

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 68, NUMBER 24

CONTENTS

DECEMBER 2003-15(II)

RAPID COMMUNICATIONS

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

- Geometry and electronic structure of α -Pu: A theoretical study (4 pages) 241101(R)
Babak Sadigh, Per Söderlind, and Wilhelm G. Wolfer
- Magnetothermopower and Nernst effect in unconventional charge density waves (4 pages) 241102(R)
Balázs Dóra, Kazumi Maki, András Ványolos, and Attila Virosztek

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

- Luttinger liquid in a finite one-dimensional wire with box-like boundary conditions (4 pages) 241301(R)
Fabrizio Anfuso and Sebastian Eggert
- Microscopic theory of the reentrant integer quantum Hall effect in the first and second excited Landau levels (4 pages) 241302(R)
M. O. Goerbig, P. Lederer, and C. Morais Smith
- Hysteretic dynamic nuclear polarization in GaAs/Al_xGa_{1-x}As (110) quantum wells (4 pages) 241303(R)
H. Sanada, S. Matsuzaka, K. Morita, C. Y. Hu, Y. Ohno, and H. Ohno
- Generalized drift-diffusion model for miniband superlattices (4 pages) 241304(R)
L. L. Bonilla, R. Escobedo, and Álvaro Perales
- Parallel magnetic-field-induced conductance fluctuations in one- and two-subband ballistic quantum dots (4 pages) 241305(R)
C. Gustin, S. Faniel, B. Hackens, S. Melinte, M. Shayegan, and V. Bayot
- Reflection phase of scattering electrons in a single-channel atomic wire (4 pages) 241306(R)
H. Q. Xu, I. C. Fasth, D. Csontos, L. B. Zhang, and Y. Zhao
- Ultrafast polarization dynamics in biased quantum wells under strong femtosecond optical excitation (4 pages) 241307(R)
D. Turchinovich, P. Uhd Jepsen, B. S. Monozon, M. Koch, S. Lahmann, U. Rossow, and A. Hangleiter
- Linear temperature dependence of conductivity in the apparent insulating regime of dilute two-dimensional holes in GaAs (4 pages) 241308(R)
Hwayong Noh, M. P. Lilly, D. C. Tsui, J. A. Simmons, L. N. Pfeiffer, and K. W. West
- Quantum magneto-oscillations in a two-dimensional Fermi liquid (4 pages) 241309(R)
Gregory W. Martin, Dmitrii L. Maslov, and Michael Yu. Reizer
- Inelastic scattering approach to the theory of a magnetic tunnel transistor source (4 pages) 241310(R)
Emmanuel I. Rashba
- Scaling approach to electron-electron interactions in a chaotic quantum dot (4 pages) 241311(R)
Shaffique Adam, Piet W. Brouwer, and Prashant Sharma



Raman spectroscopy of silicon nanowires (<i>4 pages</i>)	241312(R)
S. Piscanec, M. Cantoro, A. C. Ferrari, J. A. Zapien, Y. Lifshitz, S. T. Lee, S. Hofmann, and J. Robertson	
Si(111)-(7×7) surface probed by reflection high-energy positron diffraction (<i>4 pages</i>)	241313(R)
A. Kawasuso, Y. Fukaya, K. Hayashi, M. Maekawa, S. Okada, and A. Ichimiya	
Structural investigation of the ZnSe(001)-c(2×2) surface (<i>4 pages</i>)	241314(R)
W. Weigand, A. Müller, L. Kilian, T. Schallenberg, P. Bach, G. Schmidt, L. W. Molenkamp, O. Bunk, R. L. Johnson, C. Kumpf, and E. Umbach	
Spin currents in thermodynamic equilibrium: The challenge of discerning transport currents (<i>3 pages</i>)	241315(R)
Emmanuel I. Rashba	

Surface physics, low-dimensional systems, and related topics

Shapes of cagelike metal carbide clusters: First-principles calculations (<i>4 pages</i>)	241401(R)
G. K. Gueorguiev and J. M. Pacheco	
Oxygen vacancy mediated adsorption and reactions of molecular oxygen on the TiO ₂ (110) surface (<i>4 pages</i>)	241402(R)
Xueyuan Wu, Annabella Selloni, Michele Lazzeri, and Saroj K. Nayak	
Coalescence of nanoscale metal clusters: Molecular-dynamics study (<i>4 pages</i>)	241403(R)
S. Hendy, S. A. Brown, and M. Hyslop	
Electronic structure and rebonding in the onionlike As@Ni ₁₂ @As ₂₀ cluster (<i>4 pages</i>)	241404(R)
Tunna Baruah, Rajendra R. Zope, Steven L. Richardson, and Mark R. Pederson	
Microscopic theory for nanotube piezoelectricity (<i>3 pages</i>)	241405(R)
Na Sai and E. J. Mele	
Diameter dependent wall deformations during the compression of a carbon nanotube bundle (<i>4 pages</i>)	241406(R)
U. D. Venkateswaran, D. L. Masica, G. U. Sumanasekera, C. A. Furtado, U. J. Kim, and P. C. Eklund	

