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 60, NUMBER 4 *CONTENTS* 15 JULY 1999-II

RAPID COMMUNICATIONS

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

Dynamical electron-ion coupling in the ionic conductor α-NaSn R2135
Masayasu Miyata, Takeo Fujiwara, Susumu Yamamoto, and Takeo Hoshi

Semiconductors I: bulk

Sulfur: A donor dopant for *n*-type diamond semiconductors R2139
Isao Sakaguchi, Mikka N.-Gamo, Yuko Kikuchi, Eiji Yasu, Hajime Haneda, Toshimitsu Suzuki, and Toshihiro Ando

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

Dynamical description of the buildup process in resonant tunneling: Evidence of exponential and nonexponential contributions R2142
Roberto Romo and Jorge Villavicencio

Crystalline Si_3N_4 thin films on Si(111) and the 4×4 reconstruction on Si_3N_4(0001) R2146
Xue-sen Wang, Guangjie Zhai, Jianshu Yang, and Nelson Cue

Molecular-dynamics investigation of the surface stress distribution in a Ge/Si quantum dot superlattice R2150
I. Daruka, A.-L. Barabási, S. J. Zhou, T. C. Germann, P. S. Lomdahl, and A. R. Bishop

Maximum metallic conductivity in Si-MOS structures R2154
V. M. Pudalov, G. Brunthaler, A. Prinz, and G. Bauer

Phonon interaction of single excitons and biexcitons R2157
F. Gindele, K. Hild, W. Langbein, and U. Woggon

Effect of the spin-orbit geometric phase on the spectrum of Aharonov-Bohm oscillations in a semiconductor mesoscopic ring R2161
A. G. Mal'shukov, V. V. Shlyapin, and K. A. Chao

Local Fermi-level pinning at a single adatom (Cs) or vacancy (As) on a GaAs(110) surface R2165
S. Aloni, I. Nevo, and G. Haase

Shot-noise suppression in multimode ballistic Fermi conductors R2169
Y. Naveh, A. N. Korotkov, and K. K. Likharev

Magnetic semiconductor quantum wells in high fields to 60 Tesla: Photoluminescence linewidth annealing at magnetization steps R2173
S. A. Crooker, D. G. Rickel, S. K. Lyo, N. Samarth, and D. D. Awschalom

Ultrafast dynamics of inter- and intraband transitions in semiconductor nanocrystals: Implications for quantum-dot lasers R2177
V. I. Klimov, Ch. J. Schwarz, D. W. McBranch, C. A. Leatherdale, and M. G. Bawendi

Copyright 1999 by The American Physical Society

0163-1829(19990715)60:4;1-V

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 60, NUMBER 4** **15 JULY 1999-II**

Intraband relaxation in CdSe quantum dots R2181
Philippe Guyot-Sionnest, Moonsub Shim, Chris Matranga, and Margaret Hines
Excited states and selection rules in self-assembled InAs/GaAs quantum dots R2185
I. E. Itskevich, M. S. Skolnick, D. J. Mowbray, I. A. Trojan, S. G. Lyapin, L. R. Wilson, M. J. Steer, M. Hopkinson, L. Eaves, and P. C. Main
Electron-filling modulation reflectance in charged self-assembled $In_xGa_{1-x}As$ quantum dots R2189
T. M. Hsu, W.-H. Chang, K. F. Tsai, J.-I. Chyi, N. T. Yeh, and T. E. Nee
Radiative recombination in *p*-type δ-doped layers in GaAs R2193
Q. X. Zhao, M. Willander, P. O. Holtz, W. Lu, H. F. Dou, S. C. Shen, G. Li, and C. Jagadish

Surface physics, low-dimensional systems, and related topics

Anharmonicity of the dipole resonance of metal clusters R2197
K. Hagino
Nanometer ripple formation and self-affine roughening of ion-beam-eroded graphite surfaces R2200
S. Habenicht, W. Bolse, K. P. Lieb, K. Reimann, and U. Geyer
Epitaxial growth kinetics with interacting coherent islands R2204
H. M. Koduvely and A. Zangwill
Energetics of the oxidation and opening of a carbon nanotube R2208
M. S. C. Mazzoni, H. Chacham, P. Ordejón, D. Sánchez-Portal, J. M. Soler, and E. Artacho

