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
Suite 1NO1
2 Huntington Quadrangle
Melville, NY 11747-4502

THIRD SERIES, VOLUME 69, NUMBER 19 *CONTENTS* **MAY 2004-15(I)**

BRIEF REPORTS

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

Effect of atomic displacements on the ground state of α-TeO_2 *(4 pages)* 193101
B. R. Sahu and Leonard Kleinman

Optical properties of the pyrochlore oxide $Pb_2Ru_2O_{6.5}$ *(4 pages)* 193102
P. Zheng, N. L. Wang, J. L. Luo, R. Jin, and D. Mandrus

Sensitivity to termination morphology of light coupling in photonic-crystal waveguides *(4 pages)* 193103
Lan-Lan Lin and Zhi-Yuan Li

Changes in the electronic structure of cerium due to variations in close packing *(4 pages)* 193104
K. T. Moore, B. W. Chung, S. A. Morton, A. J. Schwartz, J. G. Tobin, S. Lazar, F. D. Tichelaar, H. W. Zandbergen, P. Söderlind, and G. van der Laan

Electronic structure of calcium hexaboride within the weighted density approximation *(4 pages)* 193105
Zhigang Wu, D. J. Singh, and R. E. Cohen

Semiconductors I: bulk

Electrical conductivity of tellurium in the liquid state *(4 pages)* 193201
D. A. Barlow

Optical and electrical properties of vanadium and erbium in 4*H*-SiC *(4 pages)* 193202
D. Prezzi, T. A. G. Eberlein, J.-S. Filhol, R. Jones, M. J. Shaw, P. R. Briddon, and S. Öberg

Measurements of deviation from Einstein relation in PVK-based photorefractive polymers by photoelectromotive-force technique *(4 pages)* 193203
S. Mansurova, S. Stepanov, V. Camacho-Pernas, R. Ramos-Garcia, F. Gallego-Gomez, E. Mecher, and K. Meerholz

Pulsed-illumination study of metastable defect creation time scales in hydrogenated amorphous silicon *(4 pages)* 193204
Stephan Heck and Howard M. Branz

Optical band-edge shift of anatase $Ti_{1-x}Co_xO_{2-\delta}$ *(4 pages)* 193205
J. R. Simpson, H. D. Drew, S. R. Shinde, R. J. Choudhary, S. B. Ogale, and T. Venkatesan

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

Energetics of growth on the $c(4\times4)$ reconstructed GaAs(001) surface and antisite formation: An *ab initio* approach *(4 pages)* 193301
Sándor Kunsági-Máté, Carsten Schür, Tamas Marek, and Horst P. Strunk

Resonant nature of phonon-induced damping of Rabi oscillations in quantum dots *(4 pages)* 193302
P. Machnikowski and L. Jacak

Copyright 2004 by The American Physical Society

(Continued)

0163-1829(20040515)69:19;1-H

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 69, NUMBER 19** **MAY 2004-15(I)**

NMR investigation of atomic ordering in $Al_xGa_{1-x}As$ thin films *(4 pages)* 193303
C. Degen, M. Tomaselli, B. H. Meier, M. M. A. J. Voncken, and A. P. M Kentgens

Radiation-induced oscillatory magnetoresistance as a sensitive probe of the zero-field spin-splitting in high-mobility $GaAs/Al_xGa_{1-x}As$ devices *(4 pages)* 193304
R. G. Mani, J. H. Smet, K. von Klitzing, V. Narayanamurti, W. B. Johnson, and V. Umansky

Resonant thermal transport in semiconductor barrier structures *(4 pages)* 193305
P. Hyldgaard

Interaction-induced dephasing of Aharonov-Bohm oscillations *(4 pages)* 193306
T. Ludwig and A. D. Mirlin

Self-assembly of quantum dots: Effect of neighbor islands on the wetting in coherent Stranski-Krastanov growth *(4 pages)* 193307
José Emilio Prieto and Ivan Markov

Surface physics, low-dimensional systems, and related topics

Chiral symmetry of double-walled carbon nanotubes detected in first-principles optical absorption spectra *(4 pages)* 193401
Xiaoping Yang, Jiangwei Chen, Hui Jiang, and Jinming Dong

