PHYSICAL REVIEW B

For editorial and subscription correspondence,
please see inside front cover
(ISSN: 1098-0121)

PERIODICALS
Postmaster send address changes to:
APS Subscription Services
Suite 1NO1
2 Huntington Quadrangle
Melville, NY 11747-4502

THIRD SERIES, VOLUME 74, NUMBER 15 *CONTENTS* **OCTOBER 2006-15(I)**

BRIEF REPORTS

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

Band-structure results for elastic waves interpreted with multiple-scattering theory *(4 pages)* 153101
Li Cai, Han Xiaoyun, and Wen Xisen

Band structure and band-gap control in photonic superlattices *(4 pages)* 153102
S. B. Cavalcanti, M. de Dios-Leyva, E. Reyes-Gómez, and L. E. Oliveira

Universality of the metal-insulator transition in three-dimensional disordered systems *(4 pages)* 153103
J. Brndiar and P. Markoš

Polaron conductivity mechanism in oxalic acid dihydrate: *ac* conductivity experiment *(4 pages)* 153104
Adrijan Levstik, Cene Filipič, Vid Bobnar, Iva Levstik, and Dušan Hadži

Semiconductors I: bulk

Light-induced hyperfine ^{69}Ga shifts in semi-insulating GaAs observed by optically polarized NMR *(4 pages)* 153201
Kannan Ramaswamy, Stacy Mui, and Sophia E. Hayes

Filling fraction limits for rare-earth atoms in $CoSb_3$: An *ab initio* approach *(4 pages)* 153202
Z. G. Mei, W. Zhang, L. D. Chen, and J. Yang

Thermodynamics of type-I and type-II Si clathrates at zero pressure: Monte Carlo simulations *(4 pages)* 153203
Caetano R. Miranda and Alex Antonelli

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

Estimation of local and nonlocal contributions to the current-induced magnetization switching *(4 pages)* 153301
T. Yang, A. Hirohata, T. Kimura, and Y. Otani

Spin-exchange interaction in ZnO-based quantum wells *(4 pages)* 153302
B. Gil, P. Lefebvre, T. Bretagnon, T. Guillet, J. A. Sans, T. Taliercio, and C. Morhain

Quantum dot dephasing by fractional quantum Hall edge states *(4 pages)* 153303
T. K. T. Nguyen, A. Crépieux, T. Jonckheere, A. V. Nguyen, Y. Levinson, and T. Martin

Elastic strain relaxation in discontinuous wetting layers and its impact on lateral ordering of heteroepitaxial dots *(4 pages)* 153304
M. Hanke, T. Boeck, A.-K. Gerlitzke, F. Syrowatka, and F. Heyroth

Copyright 2006 by The American Physical Society

1098-0121(20061015)74:15;1-S

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Oxidation of Si during the growth of SiO_x by ion-beam sputter deposition: *In situ* x-ray photoelectron spectroscopy as a function of oxygen partial pressure and deposition temperature *(4 pages)* 153305
Kyung Joong Kim, Jeong Won Kim, Moon-Seung Yang, and Jung Hoon Shin

Effects of excitons in nonlinear optical rectification in semiparabolic quantum dots *(4 pages)* 153306
Sotirios Baskoutas, Emmanuel Paspalakis, and Andreas F. Terzis

Circular dichroism in InAs/GaAs quantum dots: Confinement-induced magnetism *(4 pages)* 153307
E. W. Bogaart, J. E. M. Haverkort, T. Mano, T. van Lippen, G. J. Hamhuis, and R. Nötzel

Two-spin entanglement induced by electron scattering in nanostructures *(4 pages)* 153308
Gian Luca Giorgi and Ferdinando de Pasquale

Charge detection in a closed-loop Aharonov-Bohm interferometer *(4 pages)* 153309
Gyong Luck Khym and Kicheon Kang

Influence of band structure effects on domain-wall resistance in diluted ferromagnetic semiconductors *(4 pages)* 153310
R. Oszwałdowski, J. A. Majewski, and T. Dietl

