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 56, NUMBER 20 ***CONTENTS*** **15 NOVEMBER 1997-II**

RAPID COMMUNICATIONS

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

Large thermoelectric power in $NaCo_2O_4$ single crystals R12 685
I. Terasaki, Y. Sasago, and K. Uchinokura

Pressure-induced changes in transport properties of layered $La_{1.2}Ca_{1.8}Mn_2O_7$ R12 688
K. V. Kamenev, M. R. Lees, G. Balakrishnan, and D. McK. Paul

Resonance in a Tomonaga-Luttinger liquid R12 691
Inès Safi

Semiconductors I: bulk

Silicon incorporation in a shallow donor center in hydrogenated Czochralski-grown Si crystals: An EPR study R12 695
V. P. Markevich, T. Mchedlidze, and M. Suezawa

Semiconductor effective charges and dielectric constants in the tight-binding approach R12 698
Massimiliano Di Ventra and Pablo Fernández

Transient uv electroluminescence from poly(*p*-phenylenevinylene) conjugated polymer induced by strong voltage pulses R12 702
Haim Chayet, Roman Pogreb, and Dan Davidov

Interaction of vacancies with partial dislocations in silicon R12 706
Niklas Lehto and Sven Öberg

Silicon network relaxation in amorphous hydrogenated silicon R12 710
Z. Remeš, M. Vaněček, A. H. Mahan, and R. S. Crandall

Evidence for an enhanced magnetoresistance accompanying a continuous phase transition in semiconducting $La_{0.67}Mg_{0.33}MnO_3$ R12 714
X. Z. Zhou, H. P. Kunkel, J. H. Zhao, P. A. Stampe, and Gwyn Williams

Femtosecond degenerate four-wave mixing of GaN on sapphire: Measurement of intrinsic exciton dephasing time R12 718
S. Pau, J. Kuhl, F. Scholz, V. Haerle, M. A. Khan, and C. J. Sun

Transient four-wave-mixing spectroscopy on gallium nitride: Energy splittings of intrinsic excitonic resonances ... R12 722
R. Zimmermann, A. Euteneuer, J. Möbius, D. Weber, M. R. Hofmann, W. W. Rühle, E. O. Göbel, B. K. Meyer, H. Amano, and I. Akasaki

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

Theory of surface morphology of wurtzite GaN (0001) surfaces R12 725
Krzysztof Rapcewicz, Marco Buongiorno Nardelli, and J. Bernholc

Precursors of a Mott insulator in modulated quantum wires R12 729
Arkadi A. Odintsov, Yasuhiro Tokura, and Seigo Tarucha

Correlation analysis of self-similarity in semiconductor billiards R12 733
R. P. Taylor, A. P. Micolich, R. Newbury, and T. M. Fromhold

Assignment of rest-atom surface core-level shift through adsorption-site selectivity of methoxy on Si(111)-7×7 ... R12 737
M. N. Piancastelli, J. J. Paggel, Chr. Weindel, M. Hasselblatt, and K. Horn

Scaling and the metal-insulator transition in Si/SiGe quantum wells R12 741
J. Lam, M. D'Iorio, D. Brown, and H. Lafontaine

(Continued)

0163-1829(19971115)56:20;1-Z

PHYSICAL REVIEW B THIRD SERIES, VOLUME 56, NUMBER 20 15 NOVEMBER 1997-II

Effects of interface asymmetry on hole subband degeneracies and spin-relaxation rates in quantum wells R12 744
L. Vervoort, R. Ferreira, and P. Voisin
Elimination of spurious solutions from eight-band $\mathbf{k}\cdot\mathbf{p}$ theory R12 748
Bradley A. Foreman
Electron population inversion in photon-assisted tunneling through a quantum wire R12 752
C. Niu and D. L. Lin
From Tomonaga-Luttinger to Fermi liquid in transport through a tunneling barrier R12 756
V. V. Ponomarenko and N. Nagaosa
One-dimensional plasmons in magnetic fields R12 760
E. Ulrichs, G. Biese, C. Steinebach, C. Schüller, D. Heitmann, and K. Eberl
Metal-insulator transition at $B=0$ in p-type SiGe R12 764
P. T. Coleridge, R. L. Williams, Y. Feng, and P. Zawadzki
Spin-flip excitations in the fractional-quantum-Hall-effect regime studied by polarized photoluminescence of charged excitons R12 768
D. Gekhtman, E. Cohen, Arza Ron, and L. N. Pfeiffer
Pairing in the quantum Hall system R12 772
Kang-Hun Ahn and K. J. Chang
Evidence for a spin transition in the $\nu=\frac{2}{5}$ fractional quantum Hall effect R12 776
W. Kang, J. B. Young, S. T. Hannahs, E. Palm, K. L. Campman, and A. C. Gossard
Coherent reflected pulses of exciton polaritons in multiple quantum wells at Brewster's-angle incidence R12 780
Byung-Ryool Hyun, Tomobumi Mishina, Yasuaki Masumoto, and Masaaki Nakayama
Odd-parity excitons in semiconductor superlattices R12 784
K. Bott, J. Hader, S. W. Koch, and P. Thomas
Filling-factor dependence of the negatively-charged-exciton absorption in a CdTe quantum well R12 787
S. Lovisa, R. T. Cox, N. Magnea, and K. Saminadayar