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

Existence of broad acoustic bandgaps in three-component composite (<i>6 pages</i>)	245101
Shu Zhang and Jianchun Cheng	
Unscreened Hartree-Fock calculations for metallic Fe, Co, Ni, and Cu from <i>ab initio</i> Hamiltonians (<i>11 pages</i>)	245102
I. Schnell, G. Czycholl, and R. C. Albers	
Semiclassical action based on dynamical mean-field theory describing electrons interacting with local lattice fluctuations (<i>9 pages</i>)	245103
Stefan Blawid and Gertrud Zwicknagl	
Tight-binding theory of Faraday rotation in graphite (<i>6 pages</i>)	245104
Thomas G. Pedersen	
Theory of time-domain measurement of spin-dependent recombination with pulsed electrically detected magnetic resonance (<i>19 pages</i>)	245105
Christoph Boehme and Klaus Lips	
Applicability of the localization-interaction model to magnetoconductivity studies of polyaniline films at the metal-insulator boundary (<i>11 pages</i>)	245106
G. Tzamalís, N. A. Zaidi, and A. P. Monkman	
Water molecule by the self-consistent atomic deformation method (<i>7 pages</i>)	245107
M. M. Ossowski, L. L. Boyer, M. J. Mehl, and M. R. Pederson	
Dielectric properties and dynamical conductivity of LaTiO ₃ : From dc to optical frequencies (<i>11 pages</i>)	245108
P. Lunkenheimer, T. Rudolf, J. Hemberger, A. Pimenov, S. Tachos, F. Lichtenberg, and A. Loidl	

Signatures of an electronic nematic phase at the isotropic-nematic phase transition (5 pages)	245109
Hae-Young Kee, Eugene H. Kim, and Chung-Hou Chung	
Evaluation of lensing in photonic crystal slabs exhibiting negative refraction (7 pages)	245110
Zhi-Yuan Li and Lan-Lan Lin	
Scaling properties of the projected SO(5) model in three dimensions (6 pages)	245111
M. Jöstingmeier, A. Dorneich, E. Arrigoni, W. Hanke, and Shou-Cheng Zhang	
Green function approach for the <i>ab initio</i> calculation of the optical and magneto-optical properties of solids: Accounting for dynamical many-body effects (5 pages)	245112
A. Perlov, S. Chadov, and H. Ebert	
Electronic and optical properties of the 1T phases of TiS ₂ , TiSe ₂ , and TiTe ₂ (7 pages)	245113
Ali Hussain Reshak and S. Auluck	
Determination of pressure-induced valence changes in YbAl ₂ by resonant inelastic x-ray emission (11 pages)	245114
C. Dallera, E. Annese, J.-P. Rueff, A. Palenzona, G. Vankó, L. Braicovich, A. Shukla, and M. Grioni	
Strain-tunable optical valves at T-junction waveguides in photonic crystals (6 pages)	245115
Natalia Malkova and Venkatraman Gopalan	
On-site interaction effects on localization: Dominance of nonuniversal contributions (7 pages)	245116
Moshe Goldstein and Richard Berkovits	
Application of structural symmetries in the plane-wave-based transfer-matrix method for three-dimensional photonic crystal waveguides (20 pages)	245117
Zhi-Yuan Li and Kai-Ming Ho	
Fermi surface of UGe ₂ in the paramagnetic phase (6 pages)	245118
M. Biasini and R. Troc	
Transport properties of Kondo-insulator alloys (8 pages)	245119
L. Peche, E. V. Anda, and C. A. Büsser	
Alternative separation of exchange and correlation in density-functional theory (5 pages)	245120
R. Armiento and A. E. Mattsson	
Dynamical properties of a strongly correlated model for quarter-filled layered organic molecular crystals (15 pages)	245121
Jaime Merino, Andrés Greco, Ross H. McKenzie, and Matteo Calandra	

Semiconductors I: bulk

Atomistic simulations of the effect of Coulombic interactions on carrier fluctuations in doped silicon (5 pages)	245201
Zudian Qin and Scott T. Dunham	
Near band edge recombination mechanisms in GaTe (6 pages)	245202
A. Zubiaga, J. A. García, F. Plazaola, V. Muñoz-Sanjósé, and C. Martínez-Tomás	
Geminate pair recombination in molecular systems with correlated disorder (7 pages)	245203
Darius Abramavicius and Leonas Valkunas	
Charge dynamics of muonium centers in Si revealed by photoinduced muon spin relaxation (17 pages)	245204
R. Kadono, R. M. Macrae, and K. Nagamine	
Spin relaxation in <i>n</i> -doped GaAs due to impurity and electron-electron Elliot-Yafet scattering (5 pages)	245205
P. I. Tamborenea, M. A. Kuroda, and F. L. Bottesi	
Predicted absence of ferromagnetism in manganese-doped diamond (5 pages)	245206
Steven C. Erwin and C. Stephen Hellberg	

