

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 67, NUMBER 15

CONTENTS

APRIL 2003-15(I)

BRIEF REPORTS

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

- Theory of electric-field-induced metal-insulator transition in doped manganites (*4 pages*) 153101
R. Y. Gu, Z. D. Wang, and C. S. Ting
- Dynamic localization of two electrons in a one-dimensional lattice system driven by an oscillating electric field (*4 pages*) 153102
Ken-ichi Noba
- Equivalence of the Falicov-Kimball and Brandt-Mielsch forms for the free energy of the infinite-dimensional Falicov-Kimball model (*3 pages*) 153103
A. M. Shvaika and J. K. Freericks
- High-magnetic-field-induced insulating phase in an organic conductor (*4 pages*) 153104
J. S. Brooks, D. Graf, E. S. Choi, L. Balicas, K. Storr, C. H. Mielke, and G. C. Papavassiliou
- Stability and electronic properties of carbon phosphide compounds with 1:1 stoichiometry (*4 pages*) 153105
Jin-Cheng Zheng, Michael C. Payne, Yuan Ping Feng, and Adele Tzu-Lin Lim
- Correlated metals and the LDA+*U* method (*4 pages*) 153106
A. G. Petukhov, I. I. Mazin, L. Chioncel, and A. I. Lichtenstein
- Effects of electron-phonon coupling on the metal-insulator transition in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ superconductors (*4 pages*) 153107
Changjin Zhang and Yuheng Zhang
- Spin fluctuations in the quarter-filled Hubbard ring: Significances to LiV_2O_4 (*4 pages*) 153108
J. D. Lee
- Focusing of electromagnetic waves by periodic arrays of dielectric cylinders (*4 pages*) 153109
Bikash C. Gupta and Zhen Ye

Semiconductors I: bulk

- Coherent suppression of plasmon-phonon oscillations in a semiconductor using two ultrashort optical pulses (*4 pages*) 153201
M. I. Bakunov, A. V. Maslov, and S. N. Zhukov
- Isotherms for the liquid-gas phase transition in silicon from NPT Monte Carlo simulations (*4 pages*) 153202
D. V. Makhov and Laurent J. Lewis
- Lattice constant in diluted magnetic semiconductors (Ga,Mn)As (*4 pages*) 153203
J. Mašek, J. Kudrnovský, and F. Máca

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

- Symmetry of $\text{GaAs}_{1-x}\text{N}_x$ conduction-band minimum probed by resonant Raman scattering (*4 pages*) 153301
M. J. Seong, H. M. Cheong, S. Yoon, J. F. Geisz, and A. Mascarenhas



Polarization dynamics in self-assembled CdSe/ZnSe quantum dots: The role of excess energy (4 pages)	153302
M. Scheibner, G. Bacher, S. Weber, A. Forchel, Th. Passow, and D. Hommel	
Field-effect persistent photoconductivity in AlAs and GaAs quantum wells with $\text{Al}_x\text{Ga}_{1-x}\text{As}$ barriers (4 pages)	153303
E. P. De Poortere, Y. P. Shkolnikov, and M. Shayegan	
Shot noise in nanoscale conductors from first principles (4 pages)	153304
Yu-Chang Chen and Massimiliano Di Ventra	
Spatially resolved spectra in semiconductor quantum structures: Spatially averaged spectra compared to far-field spectra (4 pages)	153305
G. Pistone, S. Savasta, O. Di Stefano, and R. Girlanda	
Magnetotransport properties of a polarization-doped three-dimensional electron slab in graded AlGaIn (4 pages)	153306
Debdeep Jena, Sten Heikman, James S. Speck, Arthur Gossard, Umesh K. Mishra, Angela Link, and Oliver Ambacher	
Model for C defect on Si(100): The dissociative adsorption of a single water molecule on two adjacent dimers (4 pages)	153307
M. Z. Hossain, Y. Yamashita, K. Mukai, and J. Yoshinobu	