Surface physics, low-dimensional systems, and related topics

Surface structure of single-crystal cubic boron nitride (111) studied by LEED, EELS, and AES R12 791
Kian Ping Loh, Isao Sakaguchi, Mikka Nishitani-Gamo, Takashi Taniguchi, and Toshihiro Ando

ARTICLES

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

Two interacting electrons in a quasiperiodic chain 12 797
S. N. Evangelou and D. E. Katsanos
Approximate occupation functions for density-functional calculations 12 805
D. M. C. Nicholson and X.-G. Zhang
Long-wavelength behavior of the exchange-correlation kernel in the Kohn-Sham theory of periodic systems 12 811
Ph. Ghosez, X. Gonze, and R. W. Godby
Electronic excitations in cupric oxide 12 818
Manabu Takahashi and Jun-ichi Igarashi
Self-consistent cumulant expansion for the electron gas 12 825
B. Holm and F. Aryasetiawan
Improved local-field corrections to the G_0W approximation in jellium: Importance of consistency relations 12 832
M. Hindgren and C.-O. Almbladh
Phase separation as an instability of the Tomonaga-Luttinger liquid 12 840
Masaaki Nakamura and Kiyohide Nomura
Maximally localized generalized Wannier functions for composite energy bands 12 847
Nicola Marzari and David Vanderbilt
Accuracy and convergence properties of the extended linear augmented-plane-wave method 12 866
E. E. Krasovskii

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 56, NUMBER 20 15 NOVEMBER 1997-II

Surface electronic structure with the linear methods of band theory 12 874
E. E. Krasovskii and W. Schattke
Theoretical description of spin-resolved appearance potential spectroscopy 12 884
H. Ebert and V. Popescu
Spin-dependent local density of empty electronic states in $FeNi_3$ 12 893
J. Reinmuth, F. Passek, V. N. Petrov, M. Donath, V. Popescu, and H. Ebert
Electron paramagnetic resonance and microwave conductivity in pyrolyzed polyacrylonitrile chains included in zeolites 12 899
Stéphane Esnouf, François Beuneu, Patricia Enzel, and Thomas Bein
de Haas–van Alphen effect in the organic metal κ-$(BEDT\text{-}TSF)_2Cu[N(CN)_2]Br$: Crossover to two-dimensional behavior in the complete-breakdown regime 12 905
N. Harrison, C. H. Mielke, D. G. Rickel, L. K. Montgomery, and T. Burgin
Interplay of Mott transition and ferromagnetism in the orbitally degenerate Hubbard model 12 909
Raymond Frésard and Gabriel Kotliar
Low-temperature transport, thermodynamic, and optical properties of FeSi 12 916
S. Paschen, E. Felder, M. A. Chernikov, L. Degiorgi, H. Schwer, H. R. Ott, D. P. Young, J. L. Sarrao, and Z. Fisk
Transition phenomenon in Ti_2O_3 using the discrete variational $X\alpha$ cluster method and periodic shell model 12 931
H. Nakatsugawa and E. Iguchi
Electronic phase transitions in a one-dimensional spinless fermion model with competing interactions 12 939
A. K. Zhuravlev, M. I. Katsnelson, and A. V. Trefilov
Instability of the marginal commutative model of tunneling centers interacting with a metallic environment: Role of the electron-hole symmetry breaking 12 947
A. Zawadowski, G. Zaránd, P. Nozières, K. Vladár, and G. T. Zimányi
Peculiar low-temperature properties of metallic $Nd_{2-x}Ce_xCuO_4$ caused by interactions between Nd moments and conduction electrons 12 961
E. Maiser, W. Mexner, R. Schäfer, T. Schreiner, P. Adelmann, G. Czjzek, J. L. Peng, and R. L. Greene
Delocalization transition via supersymmetry in one dimension 12 970
Leon Balents and Matthew P. A. Fisher
Off-resonant spectral hole burning in CaS:Eu by time-varying Coulomb fields 12 992
S. A. Basun, M. Raukas, U. Happek, A. A. Kaplyanskii, J. C. Vial, J. Rennie, W. M. Yen, and R. S. Meltzer
Carrier generation and compensation in Y- and Nb-doped $CaTiO_3$ single crystals 12 998
K. Ueda, H. Yanagi, H. Hosono, and H. Kawazoe
Effect of configuration interaction on calculated polarized UV-VIS absorption spectra: A molecular dynamics based study 13 006
Mattias Klintenberg and John O. Thomas
Computationally based explanation of the peculiar magneto-optical properties of PtMnSb and related ternary compounds 13 012
V. N. Antonov, P. M. Oppeneer, A. N. Yaresko, A. Ya. Perlov, and T. Kraft
Nanoscopic tunneling contacts on mesoscopic multiprobe conductors 13 026
Thomas Gramespacher and Markus Büttiker
Understanding the isomer shift of Fe impurities in metallic hosts 13 035
L. A. Terrazos and S. Frota-Pessôa

