Si(001) 1322
B. S. Swartzentruber
Form of the quantum kinetic-energy operator with spatially varying effective mass 1326
F. S. A. Cavalcante, R. N. Costa Filho, J. Ribeiro Filho, C. A. S. de Almeida, and V. N. Freire
Theoretical study of magnetotunneling spectroscopy 1329
T.-J. Chow, G. Y. Wu, K.-M. Hung, and C.-W. Chen
Exciton formation rates in GaAs/Al_xGa_{1-x}As quantum wells 1333
C. Piermarocchi, F. Tassone, V. Savona, A. Quattropani, and P. Schwendimann

(Continued)

0163-1829(19970115)55:3;1-H

PHYSICAL REVIEW B THIRD SERIES, VOLUME 55, NUMBER 3 15 JANUARY 1997-I

Atomic-scale imaging of strain relaxation via misfit dislocations in highly mismatched semiconductor heteroepitaxy: InAs/GaAs(111)*A* 1337
H. Yamaguchi, J. G. Belk, X. M. Zhang, J. L. Sudijono, M. R. Fahy, T. S. Jones, D. W. Pashley, and B. A. Joyce

Nonlinear boundary oscillations in strongly correlated electron quantum wires 1341
Holger Frahm and Andrei A. Zvyagin

Incompressible liquid states in asymmetric double-layer electron systems 1345
D. S. Hirashima

Binding energy of neutral bound excitons in GaAs-$Al_xGa_{1-x}As$ quantum wells 1349
Jian-Jun Liu and Xiao-Jun Kong

Magnetoconductance of Aharonov-Bohm rings with half-bound states 1353
Massimiliano Di Ventra, Florian Gagel, and Klaus Maschke

Equilibration length of edge states in a GaAs/$In_yGa_{1-y}As$/$Al_xGa_{1-x}As$ quantum well 1357
J. Herfort, Y. Takagaki, K.-J. Friedland, R. Hey, H. Kostial, and K. Ploog

Short-range correlation effects on the plasmons in cylindrical tubules 1361
B. Tanatar

Electronic states and optical gain in strained CdS/ZnS quantum structures 1364
U. Woggon, W. Petri, A. Dinger, S. Petillon, M. Hetterich, M. Grün, K. P. O'Donnell, H. Kalt, and C. Klingshirn

Magnetically induced suppression of phase breaking in ballistic mesoscopic billiards 1368
Y. Okubo, J. P. Bird, Y. Ochia, D. K. Ferry, K. Ishibashi, Y. Aoyagi, and T. Sugano

Surface physics, low-dimensional systems, and related topics

Optical spectra of hot alkali-metal clusters from the random-matrix model 1372
V. M. Akulin, C. Bréchignac, and A. Sarfati

Collective excitations of two layers of K on Ni(111) 1376
G. Chiarello, A. Cupolillo, A. Amoddeo, L. S. Caputi, L. Papagno, and E. Colavita

Heteroepitaxial subsurface growth mode resulting in interlayer mixing 1380
P. W. Murray, S. Thorshaug, I. Stensgaard, F. Besenbacher, E. Lægsgaard, A. V. Ruban, K. W. Jacobsen, G. Kopidakis, and H. L. Skriver

Transition from three-dimensional to two-dimensional faceting of Ag(110) induced by Cu-phthalocyanine 1384
Matthias Böhringer, Richard Berndt, and Wolf-Dieter Schneider

Critical examination of prewetting and surface melting on caprolactam 1388
Gerard C. L. Wong, Wim H. de Jeu, Gertjan Bögels, Erwin P. G. van den Berg, and Piet Bennema

Photoemission study of Sm on Ta(110): Valence states in the initial growth phase 1391
F. Strisland, S. Raaen, A. Ramstad, and C. Berg

Lattice dynamics of the Ni(977) surface 1395
Gregor Witte and J. Peter Toennies

ARTICLES

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

Cyclotron-resonance transmission through potassium in a perpendicular magnetic field: Effects of the charge-density wave 1398
Mi-Ae Park and A. W. Overhauser

Hubbard one-particle Green function in the antiferromagnetic phase 1408
G. Polatsek and K. W. Becker

Optical and loss spectra of SiC polytypes from *ab initio* calculations 1422
B. Adolph, K. Tenelsen, V. I. Gavrilenko, and F. Bechstedt

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 55, NUMBER 3** **15 JANUARY 1997-I**