Growth mechanisms in Ge/Si(111) heteroepitaxy with and without Bi as a surfactant *(4 pages)* 193402
Neelima Paul, Hidehito Asaoka, Josef Mysliveček, and Bert Voigtländer

Tubular structures of GaS *(4 pages)* 193403
Th. Köhler, Th. Frauenheim, Z. Hajnal, and G. Seifert

Nanowires for spintronics: A study of transition-metal elements of groups 8–10 *(4 pages)* 193404
Tashi Nautiyal, T. H. Rho, and Kwang S. Kim

Mg(0001) surface oxidation: A two-dimensional oxide phase *(4 pages)* 193405
Elsebeth Schröder, Roman Fasel, and Adam Kiejna

Formation of carbon-gold-sulfide conductive granular molecules by a cooperation process of plasma CVD and sputtering *(4 pages)* 193406
Md. Abul Kashem and Shinzo Morita

ARTICLES

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

Exchange and correlation as a functional of the local density of states *(5 pages)* 195101
José M. Soler

Variational energy functionals tested on atoms *(12 pages)* 195102
Nils Erik Dahlen and Ulf von Barth

Modeling the crystal-field splitting of the energy levels of Er^{3+} in charge-compensated sites in lithium niobate *(10 pages)* 195103
John B. Gruber, Dhiraj K. Sardar, Raylon M. Yow, Bahram Zandi, and Edvard P. Kokanyan

Dependence of the optical and magneto-optical properties and electronic structures on the atomic order in Ni_2MnIn Heusler alloys *(9 pages)* 195104
Y. V. Kudryavtsev, Y. P. Lee, and J. Y. Rhee

Cluster-dynamical mean-field theory of the density-driven Mott transition in the one-dimensional Hubbard model *(5 pages)* 195105
M. Capone, M. Civelli, S. S. Kancharla, C. Castellani, and G. Kotliar

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 69, NUMBER 19** **MAY 2004-15(I)**

Electronic properties of alkali-metal loaded zeolites: Supercrystal Mott insulators *(5 pages)* 195106
Ryotaro Arita, Takashi Miyake, Takao Kotani, Mark van Schilfgaarde, Takashi Oka, Kazuhiko Kuroki, Yasuo Nozue, and Hideo Aoki

Fractal noise in quantum ballistic and diffusive lattice systems *(8 pages)* 195107
E. J. Amanatidis, D. E. Katsanos, and S. N. Evangelou

Analytical and numerical studies of wire-mesh metallic photonic crystals *(7 pages)* 195108
A. L. Pokrovsky

Kondo effect in systems with dynamical symmetries *(24 pages)* 195109
T. Kuzmenko, K. Kikoin, and Y. Avishai

Embedding method for conductance of DNA *(13 pages)* 195110
O. R. Davies and J. E. Inglesfield

Nature of lossy Bloch states in polaritonic photonic crystals *(10 pages)* 195111
Kerwyn Casey Huang, Elefterios Lidorikis, Xunya Jiang, John D. Joannopoulos, Keith A. Nelson, Peter Bienstman, and Shanhui Fan

Noncommuting limits and effective properties for oblique propagation of electromagnetic waves through an array of aligned fibres *(8 pages)* 195112
C. Poulton, S. Guenneau, and A. B. Movchan

Numerical atomic basis orbitals from H to Kr *(19 pages)* 195113
T. Ozaki and H. Kino

Optical investigation of the charge-density-wave phase transitions in $NbSe_3$ *(5 pages)* 195114
A. Perucchi, L. Degiorgi, and R. E. Thorne

Charge-density-wave instabilities driven by multiple umklapp scattering *(5 pages)* 195115
Peter Schmitteckert and Ralph Werner

Evolution of the electronic structure from electron-doped to hole-doped states in the two-dimensional Mott-Hubbard system $La_{1.17-x}Pb_xVS_{3.17}$ *(8 pages)* 195116
A. Ino, T. Okane, S.-I. Fujimori, A. Fujimori, T. Mizokawa, Y. Yasui, T. Nishikawa, and M. Sato

Semiconductors I: bulk

Urbach tail, disorder, and localized modes in ternary semiconductors *(5 pages)* 195201
Ismardo Bonalde, Ernesto Medina, Miguel Rodríguez, S. M. Wasim, G. Marín, C. Rincón, A. Rincón, and C. Torres

