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 62, NUMBER 4 *CONTENTS* **15 JULY 2000-II**

RAPID COMMUNICATIONS

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

Enhancement and suppression of thermal emission by a three-dimensional photonic crystal R2243
Shawn-Yu Lin, J. G. Fleming, E. Chow, Jim Bur, K. K. Choi, and A. Goldberg

Heavy photons at coupled-cavity waveguide band edges in a three-dimensional photonic crystal R2247
Mehmet Bayindir and E. Ozbay

Semiconductors I: bulk

Oxygen configurations in silica R2251
James R. Chelikowsky, D. J. Chadi, and N. Binggeli

Localization length and impurity dielectric susceptibility in the critical regime of the metal-insulator transition in homogeneously doped *p*-type Ge R2255
Michio Watanabe, Kohei M. Itoh, Youiti Ootuka, and Eugene E. Haller

Group V acceptors in CdTe: *Ab initio* calculation of lattice relaxation and the electric-field gradient R2259
Stephan Lany, Peter Blaha, Joachim Hamann, Volker Ostheimer, Herbert Wolf, and Thomas Wichert

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

Exploiting exciton-exciton interactions in semiconductor quantum dots for quantum-information processing R2263
Filippo Troiani, Ulrich Hohenester, and Elisa Molinari

NMR-based nanostructure switch for quantum logic R2267
John H. Reina, Luis Quiroga, and Neil F. Johnson

Evidence for a shear horizontal resonance in supported thin films R2271
X. Zhang, M. H. Manghnani, and A. G. Every

L-to-X crossover in the conduction-band minimum of Ge quantum dots R2275
F. A. Reboredo and Alex Zunger

Evidence of polariton stimulation in semiconductor microcavities R2279
F. Boeuf, R. André, R. Romestain, Le Si Dang, E. Péronne, J. F. Lampin, D. Hulin, and A. Alexandrou

Relaxation bottleneck and its suppression in semiconductor microcavities R2283
A. I. Tartakovskii, M. Emam-Ismail, R. M. Stevenson, M. S. Skolnick, V. N. Astratov, D. M. Whittaker, J. J. Baumberg, and J. S. Roberts

Surface physics, low-dimensional systems, and related topics

Gold clusters (Au_N, $2 \leqslant N \leqslant 10$) and their anions R2287
Hannu Häkkinen and Uzi Landman

Electronic and structural properties of carbon nanohorns R2291
Savas Berber, Young-Kyun Kwon, and David Tománek

Copyright 2000 by The American Physical Society

0163-1829(20000715)62:4;1-H

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 62, NUMBER 4** **15 JULY 2000-II**

Interaction of CO with the reconstructed Au(111) surface near atmospheric pressures R2295
P. Steadman, K. Peters, H. Isern, J. Alvarez, and S. Ferrer
Real-time study of nucleation, growth, and ripening during Fe/Fe(100) homoepitaxy using ion scattering R2299
R. Pfandzelter, T. Igel, and H. Winter
Extended energy range of Ag quantum-well states in Ag(111)/Au(111)/W(110) R2303
A. M. Shikin, D. V. Vyalikh, Yu. S. Dedkov, G. V. Prudnikova, V. K. Adamchuk, E. Weschke, and G. Kaindl
Local electronic properties of single-wall nanotube circuits measured by conducting-tip AFM R2307
M. Freitag, M. Radosavljević, W. Clauss, and A. T. Johnson