High-resolution Gd 4*d* photoemission from different intermetallic compounds 1430
Jacek Szade, Jens Lachnitt, and Manfred Neumann
Ground-state properties of the two-dimensional *t-J* model 1435
Masanori Kohno
Raman scattering in the $R\mathrm{TiO}_3$ family of Mott-Hubbard insulators 1442
M. Reedyk, D. A. Crandles, M. Cardona, J. D. Garrett, and J. E. Greedan
Pairs of Bloch electrons and magnetic translation groups 1449
Wojciech Florek
Electronic structure of light metal hydrides 1454
P. K. Khowash, B. K. Rao, T. McMullen, and P. Jena
Electron-spectroscopy study of correlation mechanisms in CuGeO_3 single crystals 1459
F. Parmigiani, L. Sangaletti, A. Goldoni, U. del Pennino, C. Kim, Z.-X. Shen, A. Revcolevschi, and G. Dhalènne
Microscopic theory of Anderson localization in a magnetic field 1469
P. Kleinert and V. V. Bryksin
Low-temperature transport properties of the filled skutterudites $\mathrm{CeFe}_{4-x}\mathrm{Co}_x\mathrm{Sb}_{12}$ 1476
Baoxing Chen, Jun-Hao Xu, Ctirad Uher, Donald T. Morelli, Gregory P. Meisner, Jean-Pierre Fleurial, Thierry Caillat, and Alex Borshchevsky
Finite-size effects and quantum phonon fluctuations in the optical absorption edge of dimerized chains 1481
Ioan Bâldea, Horst Köppel, and Lorenz S. Cederbaum
Optical absorption in the substituted phenylene-based conjugated polymers: Theory and experiment 1486
M. Chandross, S. Mazumdar, M. Liess, P. A. Lane, Z. V. Vardeny, M. Hamaguchi, and K. Yoshino
Coulomb interactions and linear, nonlinear, and triplet absorption in poly(para-phenylenevinylene) 1497
M. Chandross and S. Mazumdar

Semiconductors I: bulk

General model for the description of the third-order optical nonlinearities in conjugated systems: Application to the all-*trans* β-carotene molecule 1505
D. Beljonne, J. Cornil, Z. Shuai, J. L. Brédas, F. Rohlfing, D. D. C. Bradley, W. E. Torruellas, V. Ricci, and G. I. Stegeman
Role of nonequilibrium dynamical screening in carrier thermalization 1517
Girish S. Setlur and Yia-Chung Chang
Highly optimized tight-binding model of silicon 1528
Thomas J. Lenosky, Joel D. Kress, Inhee Kwon, Arthur F. Voter, Byard Edwards, David F. Richards, Sang Yang, and James B. Adams
Local atomic structure of semiconductor alloys using pair distribution functions 1545
Jean S. Chung and M. F. Thorpe
Plasmon-phonon coupling in δ-doped polar semiconductors 1554
Guo-Qiang Hai, Nelson Studart, and Gilmar E. Marques

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

Quantum-confined Stark effect on spatially indirect excitons in $\mathrm{CdTe/Cd}_x\mathrm{Zn}_{1-x}\mathrm{Te}$ quantum wells 1563
H. Haas, N. Magnea, and Le Si Dang
Single-electron charging and Coulomb interaction in InAs self-assembled quantum dot arrays 1568
G. Medeiros-Ribeiro, F. G. Pikus, P. M. Petroff, and A. L. Efros
Localized electronic states in coupled superlattices 1574
Maria Stęślicka and Robert Kucharczyk
Correlated conductance through a lattice of quantum dots: Metal to antiferromagnetic insulator transition 1578
Hao Chen, Jian Wu, Zhi-Qiang Li, and Yoshiyuki Kawazoe

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 55, NUMBER 3 15 JANUARY 1997-I