Surface physics, low-dimensional systems, and related topics

Site exchange in ultrathin layers of Ni on Cu(100) studied with element-specific layer-by-layer resolution (4 pages)	153401
T. C. Q. Noakes, P. Bailey, and G. van der Laan	
STM-induced photon emission at the solid-liquid interface (4 pages)	153402
Karen Perronet and Fabrice Charra	
Electronic states of epitaxial thin films of $\text{La}_{0.9}\text{Sn}_{0.1}\text{MnO}_3$ and $\text{La}_{0.9}\text{Ca}_{0.1}\text{MnO}_3$ (4 pages)	153403
J. Gao, S. Y. Dai, and T. K. Li	
Measurement of the elastic modulus of nanostructured gold and platinum thin films (4 pages)	153404
M. C. Salvadori, I. G. Brown, A. R. Vaz, L. L. Melo, and M. Cattani	
Heteroepitaxial growth of Co on W(110) investigated by scanning tunneling microscopy (4 pages)	153405
M. Pratzer, H. J. Elmers, and M. Getzlaff	
Ordered versus disordered growth of copper quantum wires on Mo and W vicinal surfaces (4 pages)	153406
Mario Mura, Paolo Ruggerone, and Vincenzo Fiorentini	

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

Fast method for force computations in electronic structure calculations (6 pages)	155101
Nicholas Choly and Efthimios Kaxiras	
Nonresonant inelastic light scattering in the Hubbard model (8 pages)	155102
J. K. Freericks, T. P. Devereaux, R. Bulla, and Th. Pruschke	
Localized U 5f electrons in UPd_3 from LDA+U calculations (10 pages)	155103
A. N. Yaresko, V. N. Antonov, and P. Fulde	
Decoherence and relaxation of a quantum bit in the presence of Rabi oscillations (7 pages)	155104
Anatoly Yu. Smirnov	
Half-metallic electronic structure of CrO_2 in resonant scattering (4 pages)	155105
E. Z. Kurmaev, A. Moewes, S. M. Butorin, M. I. Katsnelson, L. D. Finkelstein, J. Nordgren, and P. M. Tedrow	
Scaling of the conductance distribution near the Anderson transition (5 pages)	155106
Keith Slevin, Peter Markoš, and Tomi Ohtsuki	

Auger effect in high-resolution Ce 3 <i>d</i> -edge resonant photoemission (6 pages)	155107
E.-J. Cho, R.-J. Jung, B.-H. Choi, S.-J. Oh, T. Iwasaki, A. Sekiyama, S. Imada, S. Suga, T. Muro, J.-G. Park, and Y. S. Kwon	
Variationally optimized atomic orbitals for large-scale electronic structures (5 pages)	155108
T. Ozaki	
Nonuniversal properties of the single-particle density of states of a one-dimensional system with electron- phonon interactions (6 pages)	155109
Emiliano Papa	
Lifetime broadening in Compton scattering (6 pages)	155110
Friedhelm Bell	
Multiplet splitting of core-electron binding energies in chromium compounds (5 pages)	155111
I. Pollini	
Metal-insulator crossover behavior at the surface of NiS ₂ (5 pages)	155112
D. D. Sarma, S. R. Krishnakumar, E. Weschke, C. Schüßler-Langeheine, Chandan Mazumdar, L. Kilian, G. Kaindl, K. Mamiya, S.-I. Fujimori, A. Fujimori, and T. Miyadai	
Influence of Coulomb and phonon interaction on the exciton formation dynamics in semiconductor heterostructures (17 pages)	155113
Walter Hoyer, Mackillo Kira, and Stephan W. Koch	
Local density of states in three-dimensional photonic crystals: Calculation and enhancement effects (7 pages)	155114
Rongzhou Wang, Xue-Hua Wang, Ben-Yuan Gu, and Guo-Zhen Yang	

