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 70, NUMBER 4 *CONTENTS* **JULY 2004-15(II)**

RAPID COMMUNICATIONS

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

Representation of electronic structures in crystals in terms of highly localized quasiatomic minimal basis orbitals *(4 pages)* . . . . . 041101(R)
W. C. Lu, C. Z. Wang, T. L. Chan, K. Ruedenberg, and K. M. Ho

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

Transverse electron focusing in systems with spin-orbit coupling *(4 pages)* . . . . . 041301(R)
Gonzalo Usaj and C. A. Balseiro

Selective coherent destruction of tunneling in a quantum-dot array *(4 pages)* . . . . . 041302(R)
J. M. Villas-Bôas, Sergio E. Ulloa, and Nelson Studart

Suppression of the persistent spin Hall current by defect scattering *(4 pages)* . . . . . 041303(R)
Jun-ichiro Inoue, Gerrit E. W. Bauer, and Laurens W. Molenkamp

Electronic coherence in metals: Comparing weak localization and time-dependent conductance fluctuations *(4 pages)* . . . . . 041304(R)
A. Trionfi, S. Lee, and D. Natelson

Charge shelving and bias spectroscopy for the readout of a charge qubit on the basis of superposition states *(4 pages)* . . . . . 041305(R)
Andrew D. Greentree, A. R. Hamilton, and F. Green

Single 2×1 domain orientation on Si(001) surfaces using aperiodic Bi line arrays *(4 pages)* . . . . . 041306(R)
J. M. MacLeod and A. B. McLean

Surface physics, low-dimensional systems, and related topics

Strain-induced incomplete wetting at CuAu(001) surfaces *(4 pages)* . . . . . 041401(R)
W. Schweika, H. Reichert, W. Babik, O. Klein, and S. Engemann

Surface instability and evolution of nonlinear elastic heteroepitaxial thin-film structures *(4 pages)* . . . . . 041402(R)
Y. W. Zhang and D. J. Srolovitz

Magnetic properties of polymerized C_{60}: The influence of defects and hydrogen *(4 pages)* . . . . . 041403(R)
J. A. Chan, B. Montanari, J. D. Gale, S. M. Bennington, J. W. Taylor, and N. M. Harrison

Copyright 2004 by The American Physical Society

0163-1829(20040715)70:4;1-4

(Continued)

THIRD SERIES, VOLUME , NUMBER

ARTICLES

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

Systematic prediction of crystal structures: An application to sp^3 -hybridized carbon polymorphs *(7 pages)* . . . 045101
Rachel T. Strong, Chris J. Pickard, Victor Milman, Georg Thimm, and Björn Winkler

Charge disproportionation in $(TMTTF)_2SCN$ observed by ^{13}C NMR *(6 pages)* 045102
Shigeki Fujiyama and Toshikazu Nakamura

First-principles calculations of ELNES and XANES of selected wide-gap materials: Dependence on crystal structure and orientation *(10 pages)* 045103
Teruyasu Mizoguchi, Isao Tanaka, Satoru Yoshioka, Masahiro Kunisu, Tomoyuki Yamamoto, and W. Y. Ching

Charge disproportionation and spin ordering tendencies in Na_xCoO_2 *(9 pages)* 045104
K.-W. Lee, J. Kuneš, and W. E. Pickett

Interpretation of resonant photoemission spectra and electronic structure of RT_2 compounds (R=Ce, Pr, Nd; T=Co, Rh, Ir) *(7 pages)* 045105
Yu. Kucherenko, S. L. Molodtsov, A. N. Yaresko, and C. Laubschat

Effect of charge transfer on EELS integrated cross sections in Mn and Ti oxides *(10 pages)* 045106
Pavel L. Potapov, Kevin Jorissen, Dominique Schryvers, and Dirk Lamoen

Phase diagram and quasiparticle properties of the Hubbard model within cluster two-site dynamical mean-field theory *(9 pages)* 045107
E. C. Carter and A. J. Schofield

Electronic structure calculations for $PrOs_4Sb_{12}$ filled skutterudite. A theoretical approach using extended Huckel tight-binding method *(5 pages)* 045108
Donald H. Galvan and Cuauhtémoc Samaniego