ARTICLES

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

Transferable relativistic Dirac-Slater pseudopotentials 2311
Ilya Grinberg, Nicholas J. Ramer, and Andrew M. Rappe
Temperature and filling dependence of the superconducting π phase in the Penson-Kolb-Hubbard model 2315
Fabrizio Dolcini and Arianna Montorsi
Dimensional crossover of the exchange-correlation density functional 2321
P. García-González
Minimum principles and level splitting in quantum Monte Carlo excitation energies: Application to diamond 2330
M. D. Towler, Randolph Q. Hood, and R. J. Needs
Theory of orbital excitation and resonant inelastic x-ray scattering in manganites 2338
Sumio Ishihara and Sadamichi Maekawa
Excitonic order at strong coupling: Pseudospin, doping, and ferromagnetism 2346
Leon Balents
Strong-coupling approach for strongly correlated electron systems 2358
Andrij M. Shvaika
Effect of Hund coupling on one-dimensional Luttinger liquids 2372
H. C. Lee and S.-R. Eric Yang
Quantum phase transitions and collapse of the Mott gap in the $d=1+\epsilon$ dimensional Hubbard model with $2k_F$ umklapp scattering 2377
Jun-ichiro Kishine
Quantum oscillations and phase diagram of α-(BEDT-TTF)$_2$TlHg(SCN)$_4$ 2388
Cyril Proust, Alain Audouard, Alexei Kovalev, David Vignolles, Mark Kartsovnik, Luc Brossard, and Natalia Kushch
Mo cluster formation in the intercalation compound LiMoS$_2$ 2397
X. Rocquefelte, F. Boîte, P. Gressier, G. Ouvrard, P. Blaha, and K. Schwarz
Distribution function of the local density of states of a one-channel weakly disordered ring in an external magnetic field 2401
H. Feldmann, E. P. Nakhmedov, and R. Oppermann
Cyclotron effective masses in layered metals 2416
Jaime Merino and Ross H. McKenzie
Gap to transition-temperature ratio in density-wave ordering: A dynamical mean-field study 2424
Stefan Blawid and Andrew Millis
Primary photoexcitations in oligophenylenevinylene thin films probed by femtosecond spectroscopy 2429
G. Cerulo, G. Lanzani, S. De Silvestri, H.-J. Egelhaaf, L. Lüer, and D. Oelkrug
Theory of solid-state contributions to the x-ray elastic scattering amplitude 2437
A. L. Ankudinov and J. J. Rehr

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 62, NUMBER 4** **15 JULY 2000-II**

Elastic wave scattering by periodic structures of spherical objects: Theory and experiment 2446
Zhengyou Liu, C. T. Chan, Ping Sheng, A. L. Goertzen, and J. H. Page
Transfer-matrix approach for modulated structures with defects 2458
T. Kostyrko

Semiconductors I: bulk

Electronic excitations in beryllium chalcogenides from the *ab initio GW* approach 2466
A. Fleszar and W. Hanke
First-principles calculations of the thermodynamic and structural properties of strained $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ alloys 2475
L. K. Teles, J. Furthmüller, L. M. R. Scolfaro, J. R. Leite, and F. Bechstedt
Resonant states induced by shallow acceptors in uniaxially strained semiconductors 2486
M. A. Odnoblyudov, I. N. Yassievich, V. M. Chistyakov, and K. A. Chao
Capacitance transient spectroscopy models of coupled trapping kinetics among multiple defect states: Application to the study of trapping kinetics of defects in heavy-ion-damaged silicon 2496
P. K. Giri and Y. N. Mohapatra
Formation of polaron pairs and time-resolved photogeneration of free charge carriers in π-conjugated polymers 2505
Eugene Frankevich, Hisao Ishii, Yasushi Hamanaka, Takahiro Yokoyama, Akihiko Fuji, Sergey Li, Katsumi Yoshino, Arao Nakamura, and Kazuhiko Seki
Correlation effects beyond Hartree-Fock theory and polarization dependence of four-wave mixing in bulk GaAs at high magnetic field 2516
N. A. Fromer, P. Kner, D. S. Chemla, R. Lövenich, and W. Schäfer
Statistical Ga clusters and $\boldsymbol{A_1}$(TO) gap mode in $Al_xGa_{1-x}N$ alloys 2522
A. A. Klochikhin, V. Yu. Davydov, I. N. Goncharuk, A. N. Smirnov, A. E. Nikolaev, M. V. Baidakova, J. Aderhold, J. Graul, J. Stemmer, and O. Semchinova
Extension of the collision-time tensor to the case of inelastic scattering mechanisms: Application to GaAs and GaN 2536
Jean-Louis Farvacque