Spectra and energy levels of $Gd^{3+}(4f^7)$ in AlN *(7 pages)* 195202
John B. Gruber, Ulrich Vetter, Hans Hofsäss, Bahram Zandi, and Michael F. Reid

On-site Coulomb interaction and the magnetism of (GaMn)N and (GaMn)As *(7 pages)* 195203
L. M. Sandratskii, P. Bruno, and J. Kudrnovský

First-principles study of neutral oxygen vacancies in amorphous silica and germania *(10 pages)* 195204
Tomoyuki Tamura, Guang-Hong Lu, Ryoichi Yamamoto, and Masanori Kohyama

Anomalous capture and emission from internal surfaces of semiconductor voids: Nanopores in SiC *(4 pages)* 195205
D. C. Look, Z-Q. Fang, S. Soloviev, T. S. Sudarshan, and J. J. Boeckl

H_2O and O_2 molecules in amorphous SiO_2: Defect formation and annihilation mechanisms *(9 pages)* 195206
T. Bakos, S. N. Rashkeev, and S. T. Pantelides

Reverse Monte Carlo modeling of amorphous silicon *(5 pages)* 195207
Parthapratim Biswas, Raymond Atta-Fynn, and D. A. Drabold

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

Resonance approximation and charge loading and unloading in adiabatic quantum pumping *(9 pages)* 195301
Vyacheslavs Kashcheyevs, Amnon Aharony, and Ora Entin-Wohlman

Plasmon attenuation and optical conductivity of a two-dimensional electron gas *(8 pages)* 195302
E. G. Mishchenko, M. Yu. Reizer, and L. I. Glazman

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 69, NUMBER 19** **MAY 2004-15(I)**

STM characterization of the Si-P heterodimer *(5 pages)* 195303
N. J. Curson, S. R. Schofield, M. Y. Simmons, L. Oberbeck, J. L. O'Brien, and R. G. Clark
Dynamical screening effects on dark current in a quantum-well infrared photodetector *(7 pages)* 195304
S. Panda, B. K. Panda, and S. G. Mishra
Metallicity and its low-temperature behavior in dilute two-dimensional carrier systems *(15 pages)* 195305
S. Das Sarma and E. H. Hwang
Thermopower of a *p*-type $Si/Si_{1-x}Ge_x$ heterostructure *(9 pages)* 195306
C. Possanzini, R. Fletcher, M. Tsaousidou, P. T. Coleridge, R. L. Williams, Y. Feng, and J. C. Maan
Strain determination in multilayers by complementary anomalous x-ray diffraction *(8 pages)* 195307
T. U. Schülli, R. T. Lechner, J. Stangl, G. Springholz, G. Bauer, M. Sztucki, and T. H. Metzger
Coherent control of electric currents in superlattices and molecular wires: Effect of relaxation *(7 pages)* 195308
Kirill A. Pronin and Andre D. Bandrauk
Excitons in Si nanocrystals: Confinement and migration effects *(7 pages)* 195309
Johannes Heitmann, Frank Müller, Lixin Yi, Margit Zacharias, Dmitri Kovalev, and Frank Eichhorn
Numerical analysis of radio-frequency single-electron transistor operation *(13 pages)* 195310
Valentin O. Turin and Alexander N. Korotkov
Structural properties of a thallium-induced Si(111)-1×1 surface *(5 pages)* 195311
N. D. Kim, C. G. Hwang, J. W. Chung, T. C. Kim, H. J. Kim, and D. Y. Noh
Simulation of Ge/Si intermixing during heteroepitaxy *(6 pages)* 195312
Richard J. Wagner and Erdogan Gulari
Effect of surface curvature on magnetic moment and persistent currents in two-dimensional quantum rings and dots *(9 pages)* 195313
D. V. Bulaev, V. A. Geyler, and V. A. Margulis
Hall effect in the ferromagnet UGe_2 *(6 pages)* 195314
V. H. Tran, S. Paschen, R. Troć, M. Baenitz, and F. Steglich
Molecular spintronics: Coherent spin transfer in coupled quantum dots *(12 pages)* 195315
Florian Meier, Veronica Cerletti, Oliver Gywat, Daniel Loss, and D. D. Awschalom
Thermal conductivity modeling of periodic two-dimensional nanocomposites *(10 pages)* 195316
Ronggui Yang and Gang Chen
Charge-state dependence of InAs quantum-dot emission energies *(7 pages)* 195317
S. Schulz, S. Schnüll, Ch. Heyn, and W. Hansen
Time-dependent partition-free approach in resonant tunneling systems *(17 pages)* 195318
Gianluca Stefanucci and Carl-Olof Almbladh