Electronic absorption spectra of Cu^{2+} in MgO: *Ab initio* theory and experiment *(7 pages)* 045109
José Luis Pascual, B. Savoini, and R. González

Semiconductors I: bulk

Quasiclassical approach to Bose condensation in a finite potential well *(8 pages)* 045201
L. A. Bányai, A. M. Bundaru, and H. Haug

Scanning tunneling spectroscopy on organic semiconductors: Experiment and model *(13 pages)* 045202
M. Kemerink, S. F. Alvarado, P. Müller, P. M. Koenraad, H. W. M. Salemink, J. H. Wolter, and R. A. J. Janssen

Electrodeless time-resolved microwave conductivity study of charge-carrier photogeneration in regioregular poly(3-hexylthiophene) thin films *(8 pages)* 045203
Gerald Dicker, Matthijs P. de Haas, Laurens D.A. Siebbeles, and John M. Warman

Noncritically phase-matched second-harmonic-generation chalcopyrites based on $CdSiAs_2$ and $CdSiP_2$ *(7 pages)* 045204
Walter R. L. Lambrecht and Xiaoshu Jiang

Theory of spin waves in diluted-magnetic-semiconductor quantum wells *(13 pages)* 045205
Diego Frustaglia, Jürgen König, and Allan H. MacDonald

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 70, NUMBER 4** **JULY 2004-15(II)**

Wave-vector-dependent exchange interaction and its relevance for the effective exciton mass in Cu_2O *(11 pages)* 045206
G. Dasbach, D. Fröhlich, R. Klieber, D. Suter, M. Bayer, and H. Stolz

Short- and intermediate-range structural correlations in amorphous silicon carbide: A molecular dynamics study *(11 pages)* 045207
José P. Rino, Ingvar Ebbsjö, Paulo S. Branicio, Rajiv K. Kalia, Aiichiro Nakano, Fuyuki Shimojo, and Priya Vashishta

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

Ab initio and semiempirical dielectric response of superlattices *(13 pages)* 045301
Silvana Botti, Nathalie Vast, Lucia Reining, Valerio Olevano, and Lucio Claudio Andreani

Electroluminescence and photoluminescence excitation study of asymmetric coupled $GaAs/Al_xGa_{1-x}As$ V-groove quantum wires *(5 pages)* 045302
K. F. Karlsson, H. Weman, M.-A. Dupertuis, K. Leifer, A. Rudra, and E. Kapon

Surface and bulk electronic structure of ScN(001) investigated by scanning tunneling microscopy/spectroscopy and optical absorption spectroscopy *(8 pages)* 045303
Hamad A. Al-Brithen, Arthur R. Smith, and Daniel Gall

Frequency-dependent third cumulant of current in diffusive conductors *(8 pages)* 045304
S. Pilgram, K. E. Nagaev, and M. Büttiker

Structural elements on reconstructed Si and Ge(110) surfaces *(7 pages)* 045305
A. A. Stekolnikov, J. Furthmüller, and F. Bechstedt

Modification of electron-hole excitations for a quantum well embedded in an asymmetric dielectric structure *(6 pages)* 045306
Van Trong Nguyen and Günter Mahler

Atomic structure of the cleaved $Si(111)-(2\times1)$ surface refined by dynamical LEED *(7 pages)* 045307
Geng Xu, Bingcheng Deng, Zhaoxian Yu, S. Y. Tong, M. A. Van Hove, F. Jona, and I. Zasada

Break-junction tunneling spectroscopy for doped semiconductors in the hopping regime *(8 pages)* 045308
O. Bleibaum, B. Sandow, and W. Schirmacher

Correlated quantum percolation in the lowest Landau level *(13 pages)* 045309
Nancy Sandler, Hamid R. Maei, and Jané Kondev

Electron transport in two-dimensional arrays *(11 pages)* 045310
Julia S. Meyer, Alex Kamenev, and Leonid I. Glazman

Magneto-optical response of CdSe nanostructures *(12 pages)* 045311
Pochung Chen and K. Birgitta Whaley

