

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 1N01
2 Huntington Quadrangle
Melville, NY 11747-4502

THIRD SERIES, VOLUME 79, NUMBER 4

CONTENTS

JANUARY 2009-15(II)

RAPID COMMUNICATIONS

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

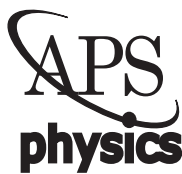
- Directive emission from high- Q photonic crystal cavities through band folding (*4 pages*) 041101(R)
Nguyen-Vi-Quynh Tran, Sylvain Combri , and Alfredo De Rossi
- All-electron Bethe-Salpeter calculations for shallow-core x-ray absorption near-edge structures (*4 pages*) 041102(R)
W. Olovsson, I. Tanaka, T. Mizoguchi, P. Puschnig, and C. Ambrosch-Draxl

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

- Photoluminescence dynamics and reduced Auger recombination in $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ superlattices under high-density photoexcitation (*4 pages*) 041301(R)
Takeshi Tayagaki, Susumu Fukatsu, and Yoshihiko Kanemitsu
- Strong magnetic coupling between an electronic spin qubit and a mechanical resonator (*4 pages*) 041302(R)
P. Rabl, P. Cappellaro, M. V. Gurudev Dutt, L. Jiang, J. R. Maze, and M. D. Lukin
- Giant frictional drag in strongly interacting bilayers near filling factor one (*4 pages*) 041303(R)
E. Tutuc, R. Pillarisetty, and M. Shayegan
- Numerical evidence for non-Abelian quantum liquids in the lowest Landau level (*4 pages*) 041304(R)
Arkadiusz W js
- Density imbalance effect on the Coulomb drag upturn in an undoped electron-hole bilayer (*4 pages*) 041305(R)
Christian P. Morath, John A. Seamons, John L. Reno, and Michael P. Lilly
- Impact of hydrogen on indium incorporation at m -plane and c -plane $\text{In}_{0.25}\text{Ga}_{0.75}\text{N}$ surfaces: First-principles calculations (*4 pages*) 041306(R)
John E. Northrup
- Spin filtering through a single impurity in a GaAs/AlAs/GaAs resonant tunneling device (*4 pages*) 041307(R)
B. Jouault, M. Gryglas, M. Baj, A. Cavanna, U. Gennser, G. Faini, and D. K. Maude
- Renormalization factor and effective mass of the two-dimensional electron gas (*4 pages*) 041308(R)
Markus Holzmann, Bernard Bernu, Valerio Olevano, Richard M. Martin, and David M. Ceperley

Surface physics, nanoscale physics, low-dimensional systems

- High-resolution surface plasmon imaging of gold nanoparticles by energy-filtered transmission electron microscopy (*4 pages*) 041401(R)
Bernhard Schaffer, Ulrich Hohenester, Andreas Tr gler, and Ferdinand Hofer



Copyright 2009 by The American Physical Society



1098-0121(20090115)79:4;1-0

(Continued)

Selected for a Viewpoint in *Physics*. Please visit <http://physics.aps.org/>.

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).

Dominant role of grain boundary scattering in the resistivity of nanometric Cu films (<i>4 pages</i>)	041402(R)
Tik Sun, Bo Yao, Andrew P. Warren, Katayun Barmak, Michael F. Toney, Robert E. Peale, and Kevin R. Coffey	
Thermal photocatalytic generation of H ₂ over CuAlO ₂ nanoparticle catalysts in H ₂ O (<i>4 pages</i>)	041403(R)
John R. Smith, Thomas H. Van Steenkiste, and Xiao-Gang Wang	
Thermoelectric properties of granular metals (<i>4 pages</i>)	041404(R)
Andreas Glatz and I. S. Beloborodov	
Structure of large gold clusters obtained by global optimization using the minima hopping method (<i>4 pages</i>)	041405(R)
Kuo Bao, Stefan Goedecker, Kenji Koga, Frédéric Lançon, and Alexey Neelov	
Hydrogen storage of calcium atoms adsorbed on graphene: First-principles plane wave calculations (<i>4 pages</i>)	041406(R)
C. Ataca, E. Aktürk, and S. Ciraci	