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

Two-dimensional electron-hole capture in a disordered hopping system (7 pages)	245301
N. C. Greenham and P. A. Bobbert	

Multiexcitons confined within a subexcitonic volume: Spectroscopic and dynamical signatures of neutral and charged biexcitons in ultrasmall semiconductor nanocrystals (5 pages)	245302
M. Achermann, J. A. Hollingsworth, and V. I. Klimov	
Cyclotron resonance of an interacting polaron gas in a quantum well: Magnetoplasmon-phonon mixing (8 pages)	245303
S. N. Klimin and J. T. Devreese	
Single scatterings in single artificial atoms: Quantum coherence and entanglement (12 pages)	245304
Ulrich Hohenester, Claudia Sifel, and Pekka Koskinen	
Fano resonances in the overlapping regime (6 pages)	245305
A. I. Magunov, I. Rotter, and S. I. Strakhova	
Spin-dependent transport through $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ diluted magnetic semiconductor quantum dots (5 pages)	245306
Shu-Shen Li, Kai Chang, Jian-Bai Xia, and Kenji Hirose	
Positron-annihilation-induced Auger electron spectroscopy studies of the (100) and (111) surfaces of silicon (6 pages)	245307
N. G. Fazleev, J. Kim, J. L. Fry, and A. H. Weiss	
Raman scattering in large single indium nitride dots: Correlation between morphology and strain (5 pages)	245308
F. Demangeot, J. Frandon, C. Pinquier, M. Caumont, O. Briot, B. Maleyre, S. Clur-Ruffenach, and B. Gil	
Effective masses of two-dimensional electron gases around cubic inclusions in hexagonal silicon carbide (7 pages)	245309
H. P. Iwata, U. Lindefelt, S. Öberg, and P. R. Briddon	
Quantized acoustoelectric current transport through a static quantum dot using a surface acoustic wave (9 pages)	245310
N. E. Fletcher, J. Ebbecke, T. J. B. M. Janssen, F. J. Ahlers, M. Pepper, H. E. Beere, and D. A. Ritchie	
Coherence and Coulomb blockade in single-electron devices: A unified treatment of interaction effects (12 pages)	245311
S. Florens, P. San José, F. Guinea, and A. Georges	
Surface electronic structures of Ca-induced reconstructions on Si(111) (6 pages)	245312
Y. K. Kim, J. W. Kim, H. S. Lee, Y. J. Kim, and H. W. Yeom	
Ballistic electron motion in a random magnetic field (10 pages)	245313
K. B. Efetov and V. R. Kogan	
Contrasting structural and bonding properties of trimethylamine and dimethylamine adsorbed on Si(001) (6 pages)	245314
Jun-Hyung Cho and Leonard Kleinman	
Induced nonequilibrium currents in the magnetization of mesoscopic dots in the quantum Hall regime (5 pages)	245315
M. P. Schwarz, D. Grundler, Ch. Heyn, D. Heitmann, D. Reuter, and A. Wieck	
Band structure of the $\text{Ca/Si(111)-(2\times 1)}$ surface (5 pages)	245316
Kazuyuki Sakamoto, H. M. Zhang, and R. I. G. Uhrberg	
Quasistates and their relation to the Dicke effect in a mesoscopic ring coupled to a reservoir (9 pages)	245317
Bernhard Wunsch and Alexander Chudnovskiy	
Interplay between quantum confinement and electron-electron interaction in deformed silicon quantum wires (10 pages)	245318
G. Parascandolo, G. Cantele, D. Ninno, and G. Iadonisi	
Optical investigation of electrical spin injection into semiconductors (13 pages)	245319
V. F. Motsnyi, P. Van Dorpe, W. Van Roy, E. Goovaerts, V. I. Safarov, G. Borghs, and J. De Boeck	
Vacuum-field Rabi splitting in quantum-well infrared photodetectors (9 pages)	245320
E. Dupont, H. C. Liu, A. J. SpringThorpe, W. Lai, and M. Extavour	