ARTICLES

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

Band approach to the excitation-energy dependence of x-ray fluorescence of TiO_2 2212
L. D. Finkelstein, E. Z. Kurmaev, M. A. Korotin, A. Moewes, B. Schneider, S. M. Butorin, J-H. Guo, J. Nordgren, D. Hartmann, M. Neumann, and D. L. Ederer
Electron-electron interactions in disordered metals: Keldysh formalism 2218
Alex Kamenev and Anton Andreev
Schwinger-Keldysh approach to disordered and interacting electron systems: Derivation of Finkelstein's renormalization-group equations 2239
Claudio Chamon, Andreas W. W. Ludwig, and Chetan Nayak
Analytical ground state for the three-band Hubbard model 2255
C. Waidacher, J. Richter, R. E. Hetzel, and K. W. Becker
Electronic structure, Fermi surface, and Curie temperature calculations for the Co-Pt system 2262
Arti Kashyap, K. B. Garg, A. K. Solanki, T. Nautiyal, and S. Auluck
Metallic state of the Hubbard model with randomly distributed Coulomb interactions 2268
Tetsuya Mutou
Nonlinear impurity in a square lattice 2276
M. I. Molina
Correlation effects in the electronic structure of $SrRuO_3$ 2281
J. Okamoto, T. Mizokawa, A. Fujimori, I. Hase, M. Nohara, H. Takagi, Y. Takeda, and M. Takano
Hopping conduction in uniaxially stressed Si:B near the insulator-metal transition 2286
S. Bogdanovich, D. Simonian, S. V. Kravchenko, M. P. Sarachik, and R. N. Bhatt
Conductivity of metallic Si:B near the metal-insulator transition: Comparison between unstressed and uniaxially stressed samples 2292
S. Bogdanovich, M. P. Sarachik, and R. N. Bhatt
Metal-insulator transition in the one-dimensional SU(N) Hubbard model 2299
Roland Assaraf, Patrick Azaria, Michel Caffarel, and Philippe Lecheminant

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 60, NUMBER 4** **15 JULY 1999-II**

Relations among reduction factors in Jahn-Teller systems of icosahedral symmetry 2319
P. B. Oliete, C. A. Bates, J. L. Dunn, and G. E. Stedman
Calculation of low-energy-electron lifetimes 2326
E. Zarate, P. Apell, and P. M. Echenique
Vibrational and low-energy optical spectra of the square-planar $Pd_3(PS_4)_2$ thiophosphate 2333
C. Calareso, V. Grasso, and L. Silipigni
Valence-band ordering in ZnO 2340
D. C. Reynolds, D. C. Look, B. Jogai, C. W. Litton, G. Cantwell, and W. C. Harsch
Analytical reconstruction of momentum density from directional Compton profiles 2345
J.-M. Gillet, C. Fluteaux, and P. J. Becker
Integrable impurity model with spin and flavor: Model inspired by resonant tunneling in quantum dots 2350
Osamu Tsuchiya, Ikuo Ichinose, and Yasuyuki Kayama
Strong-coupling perturbation theory for the two-dimensional Bose-Hubbard model in a magnetic field 2357
M. Niemeyer, J. K. Freericks, and H. Monien
Electromagnetic forces in photonic crystals 2363
M. I. Antonoyiannakis and J. B. Pendry
Local densities, distribution functions, and wave-function correlations for spatially resolved shot noise at nanocontacts 2375
Thomas Gramespacher and Markus Büttiker
Concurrent coupling of length scales: Methodology and application 2391
Jeremy Q. Broughton, Farid F. Abraham, Noam Bernstein, and Efthimios Kaxiras
Metal-centered and ligand-to-metal charge-transfer transitions of $[CrO_4]^{4-}$ and $[MnO_4]^{3-}$ in $LiNbGeO_5:Cr^{4+}$ and $Sr_5(VO_4)_3F:Mn^{5+}$ using a density-functional-theory approach 2404
F. Deghoul, H. Chermette, F. Rogemond, R. Moncorgé, C. Stückl, and C. Daul
Impurity effects in coaxial-connector photonic crystals: A quasi-one-dimensional periodic system 2410
Ranjit D. Pradhan and George H. Watson
Electronic structure of a grain-boundary model in $SrTiO_3$ 2416
Shang-Di Mo, W. Y. Ching, M. F. Chisholm, and G. Duscher
Polarization-dependent resonant-x-ray diffraction in charge- and orbital-ordering phase of $Nd_{1/2}Sr_{1/2}MnO_3$ 2425
K. Nakamura, T. Arima, A. Nakazawa, Y. Wakabayashi, and Y. Murakami
Optical transitions of paramagnetic Ge sites created by x-ray irradiation of oxygen-defect-free Ge-doped SiO_2 by the sol-gel method 2429
N. Chiodini, F. Meinardi, F. Morazzoni, A. Paleari, and R. Scotti
Angular-dependent resonant-photoemission processes at the $2p$ thresholds in nickel metal 2436
M. Magnuson, A. Nilsson, M. Weinelt, and N. Mårtensson