ARTICLES

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

Competition between Jahn-Teller coupling and orbital fluctuations in HoVO ₃ (<i>11 pages</i>)	045101
G. R. Blake, A. A. Nugroho, M. J. Gutmann, and T. T. M. Palstra	
Determination of the single-ion anisotropy energy in a $S=\frac{5}{2}$ kagome antiferromagnet using x-ray absorption spectroscopy (<i>9 pages</i>)	045102
M. A. de Vries, T. K. Johal, A. Mirone, J. S. Claydon, G. J. Nilsen, H. M. Rønnow, G. van der Laan, and A. Harrison	
Dynamics and spectral weights of shake-up valence excitations in transition metal <i>K</i> -edge resonant inelastic x-ray scattering (<i>8 pages</i>)	045103
K. H. Ahn, A. J. Fedro, and Michel van Veenendaal	
 Electron spin resonance in heavy-fermion systems (<i>6 pages</i>)	045104
P. Schlottmann	
Nonequilibrium cotunneling through a three-level quantum dot (<i>11 pages</i>)	045105
S. Schmaus, V. Koerting, J. Paaske, T. S. Jespersen, J. Nygård, and P. Wölfle	
Multicenter-type corrections to standard DFT exchange and correlation functionals (<i>5 pages</i>)	045106
Ivano Tavernelli, I-Chun Lin, and Ursula Rothlisberger	
Spin-orbit coupling in an <i>f</i> -electron tight-binding model: Electronic properties of Th, U, and Pu (<i>7 pages</i>)	045107
M. D. Jones and R. C. Albers	
Half-filled Hubbard model on a Bethe lattice with next-nearest-neighbor hopping (<i>7 pages</i>)	045108
Robert Peters and Thomas Pruschke	
Maximally localized Wannier functions for GW quasiparticles (<i>9 pages</i>)	045109
D. R. Hamann and David Vanderbilt	
Supercurrent and multiple singlet-doublet phase transitions of a quantum dot Josephson junction inside an Aharonov-Bohm ring (<i>9 pages</i>)	045110
C. Karrasch and V. Meden	

(Continued)

Model of isotropic resonant magnetism in the visible range based on core-shell clusters (9 pages)	045111
C. R. Simovski and S. A. Tretyakov	
He ³ bilayers as a simple example of deconfinement (13 pages)	045112
A. Benlagra and C. Pépin	
First-principles study of the connection between structure and electronic properties of gallium (8 pages)	045113
Elena Voloshina, Krzysztof Rosciszewski, and Beate Paulus	
Dipole-active optical phonons in YTiO ₃ : Ellipsometry study and lattice-dynamics calculations (13 pages) . . .	045114
N. N. Kovaleva, A. V. Boris, L. Capogna, J. L. Gavartin, P. Popovich, P. Yordanov, A. Maljuk, A. M. Stoneham, and B. Keimer	
Quasi-one-dimensional Fermi surface of (TMTSF) ₂ NO ₃ (5 pages)	045115
W. Kang and Ok-Hee Chung	
Spontaneous exciton condensation in 1T-TiSe ₂ : BCS-like approach (11 pages)	045116
C. Monney, H. Cercellier, F. Clerc, C. Battaglia, E. F. Schwier, C. Didiot, M. G. Garnier, H. Beck, P. Aebi, H. Berger, L. Forró, and L. Patthey	
☞ Long-wavelength correlations and transport in a marginal Fermi liquid (6 pages)	045117
A. Shekhter and C. M. Varma	
Intrinsic charge transfer gap in NiO from Ni <i>K</i> -edge x-ray absorption spectroscopy (5 pages)	045118
C. Gougousis, M. Calandra, A. Seitsonen, Ch. Brouder, A. Shukla, and F. Mauri	
Relation between nonequilibrium Green's function and Lippmann-Schwinger formalism in the first-principles quantum transport theory (5 pages)	045119
Jian Wang and Hong Guo	
Formation energies of rutile metal dioxides using density functional theory (5 pages)	045120
J. I. Martínez, H. A. Hansen, J. Rossmeisl, and J. K. Nørskov	
Evidence for charge-density-wave nature of the charge-ordered phase in La _{1/3} Sr _{2/3} FeO ₃ (5 pages)	045121
Javier Herrero-Martin, Gloria Subias, Joaquin Garcia, Javier Blasco, and M. Concepción Sánchez	
Spectrum-sensitive phonon wipeout due to a fluctuating spin state in a Fe ²⁺ coordination polymer (9 pages)	045122
V. Gnezdilov, P. Lemmens, P. Scheib, M. Ghosh, Yu. G. Pashkevich, H. Paulsen, V. Schünemann, J. A. Wolny, G. Agustí, and J. A. Real	
Structural and magnetic properties of inverse opal photonic crystals studied by x-ray diffraction, scanning electron microscopy, and small-angle neutron scattering (8 pages)	045123
S. V. Grigoriev, K. S. Napolskii, N. A. Grigoryeva, A. V. Vasilieva, A. A. Mistonov, D. Yu. Chernyshov, A. V. Petukhov, D. V. Belov, A. A. Eliseev, A. V. Lukashin, Yu. D. Tretyakov, A. S. Sinitskii, and H. Eckerlebe	
Modeling of disorder effects and optical extinction in three-dimensional photonic crystals (7 pages)	045124
Luis A. Dorado and Ricardo A. Depine	
Tuning the metal-insulator transitions of (SrMnO ₃) _n /(LaMnO ₃) _{2n} superlattices: Role of interfaces (5 pages)	045125
C. Adamo, C. A. Perroni, V. Cataudella, G. De Filippis, P. Orgiani, and L. Maritato	
Effects of bound electrons and radiation on shock Hugoniot (8 pages)	045126
Madhusmita Das and S. V. G. Menon	