Electron transport in laterally confined phosphorus δ layers in silicon *(4 pages)* 153311
S. J. Robinson, J. S. Kline, H. J. Wheelwright, J. R. Tucker, C. L. Yang, R. R. Du, B. E. Volland, I. W. Rangelow, and T.-C. Shen

Using holes in GaAs as qubits: An estimate of the Rabi frequency in the presence of an external rf field *(3 pages)* 153312
Darin Sleiter and W. F. Brinkman

Fano-Rashba effect in a quantum wire *(4 pages)* 153313
David Sánchez and Llorenç Serra

Scattering dependence of bias-controlled magnetization switching in ferromagnetic resonant tunneling diodes *(4 pages)* 153314
Swaroop Ganguly, A. H. MacDonald, L. F. Register, and S. K. Banerjee

Magnetotransport in a doubly connected two-dimensional quantum Hall system in the low magnetic field regime *(4 pages)* 153315
J. Oswald and M. Oswald

Surface physics, nanoscale physics, low-dimensional systems

Mn_n^- clusters: Size-induced transition to half metallicity *(4 pages)* 153401
Julius Jellinek, Paulo H. Acioli, Juan Garciá-Rodeja, Weijun Zheng, Owen C. Thomas, and Kit H. Bowen, Jr.

Photoluminescence polarization in individual CdSe nanowires *(4 pages)* 153402
C. X. Shan, Z. Liu, and S. K. Hark

Doping and the unique role of vacancies in promoting the magnetic ground state in carbon nanotubes and C_{60} polymers *(4 pages)* 153403
Antonis N. Andriotis, R. Michael Sheetz, and Madhu Menon

Photoluminescence quenching in peapod-derived double-walled carbon nanotubes *(4 pages)* 153404
Toshiya Okazaki, Shunji Bandow, Goshu Tamura, Yoko Fujita, Konstantin Iakoubovskii, Said Kazaoui, Nobutsugu Minami, Takeshi Saito, Kazu Suenaga, and Sumio Iijima

Emergence of macroscopic surface structure from atomistic dynamics in epitaxial film growth *(4 pages)* 153405
A. Ballestad and T. Tiedje

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Kinetics of atom rebounding in surface self-diffusion *(3 pages)* 153406
Grazyna Antczak

Focusing quantum states on surfaces: A route towards the design of ultrasmall electronic devices *(4 pages)* 153407
M. Sentef, A. P. Kampf, S. Hembacher, and J. Mannhart

Phonon band structure and electron-phonon interactions in metallic nanowires *(4 pages)* 153408
Matthieu J. Verstraete and Xavier Gonze

Ferromagnetism induced by heavy-ion irradiation in fullerene films *(4 pages)* 153409
Amit Kumar, D. K. Avasthi, J. C. Pivin, A. Tripathi, and F. Singh

First-principles absorption spectra of Si_n ($n=20-28$) clusters: Time-dependent local-density approximation versus predictions from Mie theory *(4 pages)* 153410
Juan C. Idrobo, Mingli Yang, Koblar A. Jackson, and Serdar Öğüt

Transmission of light through a single rectangular hole in a real metal *(4 pages)* 153411
F. J. García-Vidal, L. Martín-Moreno, Esteban Moreno, L. K. S. Kumar, and R. Gordon

Mechanism of low-frequency Raman scattering from the acoustic vibrations of dielectric nanoparticles *(4 pages)* 153412
M. Mattarelli, M. Montagna, F. Rossi, A. Chiasera, and M. Ferrari

Engineering of electronic structure of boron-nitride nanotubes by covalent functionalization *(4 pages)* 153413
Chunyi Zhi, Yoshio Bando, Chengchun Tang, and Dmitri Golberg

Adsorption trends for water, hydroxyl, oxygen, and hydrogen on transition-metal and platinum-skin surfaces *(4 pages)* 153414
G. S. Karlberg

Symmetry-mediated H_2O diffusion on Al{100} *(4 pages)* 153415
Jibiao Li, Ying Li, Shenglong Zhu, and Fuhui Wang