Semiconductors I: bulk

Temperature-dependent magnetization in diluted magnetic semiconductors (16 pages)	155201
S. Das Sarma, E. H. Hwang, and A. Kaminski	
Disorder and ferromagnetism in diluted magnetic semiconductors (6 pages)	155202
S.-R. Eric Yang and A. H. MacDonald	
Correlation between the antisite pair and the <i>D</i> ₁ center in SiC (5 pages)	155203
A. Gali, P. Deák, E. Rauls, N. T. Son, I. G. Ivanov, F. H. C. Carlsson, E. Janzén, and W. J. Choyke	
Stacking faults in 3 <i>C</i> -, 4 <i>H</i> -, and 6 <i>H</i> -SiC polytypes investigated by an <i>ab initio</i> supercell method (12 pages)	155204
Ulf Lindefelt, Hisaomi Iwata, Sven Öberg, and Patrick R. Briddon	
Anisotropy and large magnetoresistance in the narrow-gap semiconductor FeSb ₂ (4 pages)	155205
C. Petrovic, J. W. Kim, S. L. Bud'ko, A. I. Goldman, P. C. Canfield, W. Choe, and G. J. Miller	
Inversionless amplification of coherent terahertz radiation (4 pages)	155206
C. Janke, P. Haring Bolivar, A. Bartels, H. Kurz, and H. Künzel	
Pairing and hyperfine interactions of Cd-P complexes in silicon (7 pages)	155207
R. A. Casali and M. A. Caravaca	
Implementation of an all-electron GW approximation based on the projector augmented wave method without plasmon pole approximation: Application to Si, SiC, AlAs, InAs, NaH, and KH (10 pages)	155208
S. Lebègue, B. Arnaud, M. Alouani, and P. E. Bloechl	
Diffusion-limited recombination in polymer-fullerene blends and its influence on photocurrent collection (10 pages)	155209
Jenny Nelson	
Acceptor identification using magnetophotoluminescence of bound exciton states in InSb (14 pages)	155210
J. A. H. Stotz and M. L. W. Thewalt	

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

Fano resonance in electronic transport through a quantum wire with a side-coupled quantum dot: <i>X</i> -boson treatment (6 pages)	155301
R. Franco, M. S. Figueira, and E. V. Anda	
Amplification of a terahertz field in a semiconductor superlattice via phase-locked <i>k</i> -space bunches of Bloch oscillating electrons (4 pages)	155302
E. Schomburg, N. V. Demarina, and K. F. Renk	
Adiabatic spin pumping through a quantum dot with a single orbital level (4 pages)	155303
Tomosuke Aono	
Tunneling spectroscopy of spin-split states in quantum wells (8 pages)	155304
O. E. Raichev and P. Debray	
Collapse of odd-integer Hall gaps in double quantum wells due to edge effects (9 pages)	155305
O. G. Balev and Nelson Studart	
Interpretation of infrared and Raman spectra of amorphous carbon nitrides (20 pages)	155306
A. C. Ferrari, S. E. Rodil, and J. Robertson	
Experimental test of the planar tunneling model for ballistic electron emission spectroscopy (4 pages)	155307
Ian Appelbaum, Rahul Sheth, Ilan Shalish, K. J. Russell, and V. Narayanamurti	
Ultrafast carrier relaxation in GaN, $\text{In}_{0.05}\text{Ga}_{0.95}\text{N}$, and an $\text{In}_{0.07}\text{Ga}_{0.93}\text{N}/\text{In}_{0.12}\text{Ga}_{0.88}\text{N}$ multiple quantum well (9 pages)	155308
Ümit Özgür and Henry O. Everitt	
Electron spin relaxation in a semiconductor quantum well (9 pages)	155309
Vadim I. Puller, Lev G. Mourokh, Norman J. M. Horing, and Anatoly Yu. Smirnov	
Electron kinetics in isolated mesoscopic rings driven out of equilibrium (11 pages)	155310
V. I. Yudson and V. E. Kravtsov	
Chiral spin currents and quantum Hall effect in nanotubes (5 pages)	155311
Alex Kleiner	
Effect of the surface on the electron quantum size levels and electron <i>g</i> factor in spherical semiconductor nanocrystals (11 pages)	155312
A. V. Rodina, Al. L. Efros, and A. Yu. Alekseev	
Quantum Hall ferromagnet in a parabolic well (8 pages)	155313
G. M. Gusev, A. A. Quivy, T. E. Lamas, J. R. Leite, O. Estibals, and J. C. Portal	
Three-dimensional structures for enhanced transmission through a metallic film: Annular aperture arrays (7 pages)	155314
F. I. Baida and D. Van Labeke	
Trial state for a two-dimensional hexatic (6 pages)	155315
Anthony J. Schmidt, Orion Ciftja, and Carlos Wexler	
Adsorption and desorption of deuterium on partially oxidized Si(100) surfaces (8 pages)	155316
H. Tsurumaki, K. Iwamura, T. Karato, S. Inanaga, and A. Namiki	
Adiabatic control of the electron phase in a quantum dot (14 pages)	155317
D. Giuliano, P. Sodano, and A. Tagliacozzo	
Bethe-Salpeter equation for quantum-well exciton states in an inhomogeneous magnetic field (7 pages)	155318
Z. G. Koinov, P. Nash, and J. Witzel	
Effects of nonequilibrium electron distribution and electron-electron interaction observed in spin-split cyclotron resonance of InAs/AlSb single quantum wells at high magnetic fields (9 pages)	155319
H. Arimoto, N. Miura, and R. A. Stradling	
Multiband electron resonant Raman scattering in quantum wells in a magnetic field (10 pages)	155320
V. López-Richard, G.-Q. Hai, C. Trallero-Giner, and G. E. Marques	
Implementing the Keldysh formalism into <i>ab initio</i> methods for the calculation of quantum transport: Application to metallic nanocontacts (5 pages)	155321
E. Louis, J. A. Vergés, J. J. Palacios, A. J. Pérez-Jiménez, and E. SanFabián	