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

Domain wall formation at the $c(2\times2)$-(2×1) phase transition of the CdTe(001) surface 2542
H. Neureiter, S. Tatarenko, S. Spranger, and M. Sokolowski
Kinetics of dimer-adatom–stacking-fault reconstruction on laser-quenched Si(111) surfaces 2546
K. Shimada, T. Ishimaru, T. Watanabe, T. Yamawaki, M. Osuka, T. Hoshino, and I. Ohdomari
Screened-exchange LDA methods for films and superlattices with applications to the Si(100)2×1 surface and InAs/InSb superlattices 2552
R. Asahi, W. Mannstadt, and A. J. Freeman
Strain and crystallographic orientation effects on the valence subbands of wurtzite quantum wells 2562
Francisco Mireles and Sergio E. Ulloa
Multiple-spin exchange in a two-dimensional Wigner crystal 2573
Masafumi Katano and D. S. Hirashima
Spin interactions and switching in vertically tunnel-coupled quantum dots 2581
Guido Burkard, Georg Seelig, and Daniel Loss
Coulomb effects on the quantum cyclotron resonance from a two-dimensional electron liquid with extremely narrow Landau levels 2593
Yu. P. Monarkha, E. Teske, and P. Wyder
Laterally coupled few-electron quantum dots 2605
Andreas Wensauer, Oliver Steffens, Michael Suhrke, and Ulrich Rössler

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 62, NUMBER 4** **15 JULY 2000-II**

Pseudopotential calculations of electron and hole addition spectra of InAs, InP, and Si quantum dots 2614
Alberto Franceschetti and Alex Zunger

Temperature dependence of the Aharonov-Bohm oscillations and the energy spectrum in a single-mode ballistic ring 2624
M. Cassé, Z. D. Kvon, G. M. Gusev, E. B. Olshanetskii, L. V. Litvin, A. V. Plotnikov, D. K. Maude , and J. C. Portal

Photon-assisted Stückelberg-like oscillations in a double quantum dot 2630
O. Speer, M. E. Garcia, and K. H. Bennemann

Electron-spin polarization in magnetically modulated quantum structures 2635
Yong Guo, Bing-Lin Gu, Zhong Zeng, Jing-Zhi Yu, and Yoshiyuki Kawazoe

Quasiparticle properties of quantum Hall ferromagnets 2640
Marcus Kasner, J. J. Palacios, and A. H. MacDonald

Nonlinear acoustoelectric transport in a two-dimensional electron system 2659
A. O. Govorov, A. V. Kalameitsev, M. Rotter, A. Wixforth, J. P. Kotthaus, K.-H. Hoffmann, and N. Botkin

Photoconductivity in CdSe quantum dot solids 2669
C. A. Leatherdale, C. R. Kagan, N. Y. Morgan, S. A. Empedocles, M. A. Kastner, and M. G. Bawendi

Origin of optical anisotropies of nonpolar GaN surfaces 2681
Cecilia Noguez

Quantum-kinetic dephasing in resonantly excited semiconductor quantum wells 2686
B. Mieck, H. Haug, W. A. Hügel, M. F. Heinrich, and M. Wegener

Spin coherence and formation dynamics of charged excitons in $CdTe/Cd_{1-x-y}Mg_xZn_yTe$ quantum wells 2696
E. Vanelle, M. Paillard, X. Marie, T. Amand, P. Gilliot, D. Brinkmann, R. Lévy, J. Cibert, and S. Tatarenko

Quantum theory of phonon-assisted exciton formation and luminescence in semiconductor quantum wells 2706
A. Thränhardt, S. Kuckenburg, A. Knorr, T. Meier, and S. W. Koch

Analysis of a special model for a grating coupler 2721
W. L. Schaich

Optical properties of $GaSb/Al_{0.4}Ga_{0.6}Sb$ multiple quantum wells 2731
C. Bottazzi, A. Parisini, L. Tarricone, R. Magnanini, and A. Baraldi

Carrier capture and relaxation in Stranski-Krastanow $In_xGa_{1-x}As/GaAs(311)B$ quantum dots 2737
C. Lobo, N. Perret, D. Morris, J. Zou, D. J. H. Cockayne, M. B. Johnston, M. Gal, and R. Leon

Magnetophonon resonance in photoluminescence excitation spectra of magnetoexcitons in $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice 2743
S. Dickmann, A. I. Tartakovskii, V. B. Timofeev, V. M. Zhilin, J. Zeman, G. Martinez, and J. M. Hvam