Effect of hole diameter on terahertz surface-wave excitation in metal-hole arrays *(4 pages)* 153416
Fumiaki Miyamaru, Masaki Tanaka, and Masanori Hangyo

Vectorial method for calculating the Fresnel reflection of surface plasmon polaritons *(4 pages)* 153417
Reuven Gordon

Carbon nanowires: Phonon and π-electron confinement *(4 pages)* 153418
Alberto Milani, Matteo Tommasini, Mirella Del Zoppo, Chiara Castiglioni, and Giuseppe Zerbi

ARTICLES

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

Surface and bulk modes for periodic structures of negative index materials *(13 pages)* 155101
Ruey-Lin Chern, Chien C. Chang, and C. Chung Chang

Quantum Monte Carlo study for multiorbital systems with preserved spin and orbital rotational symmetries *(9 pages)* 155102
Shiro Sakai, Ryotaro Arita, Karsten Held, and Hideo Aoki

Electronic structure of AV_2O_4 (A=Li, Zn, and Cd) studied by x-ray photoemission spectroscopy *(5 pages)* 155103
K. Takubo, J.-Y. Son, T. Mizokawa, H. Ueda, M. Isobe, Y. Matsushita, and Y. Ueda

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Strongly disordered Hubbard model in one dimension: Spin and orbital infinite randomness and Griffiths phases *(8 pages)* 155104
R. Mélin and F. Iglói

Dynamics of photoexcited states in one-dimensional dimerized Mott insulators *(11 pages)* 155105
Nobuya Maeshima and Kenji Yonemitsu

Phononic effects and nonlocality contributions to second harmonic generation in NiO *(17 pages)* 155106
G. Lefkidis and W. Hübner

Hybridization expansion impurity solver: General formulation and application to Kondo lattice and two-orbital models *(13 pages)* 155107
Philipp Werner and Andrew J. Millis

Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides *(10 pages)* 155108
Fabien Tran, Peter Blaha, Karlheinz Schwarz, and Pavel Novák

Two-loop renormalization group theory for the quasi-one-dimensional Hubbard model at half filling *(18 pages)* 155109
M. Tsuchiizu

Possible phases of two coupled n-component fermionic chains determined using an analytic renormalization group method *(17 pages)* 155110
E. Szirmai and J. Sólyom

Electronic structure calculations of the phenalenyl-based neutral radical conductor bis(9-cyclohexylimino-1-phenalenyl) boron *(6 pages)* 155111
Johan Böhlin, Anders Hansson, and Sven Stafström

Simulating molecular conductance using real-time density functional theory *(11 pages)* 155112
Chiao-Lun Cheng, Jeremy S. Evans, and Troy Van Voorhis

Doped carrier formulation and mean-field theory of the $tt't''J$ model *(16 pages)* 155113
Tiago C. Ribeiro and Xiao-Gang Wen

Lattice-distortion-enhanced electron-phonon coupling and Fermi surface nesting in $1T$-TaS_2 *(7 pages)* 155114
F. Clerc, C. Battaglia, M. Bovet, L. Despont, C. Monney, H. Cercellier, M. G. Garnier, P. Aebi, H. Berger, and L. Forró

Temperature dependence of the conductivity sum rule in the normal state due to inelastic scattering *(11 pages)* 155115
L. Benfatto, J. P. Carbotte, and F. Marsiglio

Semiclassical motion of a multiband Bloch particle in a time-dependent field: Optical visualization *(11 pages)* 155116
S. Longhi, M. Lobino, M. Marangoni, R. Ramponi, P. Laporta, E. Cianci, and V. Foglietti

High-resolution EELS investigation of the electronic structure of ilmenites *(8 pages)* 155117
G. Radtke, S. Lazar, and G. A. Botton

Physical properties of the ferromagnetic heavy-fermion compound UIr_2Zn_{20} *(6 pages)* 155118
E. D. Bauer, A. D. Christianson, J. S. Gardner, V. A. Sidorov, J. D. Thompson, J. L. Sarrao, and M. F. Hundley