Surface physics, low-dimensional systems, and related topics

Structure and dynamics of oxygen adsorbed on Ag(100) vicinal surfaces *(12 pages)* 195401
N. Bonini, A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni
Effect of molecular wires attached to benzene: Local density-of-states study *(8 pages)* 195402
R. Kucharczyk and S. G. Davison
Ab initio calculations of adsorbate-induced stress on Ni(100) *(8 pages)* 195403
Sampyo Hong, Abdelkader Kara, Talat S. Rahman, Rolf Heid, and Klaus Peter Bohnen
Water adsorption on metal surfaces: A general picture from density functional theory studies *(13 pages)* 195404
Sheng Meng, E. G. Wang, and Shiwu Gao
(3×1)-Br/Pt(110) structure and the charge-density-wave-assisted $c(2\times2)$ to (3×1) phase transition *(13 pages)* 195405
C. Deisl, K. Swamy, N. Memmel, E. Bertel, C. Franchini, G. Schneider, J. Redinger, S. Walter, L. Hammer, and K. Heinz
Transport in ropes of carbon nanotubes: Contact barriers and Luttinger liquid theory *(4 pages)* 195406
Th. Hunger, B. Lengeler, and J. Appenzeller

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 69, NUMBER 19** **MAY 2004-15(I)**

Effect of surface stress on Ni segregation in (110) NiAl thin films *(6 pages)* 195407
J. A. Brown and Y. Mishin
Lattice dilation near a single hydrogen molecule in an interstitial channel within a nanotube bundle *(4 pages)* 195408
M. Mercedes Calbi, Ari Mizel, and Milton W. Cole
Ab initio thermodynamics of oxide surfaces: O_2 on Fe_2O_3(0001) *(12 pages)* 195409
Wolfgang Bergermayer, Hannes Schweiger, and Erich Wimmer
Adaptive quantum design of atomic clusters *(8 pages)* 195410
Jason Thalken, Yu Chen, A. F. J. Levi, and Stephan Haas
First-principles study of the effect of charge on the stability of a diamond nanocluster surface *(5 pages)* 195411
Noejung Park, Sungil Park, Nong-Moon Hwang, Jisoon Ihm, Syogo Tejima, and Hisashi Nakamura
Gold adatoms and dimers on relaxed graphite surfaces *(7 pages)* 195412
Guan Ming Wang, Joseph J. BelBruno, Steven D. Kenny, and Roger Smith
Water dissociation on a defective MgO(100) surface: Role of divacancies *(9 pages)* 195413
Benedicte Ealet, Jacek Goniakowski, and Fabio Finocchi
Imperfect wetting of vapor-deposited thin films: Monte Carlo simulations and nucleation model *(6 pages)* . . 195414
Jacques Dalla Torre, George H. Gilmer, and Mehdi Djafari Rouhani
Structural determination of iodine localization in single-walled carbon nanotube bundles by diffraction methods *(8 pages)* 195415
N. Bendiab, R. Almairac, S. Rols, R. Aznar, J.-L. Sauvajol, and I. Mirebeau
Ultrafast electron-electron scattering and energy exchanges in noble-metal nanoparticles *(13 pages)* 195416
C. Voisin, D. Christofilos, P. A. Loukakos, N. Del Fatti, F. Vallée, J. Lermé, M. Gaudry, E. Cottancin, M. Pellarin, and M. Broyer

ERRATA

Erratum: First-principles approach to the electron-phonon interaction [Phys. Rev. B **69**, 115110 (2004)] *(1 page)* . . . . . 199901(E)
Robert van Leeuwen
Erratum: Accurate ground-state phase diagram of the one-dimensional extended-Hubbard model at half filling [Phys. Rev. B **68**, 153101 (2003)] *(1 page)* . . . . . 199902(E)
G. P. Zhang

Cumulative Author Index i