Semiconductors I: bulk

Structure of high-temperature fluid selenium 2441
J. Y. Raty, A. Saùl, J. P. Gaspard, and C. Bichara
Influence of deposition conditions on long-range electronic disorder in *n*-type doped hydrogenated amorphous silicon 2449
D. Quicker and J. Kakalios
Microscopic description of exciton polaritons in direct two-band semiconductors 2456
Van Trong Nguyen and Günter Mahler
Band-gap shift in heavily doped *n*-type $Al_{0.3}Ga_{0.7}As$ alloys 2463
A. Ferreira da Silva, C. Persson, M. C. B. Marcussen, E. Veje, and A. G. de Oliveira
Imaging of ballistic carrier transport in tungsten single crystals 2468
A. Böhm, J. Heil, M. Primke, A. Gröger, P. Keppler, J. Major, and P. Wyder

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 60, NUMBER 4** **15 JULY 1999-II**

Photocapacitance study of boron-doped chemical-vapor-deposited diamond 2476
R. Zeisel, C. E. Nebel, M. Stutzmann, E. Gheeraert, and A. Deneuville

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

Atomic-resolution study of steps and ridges on arsine-exposed vicinal Ge(100) 2480
W. E. McMahon and J. M. Olson
(2×4) GaP(001) surface: Atomic structure and optical anisotropy 2488
A. M. Frisch, W. G. Schmidt, J. Bernholc, M. Pristovsek, N. Esser, and W. Richter
Atomic and electronic structure of β-SiC(001)-(3×2) 2495
Wenchang Lu, Peter Krüger, and Johannes Pollmann
Sagittal elastic waves at the interface between a superlattice and a substrate 2505
D. Bria, E. H. El Boudouti, A. Nougaoui, B. Djafari-Rouhani, and V. R. Velasco
Vertical alignment of multilayered quantum dots studied by x-ray grazing-incidence diffraction 2516
I. Kegel, T. H. Metzger, J. Peisl, J. Stangl, G. Bauer, and D. Smilgies
Ab initio optical properties of Si(100) 2522
Maurizia Palummo, Giovanni Onida, Rodolfo Del Sole, and Bernardo S. Mendoza
Geometric approach to determine the binding energy of quasi-two-dimensional biexcitons 2528
I.-K. Oh and Jai Singh
Statistics of Coulomb-blockade peak spacings within the Hartree-Fock approximation 2536
Avraham Cohen, Klaus Richter, and Richard Berkovits
Addition spectrum and Koopmans' theorem for disordered quantum dots 2541
Paul N. Walker, Gilles Montambaux, and Yuval Gefen
Enhancement of the skyrmionic excitations due to the suppression of Zeeman energy by optical orientation of nuclear spins 2554
I. V. Kukushkin, K. v. Klitzing, and K. Eberl
Current distribution in antidot arrays close to the quantum Hall regime 2561
Rolf R. Gerhardts and Johannes Groß
Current through a combined magnetostatic and electrostatic barrier system 2571
C. Heide
Temperature dependence of the electronic structure of C_{60} films adsorbed on Si(001)-(2×1) and Si(111)-(7×7) surfaces 2579
Kazuyuki Sakamoto, Daiyu Kondo, Yoshimitsu Ushimi, Masashi Harada, Akio Kimura, Akito Kakizaki, and Shozo Suto
Optical spectroscopy of quasimonolayer InAs at the onset of quantum-dot nucleation 2592
A. S. Bhatti, M. Grassi Alessi, M. Capizzi, P. Frigeri, and S. Franchi
Intraband terahertz emission from coupled semiconductor quantum wells: A model study using the exciton representation 2599
Wei Min Zhang, Torsten Meier, Vladimir Chernyak, and Shaul Mukamel
Scattering-matrix treatment of patterned multilayer photonic structures 2610
D. M. Whittaker and I. S. Culshaw
Scanning tunneling microscopy and spectroscopy at low temperatures of the (110) surface of Te-doped GaAs single crystals 2619
A. Depuydt, C. Van Haesendonck, N. S. Maslova, V. I. Panov, S. V. Savinov, and P. I. Arseev
Phonon group velocity and thermal conduction in superlattices 2627
Shin-ichiro Tamura, Yukihiro Tanaka, and Humphrey J. Maris
Hydrogen and P_b defects at the (111)Si-SiO_2 interface: An *ab initio* cluster study 2631
Blair Tuttle
Theory of exciton dephasing in semiconductor quantum dots 2638
T. Takagahara