Quantum entanglement in the $S=1/2$ spin ladder with ring exchange *(6 pages)* 155119
Jun-Liang Song, Shi-Jian Gu, and Hai-Qing Lin

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Enhanced localization of Dyakonov-like surface waves in left-handed materials *(7 pages)* 155120
L.-C. Crasovan, O. Takayama, D. Artigas, S. K. Johansen, D. Mihalache, and L. Torner

Periodic cluster perturbation theory *(5 pages)* 155121
Minh-Tien Tran

Thermodynamical stability of calcium borohydride $Ca(BH_4)_2$ *(5 pages)* 155122
Kazutoshi Miwa, Masakazu Aoki, Tatsuo Noritake, Nobuko Ohba, Yuko Nakamori, Shin-ichi Towata, Andreas Züttel, and Shin-ichi Orimo

Analysis of scanning tunneling microscopy images of the charge-density-wave phase in quasi-one-dimensional $Rb_{0.3}MoO_3$ *(6 pages)* 155123
E. Machado-Charry, P. Ordejón, E. Canadell, C. Brun, and Z. Z. Wang

Biaxial spin-nematic phase of two-dimensional disordered rotor models and $S=1$ bosons in optical lattices *(7 pages)* 155124
Jean-Sébastien Bernier, K. Sengupta, and Yong Baek Kim

Nonequilibrium magnetotransport through a quantum dot: An interpolative perturbative approach *(9 pages)* 155125
A. A. Aligia

Electronic structure of Pb- and non-Pb-based phosphate scintillators *(6 pages)* 155126
D. J. Singh, G. E. Jellison, Jr., and L. A. Boatner

Cluster model calculations of the coherent spectral weight transfer in the bandwidth-controlled $Ca_{1-x}Sr_xVO_3$ series *(5 pages)* 155127
R. J. O. Mossanek, M. Abbate, and A. Fujimori

Hidden orbital fluctuations in the solid solution $Y_{1-x}La_xTiO_3$ ($x<0.2$) *(5 pages)* 155128
L. Craco, S. Leoni, and E. Müller-Hartmann

Low-temperature magnetic and transport properties of layered Sr_xCoO_2 *(7 pages)* 155129
Y. Q. Guo, J. L. Luo, G. T. Liu, H. X. Yang, J. Q. Li, N. L. Wang, D. Jin, and T. Xiang

Optical functions of $KTaO_3$ as determined by spectroscopic ellipsometry and comparison with band structure calculations *(5 pages)* 155130
G. E. Jellison, Jr., I. Paulauskas, L. A. Boatner, and D. J. Singh

Semiconductors I: bulk

Crystal-field theory of Co^{2+} in doped ZnO *(12 pages)* 155201
R. O. Kuzian, A. M. Daré, P. Sati, and R. Hayn

Analysis of the anisotropy of excitons in pentacene single crystals using reflectivity measurements and electron energy-loss spectroscopy *(6 pages)* 155202
M. Grobosch, R. Schuster, T. Pichler, M. Knupfer, and H. Berger

Antisite effect on hole-mediated ferromagnetism in (Ga,Mn)As *(9 pages)* 155203
R. C. Myers, B. L. Sheu, A. W. Jackson, A. C. Gossard, P. Schiffer, N. Samarth, and D. D. Awschalom

Vibronic spectrum of *c*-BN measured with cathodoluminescence *(7 pages)* 155204
C. Manfredotti, R. Cossio, A. Lo Giudice, E. Vittone, and F. Fizzotti

Ab initio studies of the electronic structure of defects in PbTe *(13 pages)* 155205
Salameh Ahmad, S. D. Mahanti, Khang Hoang, and M. G. Kanatzidis

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Photoluminescence of the inorganic-organic layered semiconductor $(C_6H_5C_2H_4NH_3)_2PbI_4$: Observation of triexciton formation *(6 pages)* 155206
Makoto Shimizu, Jun-ichi Fujisawa, and Teruya Ishihara

Spin polarization control in semiconductors by electric-field gradients *(7 pages)* 155207
Dan Csontos and Sergio E. Ulloa