Anomalous temperature dependence of electrical transport in quantum Hall multilayers *(5 pages)* 045312
H. A. Walling, D. P. Dougherty, D. P. Druist, E. G. Gwinn, K. D. Maranowski, and A. C. Gossard

Electronic structure and optical properties of silicon nanowires: A study using x-ray excited optical luminescence and x-ray emission spectroscopy *(8 pages)* 045313
T. K. Sham, S. J. Naftel, P.-S. G. Kim, R. Sammynaiken, Y. H. Tang, I. Coulthard, A. Moewes, J. W. Freeland, Y.-F. Hu, and S. T. Lee

Space-charge and trap-filling effects in organic thin film field-effect transistors *(8 pages)* 045314
Marlus Koehler and Ivan Biaggio

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 70, NUMBER 4** **JULY 2004-15(II)**

Surface pattern transfer in GaAs with molecular beams of Cl_2 *(7 pages)* 045315
J. H. Schmid, T. Tiedje, R. Mar, and A. Ballestad

Near-band-gap dielectric function of $Zn_{1-x}Mn_xSe$ thin films determined by spectroscopic ellipsometry *(7 pages)* 045316
J. Kvietkova, B. Daniel, M. Hetterich, M. Schubert, D. Spemann, D. Litvinov, and D. Gerthsen

Photoelectron diffraction study of the Si-rich 3*C*-SiC(001)–(3×2) structure *(11 pages)* 045317
A. Tejeda, D. Dunham, F. J. García de Abajo, J. D. Denlinger, E. Rotenberg, E. G. Michel, and P. Soukiassian

ac gate-induced Fano resonance and peak splitting of conductance in a quantum dot *(5 pages)* 045318
Mou Yang and Shu-Shen Li

NMR linewidth and skyrmion localization in quantum Hall ferromagnets *(5 pages)* 045319
A. Villares Ferrer, R. L. Doretto, and A. O. Caldeira

Rabi oscillations in a semiconductor quantum dot: Influence of local fields *(5 pages)* 045320
G. Ya. Slepyan, A. Magyarov, S. A. Maksimenko, A. Hoffmann, and D. Bimberg

Interaction of neutral vacancies and interstitials with the Si(001) surface *(7 pages)* 045321
Taras A. Kirichenko, Sanjay K. Banerjee, and Gyeong S. Hwang

Calculations and applications of the complex band structure for carbon nanotube field-effect transistors *(8 pages)* 045322
T.-S. Xia, L. F. Register, and S. K. Banerjee

Non-Markovian dynamics in a spin star system: Exact solution and approximation techniques *(10 pages)* 045323
Heinz-Peter Breuer, Daniel Burgarth, and Francesco Petruccione

Integer filling factor phases and isospin in vertical diatomic artificial molecules *(8 pages)* 045324
D. G. Austing, S. Tarucha, H. Tamura, K. Muraki, F. Ancilotto, M. Barranco, A. Emperador, R. Mayol, and M. Pi

Surface physics, low-dimensional systems, and related topics

Diamond fragments as building blocks of functional nanostructures *(8 pages)* 045401
Gregory C. McIntosh, Mina Yoon, Savas Berber, and David Tománek

Catalytic surface oxidation by rare-earth metals: A photoemission study of Gd- and Y-promoted oxidation of W(110) *(8 pages)* 045402
R. I. R. Blyth, C. Searle, N. P. Tucker, and S. D. Barrett

Self-organized structures in $CoCr_2O_4$(001) thin films: Tunable growth from pyramidal clusters to a {111} fully faceted surface *(6 pages)* 045403
U. Lüders, F. Sánchez, and J. Fontcuberta

Improved mechanical load transfer between shells of multiwalled carbon nanotubes *(8 pages)* 045404
M. Huhtala, A. V. Krasheninnikov, J. Aittoniemi, S. J. Stuart, K. Nordlund, and K. Kaski

Self-organization of Pb thin films on Cu(111) induced by quantum size effects *(5 pages)* 045405
J. H. Dil, J. W. Kim, S. Gokhale, M. Tallarida, and K. Horn