Analytic calculations of trial wave functions of the fractional quantum Hall effect on the sphere 1582
Carmem Lucia de Souza Batista and Dingping Li
Exciton states in isolated quantum wires 1596
Jian-Bai Xia and K. W. Cheah
Band alignment in $ZnSe/Zn_{1-x-y}Cd_xMn_ySe$ quantum-well structures 1602
W. Y. Yu, M. S. Salib, A. Petrou, B. T. Jonker, and J. Warnock
Angle-resolved studies of the spin-flip Raman scattering of holes bound to acceptors in *p*-type nitrogen-doped zinc selenide 1607
Catherine Orange, Bernhard Schlichtherle, Daniel Wolverson, J. John Davies, Tobias Ruf, Ken-ichi Ogata, and Shigeo Fujita
Far-infrared magneto-optical study of two-dimensional electrons and holes in $InAs/Al_xGa_{1-x}Sb$ quantum wells ... 1617
J. Kono, B. D. McCombe, J.-P. Cheng, I. Lo, W. C. Mitchel, and C. E. Stutz
Conductance fluctuations at the integer quantum Hall plateau transition 1637
Sora Cho and Matthew P. A. Fisher
Local-density-derived semiempirical nonlocal pseudopotentials for InP with applications to large quantum dots ... 1642
Huaxiang Fu and Alex Zunger
Polarization choices in exciton-biexciton system of GaAs quantum wells 1654
S. Adachi, T. Miyashita, S. Takeyama, Y. Takagi, A. Tackeuchi, and M. Nakayama
Tunneling into a periodically modulated Luttinger liquid 1661
A. Gramada and M. E. Raikh
Dynamics of excitons and biexcitons in CuCl nanocrystals embedded in NaCl at 2 K 1667
S. Yano, T. Goto, T. Itoh, and A. Kasuya
Effects of quantum size and potential shape on the spectra of an electron and a donor in quantum dots 1673
Jia-Lin Zhu, Jian Wu, R. T. Fu, Hao Chen, and Yoshiyuki Kawazoe
Binding energy of an oxygen-related defect in modulation-doped quantum wires 1680
F. A. Reboredo and C. R. Proetto
Nonuniform segregation of Ga at AlAs/GaAs heterointerfaces 1689
Wolfgang Braun, Achim Trampert, Lutz Däweritz, and Klaus H. Ploog
Low-frequency shot noise in phonon-assisted resonant magnetotunneling 1696
Ø. Lund Bø and Yu. Galperin
Scattering of vibrational waves in perturbed quasi-one-dimensional multichannel waveguides 1707
A. Fellay, F. Gagel, K. Maschke, A. Virlouvet, and A. Khater
Valence-band offsets at the $Al_xGa_{0.5-x}In_{0.5}P$-ZnSe(001) lattice-matched interface 1718
F. Bernardini and R. M. Nieminen
Band-offset determination of the CdTe/(Cd,Mn)Te interface 1724
T. Lebihen, E. Deleporte, and C. Delalande
Birefringence in ordered (Al)GaInP 1730
R. Wirth, A. Moritz, C. Geng, F. Scholz, and A. Hangleiter

Surface physics, low-dimensional systems, and related topics

Dynamical screening in the scanning tunneling microscope and metal-insulator-metal junctions 1741
D. Šestović, L. Marušić, and M. Šunjić
First-principles real-space tight-binding LMTO calculation of electronic structures for atomic clusters 1748
Z. L. Xie, K. S. Dy, and S. Y. Wu
Theory of ionic-surface electrical conduction in porous media 1757
A. Revil and P. W. J. Glover
Influence of compressive biaxial strain on the hydrogen uptake of ultrathin single-crystal vanadium layers 1774
G. Andersson, B. Hjörvarsson, and P. Isberg
Mode damping in a commensurate monolayer solid 1782
L. W. Bruch and F. Y. Hansen

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 55, NUMBER 3** **15 JANUARY 1997-I**

X-ray diffraction peaks due to misfit dislocations in heteroepitaxial structures 1793
V. M. Kaganer, R. Köhler, M. Schmidbauer, R. Opitz, and B. Jenichen
Decay of isolated surface features driven by the Gibbs-Thomson effect in an analytic model and a simulation 1811
James G. McLean, B. Krishnamachari, D. R. Peale, E. Chason, James P. Sethna, and B. H. Cooper
Scattering of surface-plasmon polaritons by dipoles near a surface: Optical near-field localization 1824
Mufei Xiao, Anatoly Zayats, and Jesús Siqueiros
Intermediate metastable structure of the C{111}/(1×1)H-C{111}/(2×1) surface phase transition 1838
Leonid V. Zhigilei, Deepak Srivastava, and Barbara J. Garrison
Cesium adsorption on TiO_2(110) 1844
Ann W. Grant and Charles T. Campbell
Picosecond ultrasonic study of phonon reflection from solid-liquid interfaces 1852
Guray Tas and Humphrey J. Maris
Percolative behavior of an anisotropic two-dimensional network: Growth of tellurium onto an oriented polymer film 1858
T. Hoffmann, J. Martínez-Salazar, P. Herrero, and J. Petermann
Observation of Si(001) surface topography at temperatures below 1140 °C using a reflection electron microscope 1864
Takahisa Doi, Masakazu Ichikawa, and Shigeyuki Hosoki
Surface photoemission in Ag(100) 1871
E. D. Hansen, T. Miller, and T.-C. Chiang
Quantum kinetic theory of vibrational heating and bond breaking by hot electrons 1876
Shiwu Gao
Molecular beam epitaxy in the presence of phase separation 1887
François Léonard, Mohamed Laradji, and Rashmi C. Desai
Theoretical study of oxygenated (100) diamond surfaces in the presence of hydrogen 1895
Sergei Skokov, Brian Weiner, and Michael Frenklach

Errata

Erratum: Strong effects of photonic band structures on the diffraction of colloidal crystals [Phys. Rev. B **53**, 16 231 (1996)] 1903
Willem L. Vos, Rudolf Sprik, Alfons van Blaaderen, Arnout Imhof, Ad Lagendijk, and Gerard H. Wegdam
Erratum: Model-dependent electronic structure of the Si(111)2×1 surface [Phys. Rev. B **54**, 1482 (1996)] 1903
Sung-Hoon Lee and Myung-Ho Kang

Cumulative Author Index 1904