Vibrational spectra of vitreous germania from first-principles *(15 pages)* 155208
Luigi Giacomazzi, P. Umari, and Alfredo Pasquarello

Excitonic contribution to the optical absorption in zinc-blende III-V semiconductors *(11 pages)* 155209
S. Shokhovets, G. Gobsch, and O. Ambacher

Doping front propagation in light-emitting electrochemical cells *(5 pages)* 155210
Nathaniel D. Robinson, Joon-Ho Shin, Magnus Berggren, and Ludvig Edman

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

Emission from a highly excited single InAs-GaAs quantum dot in magnetic fields: An excitonic Fock-Darwin diagram *(5 pages)* 155301
A. Babinski, M. Potemski, S. Raymond, J. Lapointe, and Z. R. Wasilewski

Structural and electronic properties of Bi-adsorbate-stabilized reconstructions on the InP(100) and $GaAs_xN_{1-x}$(100) surfaces *(6 pages)* 155302
P. Laukkanen, J. Pakarinen, M. Ahola-Tuomi, M. Kuzmin, R. E. Perälä, I. J. Väyrynen, A. Tukiainen, J. Konttinen, P. Tuomisto, and M. Pessa

Nitrogen-induced perturbation of the valence band states in $GaP_{1-x}N_x$ alloys *(6 pages)* 155303
S. V. Dudiy, Alex Zunger, M. Felici, A. Polimeni, M. Capizzi, H. P. Xin, and C. W. Tu

Electronic and optical properties of InAs/GaAs nanowire superlattices *(9 pages)* 155304
Y. M. Niquet

Real-space description of current-constrained molecular junctions *(10 pages)* 155305
Anna Painelli

Localized states in continuum in low-dimensional systems *(7 pages)* 155306
Khee-Kyun Voo and C. S. Chu

Conservation of spin current: Model including self-consistent spin-spin interaction *(5 pages)* 155307
Jian Wang, Baigeng Wang, Wei Ren, and Hong Guo

Surface states of wurtzite semiconductor nanowires with identical lateral facets: A transfer-matrix approach *(8 pages)* 155308
N. Malkova and C. Z. Ning

Two-impurity Anderson model for the transport through two quantum dots coupled via a quantum wire *(13 pages)* 155309
P. Durganandini

Optical study of excitation and deexcitation of Tm in GaN quantum dots *(6 pages)* 155310
Thomas Andreev, Nguyen Quang Liem, Yuji Hori, Mitsuhiro Tanaka, Osamu Oda, Daniel Le Si Dang, Bruno Daudin, and Bruno Gayral

Engineering the spatial confinement of exciton polaritons in semiconductors *(8 pages)* 155311
R. Idrissi Kaitouni, O. El Daïf, A. Baas, M. Richard, T. Paraiso, P. Lugan, T. Guillet, F. Morier-Genoud, J. D. Ganière, J. L. Staehli, V. Savona, and B. Deveaud

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Polarization ratio and effective mass in InP nanowires: Effect of crystallographic axis *(10 pages)* 155312
Dileep Karanth and Huaxiang Fu

Accumulation of opposite spins on the transverse edges of a two-dimensional electron gas in a longitudinal electric field *(5 pages)* 155313
Yanxia Xing, Qing-feng Sun, Liang Tang, and JiangPing Hu

Enhancing Kerr nonlinearity in an asymmetric double quantum well via Fano interference *(5 pages)* 155314
Hui Sun, Shangqing Gong, Yueping Niu, Shiqi Jin, Ruxin Li, and Zhizhan Xu

Quantum theory of luminescence in multiple-quantum-well Bragg structures *(11 pages)* 155315
M. Schäfer, M. Werchner, W. Hoyer, M. Kira, and S. W. Koch

Spin relaxation in narrow wires of a two-dimensional electron gas *(5 pages)* 155316
Peter Schwab, Michael Dzierzawa, Cosimo Gorini, and Roberto Raimondi