Molecular-dynamics simulations of nanoscale surface modification of Si(111) via local excitation 2751
Magnus Hedström and Hai-Ping Cheng

Hydrodynamics beyond local equilibrium: Application to electron gas 2759
I. V. Tokatly and O. Pankratov

Internal transitions of confined neutral magnetoexcitons in $GaAs/Al_xGa_{1-x}As$ quantum wells 2773
H. A. Nickel, G. Kioseoglou, T. Yeo, H. D. Cheong, A. Petrou, B. D. McCombe, D. Broido, K. K. Bajaj, and R. A. Lewis

Diffusion and transport coefficients in synthetic opals 2780
J. O. Sofo and G. D. Mahan

Microscopic derivation of transport coefficients and boundary conditions in discrete drift-diffusion models of weakly coupled superlattices 2786
L. L. Bonilla, G. Platero, and D. Sánchez

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 62, NUMBER 4** **15 JULY 2000-II**

Surface physics, low-dimensional systems, and related topics

Simulation of scanning tunneling spectroscopy of supported carbon nanotubes 2797
Géza I. Márk, László P. Biró, József Gyulai, Paul A. Thiry, Amand A. Lucas, and Philippe Lambin
Solitons in carbon nanotubes 2806
Claudio Chamon
Intergranular segregation and ordering effect: A mixed Monte Carlo mean-field approach 2813
Jérôme Creuze, Fabienne Berthier, Robert Tétot, and Bernard Legrand
Deposition of Au_N clusters on Au(111) surfaces. I. Atomic-scale modeling 2825
Q. Hou, M. Hou, L. Bardotti, B. Prével, P. Mélinon, and A. Perez
Deposition of Au_N clusters on Au(111) surfaces. II. Experimental results and comparison with simulations 2835
L. Bardotti, B. Prével, P. Mélinon, A. Perez, Q. Hou, and M. Hou
Thin films of Co on Pt(111): Strain relaxation and growth 2843
E. Lundgren, B. Stanka, M. Schmid, and P. Varga
Phase transitions in the adsorption system Li/Mo(112) 2852
A. Fedorus, D. Kolthoff, V. Koval, I. Lyuksyutov, A. G. Naumovets, and H. Pfnür
Interpreting STM images of the MnCu/Cu(100) surface alloy 2862
D. Wortmann, S. Heinze, G. Bihlmayer, and S. Blügel
Modeling of metal thin film growth: Linking angstrom-scale molecular dynamics results to micron-scale film topographies 2869
U. Hansen, S. Rodgers, and K. F. Jensen
Nonmonotonic roughness evolution in unstable growth 2879
Claudio Castellano and Joachim Krug
Submonolayer epitaxy with impurities: Kinetic Monte Carlo simulations and rate-equation analysis 2889
Miroslav Kotrla, Joachim Krug, and Pavel Šmilauer
Density-functional study of bulk and surface properties of titanium nitride using different exchange-correlation functionals 2899
M. Marlo and V. Milman
Coherent lattice vibration of interlayer shearing mode of graphite 2908
Tomobumi Mishina, Kazuki Nitta, and Yasuaki Masumoto
Surface color centers on epitaxial NaCl films 2912
V. Zielasek, T. Hildebrandt, and M. Henzler
Molecular-dynamics simulation of thermal stress at the (100) diamond/substrate interface: Effect of film continuity 2920
Irina Rosenblum, Joan Adler, Simon Brandon, and Alon Hoffman
Critical cluster size of metallic Cr and Mo nanoclusters 2937
S. H. Huh, H. K. Kim, J. W. Park, and G. H. Lee
Evidence of $c(2\times2)$ antiferromagnetic order of Mn in an ideal monolayer on Ag(001) 2944
P. Schieffer, C. Krembel, M.-C. Hanf, G. Gewinner, and Y. Gauthier

ERRATA

Erratum: Cohesion and conductance of disordered metallic point contacts [Phys. Rev. B **60**, 5000 (1999)] 2956
J. Bürki, C. A. Stafford, X. Zotos, and D. Baeriswyl

Cumulative Author Index 2957