Electromagnetic characteristics of bilayer quantum Hall systems in the presence of interlayer coherence and tunneling (9 pages)	155322
K. Shizuya	
Unified algebraic approach to few- and many-body correlated systems (10 pages)	155323
N. Gurappa and Prasanta K. Panigrahi	
<i>Ab initio</i> valence band offsets between Si(100) and SiO ₂ from microscopic models (10 pages)	155324
B. R. Tuttle	
Photoemission investigation of the alkali-metal-induced two-dimensional electron gas at the Si(111)(1×1):H surface (7 pages)	155325
Roberto Biagi, Paolo Fantini, Valentina De Renzi, Maria Grazia Betti, Carlo Mariani, and Umberto del Pennino	
Simulation of ellipsometric spectra from nanocrystalline silicon floating gate structures (7 pages)	155326
Kyung Hoon Jun, Seung Jae Baik, Koeng Su Lim, Ho Seong Lee, and Jeong Yong Lee	
First-principles calculation of the band offset at BaO/BaTiO ₃ and SrO/SrTiO ₃ interfaces (12 pages)	155327
Javier Junquera, Magali Zimmer, Pablo Ordejón, and Philippe Ghosez	
Thermopower of a double quantum well based on GaAs (11 pages)	155328
T. Smith, M. Tsaousidou, R. Fletcher, P. T. Coleridge, Z. R. Wasilewski, and Y. Feng	
Magnetization measurements of high-mobility two-dimensional electron gases (6 pages)	155329
M. Zhu, A. Usher, A. J. Matthews, A. Potts, M. Elliott, W. G. Herrenden-Harker, D. A. Ritchie, and M. Y. Simmons	