Impact of surface bond-order loss on phonon dispersion relations and thermal conductivity of cylindrical Si nanowires *(10 pages)* 155317
T. C. Au Yeung, M. X. Gu, Chang Q. Sun, George C. K. Chen, D. W. K. Wong, and V. Nosik

Relation between growth procedure and confinement properties of CdSe/ZnSe quantum dots *(13 pages)* 155318
Ivan-Christophe Robin, Régis André, and Jean-Michel Gérard

Static local-field factors in a two-dimensional electron liquid *(6 pages)* 155319
R. Asgari, A. L. Subaşı, A. A. Sabouri-Dodaran, and B. Tanatar

Switching the sign of photon-induced exchange interactions in semiconductor microcavities with finite quality factors *(7 pages)* 155320
G. Chiappe, E. Louis, and E. V. Anda

Spin separation and spin Hall effect in quantum wires due to lateral-confinement-induced spin-orbit-coupling *(6 pages)* 155321
Kiminori Hattori and Hiroaki Okamoto

Interrelation of structural and electronic properties in $In_xGa_{1-x}N/GaN$ quantum dots using an eight-band $\mathbf{k}\cdot\mathbf{p}$ model *(12 pages)* 155322
Momme Winkelnkemper, Andrei Schliwa, and Dieter Bimberg

Statistical model for analyzing the dephasing effects in a one-dimensional scattering chain *(7 pages)* 155323
Huaixiu Zheng, Zhengfei Wang, Qinwei Shi, Xiaoping Wang, and Jie Chen

Measuring fractional charge and statistics in fractional quantum Hall fluids through noise experiments *(23 pages)* 155324
Eun-Ah Kim, Michael J. Lawler, Smitha Vishveshwara, and Eduardo Fradkin

Response functions and superfluid density in a weakly interacting Bose gas with nonquadratic dispersion *(5 pages)* 155325
Jonathan Keeling

Local equilibrium and global relaxation of strained SiGe/Si(001) layers *(5 pages)* 155326
M. Stoffel, A. Rastelli, J. Tersoff, T. Merdzhanova, and O. G. Schmidt

Numerical self-consistent field calculation of a ferromagnetic ZnMnO quantum well *(5 pages)* 155327
Nammee Kim, H. Kim, J. W. Kim, S. J. Lee, and T. W. Kang

Probing the hot-electron transport properties and interface band structure of Fe/Si (001) and $Fe_{81}C_{19}$/Si (001) Schottky diodes *(4 pages)* 155328
A. J. Stollenwerk, M. R. Krause, D. H. Idell, R. Moore, and V. P. LaBella

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Tunnel conductance via interfacial states in semimetal/semiconductor/semimetal junctions *(9 pages)* 155329
Syuta Honda, Taku Kondo, Hiroyoshi Itoh, and Jun-ichiro Inoue

Stark shift of transmission resonance in scanning tunneling spectroscopy *(4 pages)* 155330
W. B. Su, S. M. Lu, C. L. Jiang, H. T. Shih, C. S. Chang, and Tien T. Tsong

Surface physics, nanoscale physics, low-dimensional systems

Heat conduction of single-walled carbon nanotube isotope superlattice structures: A molecular dynamics study *(6 pages)* 155401
Junichiro Shiomi and Shigeo Maruyama

Adsorption of phenol on graphite(0001) and α-Al_2O_3(0001): Nature of van der Waals bonds from first-principles calculations *(7 pages)* 155402
Svetla D. Chakarova-Käck, Øyvind Borck, Elsebeth Schröder, and Bengt I. Lundqvist

Effects of short-range attraction in unstable metal (110) epitaxial growth: Molecular dynamics simulations for Cu, Ag, and Al *(5 pages)* 155403
Jianguo Yu and Jacques G. Amar

Nonlinear deformation and progressive failure of multiwalled carbon nanotubes under internal radial pressure *(7 pages)* 155404
J. R. Xiao and J. W. Gillespie, Jr.