Semiconductors I: bulk

Magneto-optical investigations of Eu-based diluted magnetic lead chalcogenides 13 042
F. Geist, W. Herbst, C. Mejía-García, H. Pascher, R. Rupprecht, Y. Ueta, G. Springholz, G. Bauer, and M. Tacke

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 56, NUMBER 20 15 NOVEMBER 1997-II

Electronic properties of the crystalline phases of the Sb_2S_3-Tl_2S system 13 054
P. E. Lippens, J. Olivier-Fourcade, J. C. Jumas, A. Gheorghiu, S. Dupont, and C. Sénémaud
Dynamics associated with Bose-Einstein statistics of orthoexcitons generated by resonant excitations in cuprous oxide 13 066
M. Y. Shen, T. Yokouchi, S. Koyama, and T. Goto
Defect complexes in GaAs: First-principles calculations 13 073
A. Janotti, A. Fazzio, P. Piquini, and R. Mota
Electronic structure of defects and impurities in III-V nitrides. II. Be, Mg, and Si in cubic boron nitride 13 077
V. A. Gubanov, E. A. Pentaleri, C. Y. Fong, and B. M. Klein
Two-photon and three-photon spectroscopy of ZnO under uniaxial stress 13 087
J. Wrzesinski and D. Fröhlich
Strain broadening of the magnetization steps in diluted magnetic semiconductors 13 094
Yuri G. Rubo, M. F. Thorpe, and Normand Mousseau
Interplay between the magnetic and transport properties in the III-V diluted magnetic semiconductor $Ga_{1-x}Mn_xAs$ 13 103
A. Van Esch, L. Van Bockstal, J. De Boeck, G. Verbanck, A. S. van Steenbergen, P. J. Wellmann, B. Grietens, R. Bogaerts, F. Herlach, and G. Borghs
Magnetic-field-induced resonant coupling between $1s$- and $3d$-exciton states 13 113
A. El Ouazzani, D. Coquillat, J. P. Lascaray, Yu. G. Rubo, and A. V. Kavokin
Interactions of hydrogen molecules with bond-centered interstitial oxygen and another defect center in silicon 13 118
R. E. Pritchard, M. J. Ashwin, J. H. Tucker, R. C. Newman, E. C. Lightowlers, M. J. Binns, S. A. McQuaid, and R. Falster
Far-infrared reflection studies in ordered $GaInP_2$ 13 126
F. Alsina, H. M. Cheong, J. D. Webb, A. Mascarenhas, J. F. Geisz, and J. M. Olson
Structure and optical properties of the planar silicon compounds polysilane and Wöhler siloxene 13 132
U. Dettlaff-Weglikowska, W. Hönle, A. Molassioti-Dohms, S. Finkbeiner, and J. Weber
Dephasing of LO-phonon–plasmon hybrid modes in n-type GaAs 13 141
F. Vallée, F. Ganikhanov, and F. Bogani
Site- and symmetry-projected band structure measured by resonant inelastic soft x-ray scattering 13 147
J. Lüning, J.-E. Rubensson, C. Ellmers, S. Eisebitt, and W. Eberhardt
X-ray-absorption near-edge structure of $CuGaSe_2$ and ZnSe: Experiment and theory 13 151
O. Šipr, P. Machek, A. Šimůnek,, J. Vackář, and J. Horák
Interchain coupling and localized vibration modes in conjugated polymers of finite length 13 162
Shi-jie Xie, Jian-Hua Wei, De-Sheng Liu, Liang-Mo Mei, and D. L. Lin
Raman scattering on α-Sn: Dependence on isotopic composition 13 167
D. T. Wang, A. Göbel, J. Zegenhagen, and M. Cardona
As-vacancy interaction and ring mechanism of diffusion in Si 13 172
Oleg Pankratov, Hanchen Huang, Tomas Diaz de la Rubia, and Christian Mailhiot
Density-matrix approach to nonequilibrium free-carrier screening in semiconductors 13 177
U. Hohenester and W. Pötz