Nanoparticle diffusion on desorbing solids: The role of elementary excitations in buffer-layer-assisted growth *(8 pages)* 045406
V. N. Antonov, J. S. Palmer, P. S. Waggoner, A. S. Bhatti, and J. H. Weaver

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 70, NUMBER 4** **JULY 2004-15(II)**

Structural and electronic properties of MgO nanotube clusters *(6 pages)* 045407
G. Bilalbegović

Conductance fluctuations in metallic nanocontacts *(5 pages)* 045408
E. Louis, A. J. Pérez-Jiménez, J. J. Palacios, J. A. Vergés, Y. García, and E. SanFabián

Effective transition rates for epitaxial growth using fast modulation *(10 pages)* 045409
Martha A. Gallivan, David G. Goodwin, and Richard M. Murray

Phase diagram of carbon nanotube ropes *(14 pages)* 045410
J. González and J. V. Alvarez

Strain-related structural and vibrational properties of thin epitaxial AlN layers *(10 pages)* 045411
V. Darakchieva, J. Birch, M. Schubert, T. Paskova, S. Tungasmita, G. Wagner, A. Kasic, and B. Monemar

Pseudomorphic-to-bulk fcc phase transition of thin Ni films on Pd(100) *(8 pages)* 045412
G. A. Rizzi, A. Cossaro, M. Petukhov, F. Sedona, G. Granozzi, F. Bruno, D. Cvetko, A. Morgante, and L. Floreano

Ab initio total energy study of ZnO adsorption on a sapphire (0001) surface *(8 pages)* 045413
Yang Chun, Li Yan-rong, and Li Jin-shan

Nitrogen ion irradiation of Au(110): Photoemission spectroscopy and possible crystal structures of gold nitride *(5 pages)* 045414
S. Krishnamurthy, M. Montalti, M. G. Wardle, M. J. Shaw, P. R. Briddon, K. Svensson, M. R. C. Hunt, and L. Šiller

Two-photon photoemission spectroscopy of TiO_2(110) surfaces modified by defects and O_2 or H_2O adsorbates *(11 pages)* 045415
Ken Onda, Bin Li, and Hrvoje Petek

Classical Stern-Gerlach profiles of Mn_5 and Mn_6 clusters *(5 pages)* 045416
N. O. Jones, S. N. Khanna, Tunna Baruah, and M. R. Pederson

Ballistic conductance of magnetic Co and Ni nanowires with ultrasoft pseudopotentials *(9 pages)* 045417
Alexander Smogunov, Andrea Dal Corso, and Erio Tosatti

Heat current and spin current through a carbon-nanotube-based molecular quantum pump *(9 pages)* 045418
Yadong Wei, Langhui Wan, Baigeng Wang, and Jian Wang

Temperature-dependent photoluminescence from single-walled carbon nanotubes *(8 pages)* 045419
J. Lefebvre, P. Finnie, and Y. Homma

Phase diagram of oxygen adsorbed on platinum (111) by first-principles investigation *(10 pages)* 045420
Hairong Tang, Anton Van der Ven, and Bernhardt L. Trout

Coupled surface plasmon polaritons on thin metal slabs corrugated on both surfaces *(14 pages)* 045421
I. R. Hooper and J. R. Sambles

Stability of reduced V_2O_5(001) surfaces *(13 pages)* 045422
M. V. Ganduglia-Pirovano and J. Sauer

Composition-induced structural transitions in mixed rare-gas clusters *(12 pages)* 045423
F. Calvo and E. Yurtsever

Photon energy dependence of the dynamic final-state effect for metal clusters at surfaces *(5 pages)* 045424
H. Hövel, I. Barke, H.-G. Boyen, P. Ziemann, M. G. Garnier, and P. Oelhafen

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 70, NUMBER 4** **JULY 2004-15(II)**

ERRATA

Publisher's Note: Electroluminescence and photoluminescence excitation study of asymmetric coupled $GaAs/Al_xGa_{1-x}As$ V-groove quantum wires [Phys. Rev. B **70**, 045302 (2004)] *(1 page)* . . . . . 049901(E)
K. F. Karlsson, H. Weman, M.-A. Dupertuis, K. Leifer, A. Rudra, and E. Kapon

Cumulative Author Index i