Emergence of quasimetallic state in a disordered two-dimensional electron gas due to strong interactions (18 pages)	245321
B. Rosenstein and Tran Minh-Tien	
Rashba effect in two-dimensional mesoscopic systems with transverse magnetic field (11 pages)	245322
S. Bellucci and P. Onorato	
Kondo resonance in a quantum dot molecule (5 pages)	245323
A.D. Güçlü, Qing Feng Sun, and Hong Guo	
Surface physics, low-dimensional systems, and related topics	
Effects of three-dimensional atomic forces in topographical imaging of atoms with an atom force microscope (9 pages)	245401
Wei Li Wang, S. Jack Hu, and Roy Clarke	
Structure and energetics of clean and hydrogenated Ni surfaces and symmetrical tilt grain boundaries using the embedded-atom method (8 pages)	245402
Motoyuki Shiga, Masatake Yamaguchi, and Hideo Kaburaki	
Phonons and specific heat of neon and methane on the surface of a nanotube bundle (12 pages)	245403
Milen K. Kostov, M. Mercedes Calbi, and Milton W. Cole	
Simulations of denuded-zone formation during growth on surfaces with anisotropic diffusion (10 pages)	245404
C. Ebner, K.-B. Park, J.-F. Nielsen, and J. P. Pelz	
Definition and measurement of the local density of electromagnetic states close to an interface (10 pages)	245405
Karl Joulain, Rémi Carminati, Jean-Philippe Mulet, and Jean-Jacques Greffet	
Phonon transport in nanowires coated with an amorphous material: An atomistic Green's function approach (12 pages)	245406
N. Mingo and Liu Yang	
Relativistic effects in EELS of nanoporous alumina membranes (13 pages)	245407
N. Zabala, A. G. Pattantyus-Abraham, A. Rivacoba, F. J. García de Abajo, and M. O. Wolf	
Thermal expansion of the Ag(110) surface studied by low-energy electron diffraction and density-functional theory (8 pages)	245408
V. B. Nascimento, E. A. Soares, V. E. de Carvalho, E. L. Lopes, R. Paniago, and C. M. C. de Castilho	
Competing stabilization mechanism for the polar ZnO(0001)-Zn surface (15 pages)	245409
Georg Kresse, Olga Dulub, and Ulrike Diebold	
From erosion to bombardment-induced growth on Ir(111) (9 pages)	245410
Ansgar Petersen, Carsten Busse, Celia Polop, Udo Linke, and Thomas Michely	
Enhanced electronic emission by excitation of an interface resonance in metallic bilayer gratings irradiated by short laser pulses (12 pages)	245411
Serena Bastiani-Ceccotti, Patrick Monchicourt, and Thierry Lehner	
Nitrogen adsorption on carbon nanotube bundles: Role of the external surface (9 pages)	245412
Jianwen Jiang and Stanley I. Sandler	
<i>d</i> -band quantum well states in ultrathin silver films on V(100) (8 pages)	245413
M. Kralj, P. Pervan, M. Milun, T. Valla, P. D. Johnson, and D. P. Woodruff	
Aperiodic incommensurate phase of a C ₆₀ monolayer on Ag(100) (12 pages)	245414
Ching-Ling Hsu and Woei Wu Pai	
Electronic excitations and tunneling spectra of metallic nanograins (8 pages)	245415
Gustavo A. Narvaez and George Kirczenow	
Reconstruction of charged surfaces: General trends and a case study of Pt(110) and Au(110) (18 pages)	245416
Alexander Y. Lozovoi and Ali Alavi	
Calculation of surface stress for fcc transition metals (5 pages)	245417
J. Kollár, L. Vitos, J. M. Osorio-Guillén, and R. Ahuja	
Local morphology and correlation lengths of reactive NiO/Cu(111) interfaces (7 pages)	245418
A. Barbier, S. Stanescu, C. Boeglin, and J.-P. Deville	

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 68, NUMBER 24

DECEMBER 2003-15(II)

Ring formation of single-walled carbon nanotubes: Competition between conformation energy and entropy (7 pages)	245419
Shengli Zhang, Shumin Zhao, Minggang Xia, Erhu Zhang, and Tao Xu	
Collective modes of interacting dielectric spheres (8 pages)	245420
Rodrigo Arias and D. L. Mills	
Laser-driven electron transfer through metal-insulator-metal contacts: Time-dependent configuration interaction singles calculations for a jellium model (7 pages)	245421
Tillmann Klamroth	

ERRATA

Erratum: $\text{Nd}^{3+} \rightarrow \text{Yb}^{3+}$ energy transfer in the $\text{YAl}_3(\text{BO}_3)_4$ nonlinear laser crystal [Phys. Rev. B 68 , 035118 (2003)] (1 page)	249901(E)
D. Jaque, M. O. Ramirez, L. E. Bausa, J. García Solé, A. Speghini, M. Bettinelli, and E. Cavalli	
Publisher's Note: <i>Ab initio</i> study of Ti-contacted single-walled carbon nanotube [Phys. Rev. B 68 , 193409 (2003)] (1 page)	249902(E)
Yi Liu, Brian Larade, and Hong Guo	

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