Electronic excitations of the H:Si(001)-(2×1) monohydride surface: First-principles calculations *(9 pages)* 155405
Neng-Ping Wang, Michael Rohlfing, Peter Krüger, and Johannes Pollmann

Iron silicides grown by solid phase epitaxy on a Si(111) surface: Schematic phase diagram *(8 pages)* 155406
K. Kataoka, K. Hattori, Y. Miyatake, and H. Daimon

Surface-plasmon-enhanced light transmission through planar metallic films *(6 pages)* 155407
L. Lin, R. J. Reeves, and R. J. Blaikie

Coherent treatment of the self-consistency and the environment-dependency in a semi-empirical Hamiltonian: Applications to bulk silicon, silicon surfaces, and silicon clusters *(13 pages)* 155408
C. Leahy, M. Yu, C. S. Jayanthi, and S. Y. Wu

Transition level dependence of Raman intensities in carbon nanotubes: Role of exciton decay *(6 pages)* 155409
B. C. Satishkumar, S. V. Goupalov, E. H. Haroz, and S. K. Doorn

Electrostatics of straight and bent single-walled carbon nanotubes *(5 pages)* 155410
E. G. Mishchenko and M. E. Raikh

Exciton absorption of perpendicularly polarized light in carbon nanotubes *(9 pages)* 155411
Seiji Uryu and Tsuneya Ando

Surface reconstructions of epitaxial MnAs films grown on GaAs(111)B *(7 pages)* 155412
A. Ouerghi, M. Marangolo, M. Eddrief, B. B. Lipinski, V. H. Etgens, M. Lazzeri, H. Cruguel, F. Sirotti, A. Coati, and Y. Garreau

Seeking optimal performance of multiwall carbon nanotubes in field emission: Tight-binding approach *(5 pages)* 155413
Shi-Dong Liang, Shao Zhi Deng, and Ning Sheng Xu

Zero-bias anomaly and possible superconductivity in single-walled carbon nanotubes *(8 pages)* 155414
Jian Zhang, Alexander Tselev, Yanfei Yang, Kyle Hatton, Paola Barbara, and Serhii Shafraniuk

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Quantum Hall effect and the topological number in graphene *(5 pages)* 155415
Yasumasa Hasegawa and Mahito Kohmoto

Structural and chemical embrittlement of grain boundaries by impurities: A general theory and first-principles calculations for copper *(13 pages)* 155416
A. Y. Lozovoi, A. T. Paxton, and M. W. Finnis

Growth dynamics of ultrasmooth hydrogenated amorphous carbon films *(7 pages)* 155417
J. G. Buijnsters, M. Camero, and L. Vázquez

Critical behavior of repulsive linear *k*-mers on triangular lattices *(8 pages)* 155418
P. M. Pasinetti, F. Romá, J. L. Riccardo, and A. J. Ramirez-Pastor

Adsorption of phenylglycine on copper: Density functional calculations *(7 pages)* 155419
S. Blankenburg and W. G. Schmidt

Light-harvesting function of β-carotene inside carbon nanotubes *(5 pages)* 155420
Kazuhiro Yanagi, Konstantin Iakoubovskii, Said Kazaoui, Nobutsugu Minami, Yutaka Maniwa, Yasumitsu Miyata, and Hiromichi Kataura

Phonon confinement and laser heating effects in Germanium nanowires *(6 pages)* 155421
R. Jalilian, G. U. Sumanasekera, H. Chandrasekharan, and M. K. Sunkara

Unified theory of linear instability of anisotropic surfaces and interfaces under capillary, electrostatic, and elastostatic forces: The regrowth of epitaxial amorphous silicon *(25 pages)* 155422
Tarik Omer Ogurtani

Fe_3O_4(001) films on Fe(001): Termination and reconstruction of iron-rich surfaces *(5 pages)* 155423
N. Spiridis, J. Barbasz, Z. Łodziana, and J. Korecki

Activated boron nitride nanotubes: A potential material for room-temperature hydrogen storage *(4 pages)* 155424
Seung-Hoon Jhi

Ab initio study of native defects in SiC nanotubes *(8 pages)* 155425
R. J. Baierle, P. Piquini, L. P. Neves, and R. H. Miwa