Surface physics, low-dimensional systems, and related topics

Influence of strain in Ag on Al(111) and Al on Ag(100) thin film growth (6 pages)	155401
V. Fournée, J. Ledieu, T. Cai, and P. A. Thiel	
Qubits with electrons on liquid helium (15 pages)	155402
M. I. Dykman, P. M. Platzman, and P. Seddighrad	
Capture numbers in rate equations and scaling laws for epitaxial growth (4 pages)	155403
Frédéric Gibou, Christian Ratsch, and Russel Caflisch	
Raman scattering in C ₆₀ and C ₄₈ N ₁₂ aza-fullerene: First-principles study (9 pages)	155404
Rui-Hua Xie, Garnett W. Bryant, and Vedene H. Smith, Jr.	
Electronic structures of lead iodide based low-dimensional crystals (6 pages)	155405
T. Umebayashi, K. Asai, T. Kondo, and A. Nakao	
Collective diffusion in a twin-spin model of O/W(110) (7 pages)	155406
Magdalena A. Załuska-Kotur, Stanisław Krukowski, and Łukasz A. Turski	
Dynamic light scattering from acoustic modes in single-walled carbon nanotubes (6 pages)	155407
C.E. Bottani, A. Li Bassi, M.G. Beghi, A. Podestà, P. Milani, A. Zakhidov, R. Baughman, D.A. Walters, and R.E. Smalley	
Relevance of the electron energy-loss spectroscopy for <i>in situ</i> studies of the growth mechanism of copper phthalocyanine molecules on metal surfaces: Al(100) (7 pages)	155408
A. Ruocco, M. P. Donzello, F. Evangelista, and G. Stefani	
Size and composition dependence in the optical properties of mixed (transition metal/noble metal) embedded clusters (10 pages)	155409
M. Gaudry, E. Cottancin, M. Pellarin, J. Lermé, L. Arnaud, J. R. Huntzinger, J. L. Vialle, M. Broyer, J. L. Rousset, M. Treilleux, and P. Mélinon	
Polaron in a one-dimensional C ₆₀ crystal (8 pages)	155410
V. R. Belosludov, T. M. Inerbaev, R. V. Belosludov, and Y. Kawazoe	
Vicinal interface sensitive magneto-optical Kerr effect: Application to Co/Au(322) (7 pages)	155411
J. Hamrle, J. Ferré, J. P. Jamet, V. Repain, G. Baudot, and S. Rousset	

Scattering angle dependence of the surface excitation probability in reflection electron energy loss spectra (9 pages)	155412
Wolfgang S. M. Werner, Christoph Eisenmenger-Sittner, Josef Zemek, and Petr Jiricek	
Defects and external field effects on the electronic properties of a carbon nanotube torus (7 pages)	155413
A. Latgé, C. G. Rocha, L. A. L. Wanderley, M. Pacheco, P. Orellana, and Z. Barticevic	
Electronic and nuclear thermal spike effects in sputtering of metals with energetic heavy ions (12 pages)	155414
H. D. Mieskes, W. Assmann, F. Grüner, H. Kucal, Z. G. Wang, and M. Toulemonde	
Modulations of valence-band photoemission spectrum from C ₆₀ monolayers on Ag(111) (6 pages)	155415
C. Ton-That, A. G. Shard, S. Egger, V. R. Dhanak, and M. E. Welland	
Interaction of CO, O, and S with metal nanoparticles on Au(111): A theoretical study (10 pages)	155416
Ping Liu, José A. Rodriguez, James T. Muckerman, and Jan Hrbek	
Nanoscale strain distribution at the Ag/Ru(0001) interface (8 pages)	155417
H. Zajonz, Doon Gibbs, A. P. Baddorf, and D. M. Zehner	
Phonons in a nanoparticle mechanically coupled to a substrate (10 pages)	155418
Kelly R. Patton and Michael R. Geller	
Localized helium excitations in ⁴ He _N -benzene clusters (14 pages)	155419
Patrick Huang and K. Birgitta Whaley	
Monte Carlo simulations of surface phase transitions in a modulated layered structure (7 pages)	155420
Da Gao and John A. Jaszczak	
First-principles calculations of Fe on GaAs(100) (9 pages)	155421
S. Mirbt, B. Sanyal, C. Isheden, and B. Johansson	
Ni-induced giant stress and surface relaxation in W(110) (4 pages)	155422
H. L. Meyerheim, D. Sander, R. Popescu, J. Kirschner, O. Robach, S. Ferrer, and P. Steadman	

ERRATA

Erratum: Dynamic correlations of the spinless Coulomb Luttinger liquid [Phys. Rev. B 65 , 125109 (2002)] (1 page)	159901(E)
Yasha Gindikin and V. A. Sablikov	
Erratum: Magnetic-field-induced transformations of Wigner-molecule symmetry in quantum dots [Phys. Rev. B 67 , 045311 (2003)] (1 page)	159902(E)
B. Szafran, S. Bednarek, and J. Adamowski	

Cumulative Author Index	i
-------------------------------	---