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

Initial oxygen reaction on Ge(100) 2×1 surfaces 13 190
T. Fukuda and T. Ogino
Phonons in {110} surfaces of III-V compound semiconductors 13 194
Hermann Nienhaus
Pinning behavior of gold-related levels in Si using $Si_{1-x}Ge_x$ alloy layers 13 202
A. Mesli, P. Kringhøj, and A. Nylandsted Larsen

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 56, NUMBER 20 15 NOVEMBER 1997-II

Conductance and its universal fluctuations in the directed network model at the crossover to the quasi-one-dimensional regime 13 218
Ilya A. Gruzberg, N. Read, and Subir Sachdev

Spectral functions of quantum dots in the integer and fractional quantum Hall regime 13 227
Arkadiusz Wójs and Pawel Hawrylak

Nonlinear transport through coupled double-quantum-dot systems 13 235
R. Kotlyar and S. Das Sarma

k·**p** finite-difference method: Band structures and cyclotron resonances of $Al_xGa_{1-x}Sb/InAs$ quantum wells 13 242
Shiow-Fon Tsay, Jih-Chen Chiang, Z. M. Chau, and Ikai Lo

Edge magnetoplasmons for very low temperatures and sharp density profiles 13 252
O. G. Balev and P. Vasilopoulos

Localization scaling relation in two dimensions: Comparison with experiment 13 263
F. W. Van Keuls, H. Mathur, H. W. Jiang, and A. J. Dahm

Sequential tunneling in doped superlattices: Fingerprints of impurity bands and photon-assisted tunneling 13 268
Andreas Wacker, Antti-Pekka Jauho, Stefan Zeuner, and S. James Allen

Microscopic picture of a chiral Luttinger liquid: Composite fermion theory of edge states 13 279
Yue Yu, Wenjun Zheng, and Zhongyuan Zhu

Application of Fermi-hypernetted-chain theory to composite-fermion quantum Hall states 13 290
O. Ciftja and S. Fantoni

Addition-spectrum oscillations in fractional quantum Hall dots 13 296
Eyal Goldmann and Scot R. Renn

Coulomb drag at the onset of Anderson insulators 13 301
Efrat Shimshoni

Infrared optical properties of mixed-phase thin films studied by spectroscopic ellipsometry using boron nitride as an example 13 306
M. Schubert, B. Rheinländer, E. Franke, H. Neumann, T. E. Tiwald, J. A. Woollam, J. Hahn, and F. Richter

Effect of carrier emission and retrapping on luminescence time decays in InAs/GaAs quantum dots 13 314
Weidong Yang, Roger R. Lowe-Webb, Hao Lee, and Peter C. Sercel

Excitonic properties of weakly coupled GaAs single quantum wells investigated with high-resolution photoluminescence excitation spectroscopy 13 321
L. Schrottke, H. T. Grahn, and K. Fujiwara

Valence-band photoemission from GaN(001) and GaAs: GaN surfaces 13 326
T. Strasser, F. Starrost, C. Solterbeck, and W. Schattke

Formation of the Zn/CdTe(100) interface: Interdiffusion, segregation, and Cd-Zn exchange studied by photoemission 13 335
C. Heske, U. Winkler, D. Eich, R. Fink, E. Umbach, Ch. Jung, and P. R. Bressler

Patterns in bistable resonant-tunneling structures 13 346
B. A. Glavin, V. A. Kochelap, and V. V. Mitin