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 60, NUMBER 4** **15 JULY 1999-II**

Magneto-optical properties of $Zn_{0.95}Mn_{0.05}Se/Zn_{0.76}Be_{0.08}Mg_{0.16}Se$ quantum wells and $Zn_{0.91}Mn_{0.09}Se/Zn_{0.972}Be_{0.028}Se$ spin superlattices 2653
B. König, U. Zehnder, D. R. Yakovlev, W. Ossau, T. Gerhard, M. Keim, A. Waag, and G. Landwehr
Harmonic-potential traps for indirect excitons in coupled quantum wells 2661
V. Negoita, D. W. Snoke, and K. Eberl
Microscopic analysis of shot-noise suppression in nondegenerate diffusive conductors 2670
T. González, J. Mateos, D. Pardo, O. M. Bulashenko, and L. Reggiani
Weak localization in ballistic quantum dots 2680
R. Akis, D. K. Ferry, J. P. Bird, and D. Vasileska
Temperature-induced turnover of the well and barrier layers in $ZnSe/Zn_{0.84}Mn_{0.16}Se$ superlattices 2691
Zuo-Ming Zhu, Guo-Hua Li, Wang Zhang, He-Xiang Han, Zhao-Ping Wang, Jie Wang, and Xun Wang
Hartree-Fock studies of surface properties of $BaTiO_3$ 2697
L. Fu, E. Yaschenko, L. Resca, and R. Resta
Optical and electronic properties of Si nanoclusters synthesized in inverse micelles 2704
J. P. Wilcoxon, G. A. Samara, and P. N. Provencio