Spin-orbit coupling in curved graphene, fullerenes, nanotubes, and nanotube caps *(15 pages)* 155426
Daniel Huertas-Hernando, F. Guinea, and Arne Brataas

Formation of nanoripples in Al films during O_2^+ sputtering *(6 pages)* 155427
P. Mishra and D. Ghose

Ab initio density-functional theory study of NH_x dehydrogenation and reverse reactions on the Rh(111) surface *(10 pages)* 155428
C. Popa, W. K. Offermans, R. A. van Santen, and A. P. J. Jansen

Effect of nitrogen on the electronic properties of ultrananocrystalline diamond thin films grown on quartz and diamond substrates *(7 pages)* 155429
P. Achatz, O. A. Williams, P. Bruno, D. M. Gruen, J. A. Garrido, and M. Stutzmann

Transport through the intertube links between two parallel carbon nanotubes *(5 pages)* 155430
Jia-Lin Zhu, Fu-Fang Xu, and Yu-Feng Jia

Persistent orbital degeneracy in carbon nanotubes *(6 pages)* 155431
A. Makarovski, L. An, J. Liu, and G. Finkelstein

Constrained evolution of nanocrystallites *(11 pages)* 155432
M. Degawa, K. Thürmer, and E. D. Williams

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 74, NUMBER 15** **OCTOBER 2006-15(I)**

Spin relaxation rates in quasi-one-dimensional coupled quantum dots *(5 pages)* 155433
C. L. Romano, P. I. Tamborenea, and S. E. Ulloa

Analytic approach to the linear susceptibility of zigzag carbon nanotubes *(7 pages)* 155434
Abbas Zarifi and Thomas Garm Pedersen

Controlling the interaction between localized and delocalized surface plasmon modes: Experiment and numerical calculations *(8 pages)* 155435
A. Christ, T. Zentgraf, S. G. Tikhodeev, N. A. Gippius, J. Kuhl, and H. Giessen

Quantized conductance in an AlAs two-dimensional electron system quantum point contact *(8 pages)* 155436
O. Gunawan, B. Habib, E. P. De Poortere, and M. Shayegan

Effects of surface defects on surface stress of Cu(001) and Cu(111) *(8 pages)* 155437
Chun-Wei Pao, David J. Srolovitz, and Carl V. Thompson

Characterization of antiphase boundary network in Fe_3O_4(111) epitaxial thin films: Effect on anomalous magnetic behavior *(11 pages)* 155438
A. M. Bataille, L. Ponson, S. Gota, L. Barbier, D. Bonamy, M. Gautier-Soyer, C. Gatel, and E. Snoeck

Energetics of CO on stepped and kinked Cu surfaces: A comparative theoretical study *(9 pages)* 155439
Faisal Mehmood, Abdelkader Kara, Talat S. Rahman, and Klaus Peter Bohnen

High-resolution x-ray diffraction study of MnO nanostructured within a MCM-48 silica matrix with a gyroidal system of channels *(5 pages)* 155440
I. V. Golosovsky, I. Mirebeau, F. Fauth, M. Mazaj, D. A. Kurdyukov, and Yu. A. Kumzerov

Molecular dynamics simulation study of the melting and structural evolution of bimetallic Pd-Pt nanowires *(12 pages)* 155441
Subramanian K. R. S. Sankaranarayanan, Venkat R. Bhethanabotla, and Babu Joseph

Linear augmented cylindrical wave method for calculating the electronic structure of double-wall carbon nanotubes *(13 pages)* 155442
P. N. D'yachkov and D. V. Makaev

Quantum mechanical study of resonant scattering in a nuclear Λ scheme *(17 pages)* 155443
S. Gheysen and J. Odeurs

ERRATA

Publisher's Note: Light-induced hyperfine ^{69}Ga shifts in semi-insulating GaAs observed by optically polarized NMR [Phys. Rev. B **74**, 153201 (2006)] *(1 page)* . . . . . 159901(E)
Kannan Ramaswamy, Stacy Mui, and Sophia E. Hayes