Theoretical study of Landau-Zener tunneling at the $M+N$ level crossing 13 360
Tatsuya Usuki

Second-harmonic spectroscopy of a Si(001) surface during calibrated variations in temperature and hydrogen coverage 13 367
J. I. Dadap, Z. Xu, X. F. Hu, M. C. Downer, N. M. Russell, J. G. Ekerdt, and O. A. Aktsipetrov

N K-edge x-ray-absorption study of heteroepitaxial GaN films 13 380
M. Katsikini, E. C. Paloura, M. Fieber-Erdmann, J. Kalomiros, T. D. Moustakas, H. Amano, and I. Akasaki

Atomic vibrations in thin $(GaAs)_n(AlAs)_n$ superlattices 13 387
K. Lambert and G. P. Srivastava

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 56, NUMBER 20** **15 NOVEMBER 1997-II**

Localization and fluctuations of local spectral density on treelike structures with large connectivity: Application to the quasiparticle line shape in quantum dots 13 393
Alexander D. Mirlin and Yan V. Fyodorov

Determination of interface preference by observation of linear-to-circular polarization conversion under optical orientation of excitons in type-II GaAs/AlAs superlattices 13 405
R. I. Dzhioev, H. M. Gibbs, E. L. Ivchenko, G. Khitrova, V. L. Korenev, M. N. Tkachuk, and B. P. Zakharchenya

Lateral superlattices as voltage-controlled traps for excitons 13 414
S. Zimmermann, A. O. Govorov, W. Hansen, J. P. Kotthaus, M. Bichler, and W. Wegscheider

Quantum Monte Carlo study of the transport through a small interacting system 13 422
Akira Oguri

Electron-phonon scattering rates in semiconductor quantum wells with thin AlAs layers 13 428
Cynthia R. McIntyre and T. L. Reinecke

Electronic states and magnetotransport in quantum waveguides with nonuniform magnetic fields 13 434
Ben-Yuan Gu, Wei-Dong Sheng, Xue-Hua Wang, and Jian Wang

Surface physics, low-dimensional systems, and related topics

Growth mode and asymptotic smoothing of sputtered Fe/Au multilayers studied by x-ray diffuse scattering 13 442
R. Paniago, R. Forrest, P. C. Chow, S. C. Moss, S. S. P. Parkin, and D. Cookson

Surface-reconstruction-induced geometries of Si clusters 13 455
Efthimios Kaxiras

Scanning tunneling microscopy studies of the TiO_2(110) surface: Structure and the nucleation growth of Pd 13 464
C. Xu, X. Lai, G. W. Zajac, and D. W. Goodman

Correlation between island-formation kinetics, surface roughening, and RHEED oscillation damping during GaAs homoepitaxy 13 483
Ch. Heyn, T. Franke, R. Anton, and M. Harsdorff

Temperature-dependent growth and structure of Cr deposited on Co(0001) 13 490
F. Scheurer, P. Ohresser, H. Bulou, J. P. Deville, B. Carrière, and A. Dobroiu

Calorimetric measurements of the energetics of Pb adsorption and adhesion to Mo(100) 13 496
J. T. Stuckless, D. E. Starr, D. J. Bald, and Charles T. Campbell

Ab initio study of the anomalies in the He-atom-scattering spectra of H/Mo(110) and H/W(110) 13 503
Bernd Kohler, Paolo Ruggerone, and Matthias Scheffler

Self-consistent Thomas-Fermi calculation of potential and current distributions in a two-dimensional Hall bar geometry 13 519
J. H. Oh and Rolf R. Gerhardts

Auger spectroscopy of hydrogenated diamond surfaces 13 529
I. L. Krainsky, V. M. Asnin, A. G. Petukhov, and M. Foygel

Atomic control of layer-by-layer epitaxial growth on $SrTiO_3$(001): Molecular-dynamics simulations 13 535
Momoji Kubo, Yasunori Oumi, Ryuji Miura, Andras Stirling, Akira Miyamoto, Masashi Kawasaki, Mamoru Yoshimoto, and Hideomi Koinuma

Empirical potential for methyl-radical association with diamond surfaces 13 543
Pascal de Sainte Claire and William L. Hase

Relativistic calculations on the adsorption of CO on the (111) surfaces of Ni, Pd, and Pt within the zeroth-order regular approximation 13 556
P. H. T. Philipsen, E. van Lenthe, J. G. Snijders, and E. J. Baerends

Cumulative Author Index 13 563