Surface physics, low-dimensional systems, and related topics

Dynamics of Au-adsorption-induced step bunching on a Si(001) vicinal surface studied by reflection electron microscopy 2715
Hiroki Minoda and Katsumichi Yagi
Extended statistical analysis of rough growth fronts in gold films prepared by thermal evaporation 2720
A. I. Oliva, E. Anguiano, J. L. Sacedón, M. Aguilar, J. A. Méndez, and J. A. Aznárez
Full symmetry, optical activity, and potentials of single-wall and multiwall nanotubes 2728
M. Damnjanović, I. Milošević, T. Vuković, and R. Sredanović
Computer simulation of general grain boundaries in rocksalt oxides 2740
J. H. Harding, D. J. Harris, and S. C. Parker
Annealing of ion-implanted defects in diamond by MeV ion-beam irradiation 2747
Jyoji Nakata
Tight-binding molecular-dynamics study of amorphous carbon deposits over silicon surfaces 2762
Chu-Chun Fu and Mariana Weissmann
General solution for three-dimensional surface structures using direct methods 2771
L. D. Marks
Pt/Co(0001) superstructures in the submonolayer range: A tight-binding quenched-molecular-dynamics study 2781
C. Goyhenex, H. Bulou, J.-P. Deville, and G. Tréglia
Unified model of diffractive and multiphonon He atom scattering from adsorbates: Holstein renormalization of the interactions and the complete Debye-Waller factor 2789
Branko Gumhalter and David C. Langreth
Modeling of the fluid-phase interfacial effect on the growth morphology of crystals 2810
X. Y. Liu
Substrate-dependent lateral order in naphthalene-tetracarboxylic-dianhydride monolayers 2818
R. Fink, D. Gador, U. Stahl, Y. Zou, and E. Umbach
Interaction of Ti with the (0001) surface of highly oriented pyrolitic graphite 2827
Qing Ma and Richard A. Rosenberg
Hole formation induced by 488.0-nm light in 10-μm-thick amorphous as-evaporated As_2S_3 films 2833
Olli Nordman and Nina Nordman
Growth characteristics and surface roughening of vapor-deposited MgO thin films 2839
Jong-Gul Yoon, Hun Kyoo Oh, and Sung Jong Lee
Brillouin spectroscopy of surface modes in thin-film Si_3N_4 on GaAs 2844
Pavel Zinin, Murli H. Manghnani, Sergei Tkachev, Vahid Askarpour, Odile Lefeuvre, and Arthur Every

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 60, NUMBER 4** **15 JULY 1999-II**

Electronic correlations on a metallic nanosphere 2851
D. N. Aristov
Electronic structure of graphitic boron at a $TaB_2(0001)$ surface 2855
H. Kawanowa, R. Souda, K. Yamamoto, S. Otani, and Y. Gotoh
Periodic lattice distortion accompanying the charge-density-wave transition for Sn/Ge(111) 2860
Jiandi Zhang, Ismail, P. J. Rous, A. P. Baddorf, and E. W. Plummer
Dynamical Kohn anomaly in surface acoustic wave response in quantum Hall systems near $\nu=1/2$ 2864
Nataliya A. Zimbovskaya and Joseph L. Birman
Geometry and material parameter dependence of InAs/GaAs quantum dot electronic structure 2869
Craig Pryor
Transfer matrices combined with Green's functions for the multiple-scattering simulation of electronic projection imaging 2875
A. Mayer and J.-P. Vigneron
Raman and resonance Raman investigation of MoS_2 nanoparticles 2883
Gitti L. Frey, Reshef Tenne, Manyalibo J. Matthews, M. S. Dresselhaus, and G. Dresselhaus
Unconventional MBE strategies from computer simulations for optimized growth conditions 2893
S. Schinzer, M. Sokolowski, M. Biehl, and W. Kinzel
XPS/HREELS study of NiO films grown on Ni(111) 2900
G. T. Tyuliev and K. L. Kostov
Molecular-dynamics study of the structural rearrangements of Cu and Au clusters softly deposited on a Cu(001) surface 2908
F. J. Palacios, M. P. Iñiguez,, M. J. López, and J. A. Alonso
$Al_{10}Li_8$: A magic compound cluster 2916
Vijay Kumar
Bridging the gap over size scales: A Green's-function method to combine tight-binding and semiempirical force calculations 2921
J. A. Nieminen and S. Paavilainen
Soft-x-ray photoelectron, x-ray absorption, and autoionization spectroscopy of 1,5-cyclooctadiene on Si(001)-2×1 2930
Florence Jolly, Fabrice Bournel, François Rochet, Georges Dufour, Fausto Sirotti, and Amina Taleb
Signature of surface states on NMR chemical shifts: A theoretical prediction 2941
Francesco Mauri, Bernd G. Pfrommer, and Steven G. Louie
Spin-dependent surface band structure of hcp Co($10\bar{1}0$) 2946
Sven Bode, Kai Starke, and Günter Kaindl

Cumulative Author Index 2953