(Continued)

Nonadiabatic wavepacket dynamics: k -space formulation (7 pages)	045127
J. M. Pruneda and Ivo Souza	
Theory of defect production in nonlinear quench across a quantum critical point (9 pages)	045128
Shreyoshi Mondal, K. Sengupta, and Diptiman Sen	
Mechanism for slow waves near cutoff frequencies in periodic waveguides (5 pages)	045129
R. V. Craster, S. Guenneau, and S. D. M. Adams	
Embedding approach for dynamical mean-field theory of strongly correlated heterostructures (8 pages)	045130
H. Ishida and A. Liebsch	
Wide-angle infrared absorber based on a negative-index plasmonic metamaterial (5 pages)	045131
Yoav Avitzour, Yaroslav A. Urzhumov, and Gennady Shvets	
Generic short-range interactions in two-leg ladders (11 pages)	045132
J. E. Bunder and Hsiu-Hau Lin	
☞ Dual fermion approach to the two-dimensional Hubbard model: Antiferromagnetic fluctuations and Fermi arcs (15 pages)	045133
A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and A. Georges	
Negative plasmon dispersion in the transition-metal dichalcogenide $2H$ -TaSe ₂ (5 pages)	045134
R. Schuster, R. Kraus, M. Knupfer, H. Berger, and B. Büchner	
Semiconductors I: bulk	
Observation of Fermi-edge excitons and exciton-phonon complexes in the optical response of heavily doped n -type wurtzite GaN (11 pages)	045201
S. Shokhovets, K. Köhler, O. Ambacher, and G. Gobsch	
Highly oriented poly(paraphenylene vinylene): Polarized optical spectroscopy under pressure (8 pages)	045202
Valentina Morandi, Matteo Galli, Franco Marabelli, and Davide Comoretto	
Theoretical study of pressure effect on the dislocation core properties in semiconductors (7 pages)	045203
L. Pizzagalli, J.-L. Demenet, and J. Rabier	
Hole spin quantum beats in bulk ZnO (5 pages)	045204
D. Lagarde, A. Balocchi, P. Renucci, H. Carrère, T. Amand, X. Marie, Z. X. Mei, and X. L. Du	
☞ Spin-wave resonances and surface spin pinning in Ga _{1-x} Mn _x As thin films (11 pages)	045205
C. Bihler, W. Schoch, W. Limmer, S. T. B. Goennenwein, and M. S. Brandt	
Electronic and optical properties of boron-doped nanocrystalline diamond films (14 pages)	045206
W. Gajewski, P. Achatz, O. A. Williams, K. Haenen, E. Bustarret, M. Stutzmann, and J. A. Garrido	
Defects in AlSb: A density functional study (7 pages)	045207
Mao-Hua Du	
All-optical coherently controlled terahertz ac charge currents from excitons in semiconductors (7 pages)	045208
Christian Sames, Jean-Michel Ménard, Markus Betz, Arthur L. Smirl, and Henry M. van Driel	
Anisotropic exchange coupling in diluted magnetic semiconductors: <i>Ab initio</i> spin-density functional theory (6 pages)	045209
H. Ebert and S. Mankovsky	
Impurity band structure of boron-doped homoepitaxial diamond (6 pages)	045210
Takashi Inushima, Rinat F. Mamin, and Hiromu Shiomi	

(Continued)

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

Size-dependent oscillator strength and quantum efficiency of CdSe quantum dots controlled via the local density of states (9 pages)	045301
M. D. Leistikow, J. Johansen, A. J. Kettelarij, P. Lodahl, and W. L. Vos	
Spin-orbit interaction and spin relaxation in a two-dimensional electron gas (6 pages)	045302
M. Studer, S. Schön, K. Ensslin, and G. Salis	
Splitting electrons into quasiparticles with a fractional edge-state Mach-Zehnder interferometer (13 pages) ...	045303
V. V. Ponomarenko and D. V. Averin	
Electronic structure of the Si(110)-(16×2) surface: High-resolution ARPES and STM investigation (6 pages)	045304
Kazuyuki Sakamoto, Martin Setvin, Kenji Mawatari, P. E. J. Eriksson, Kazushi Miki, and R. I. G. Uhrberg	
Magnetoasymmetric current fluctuations of single-electron tunneling (5 pages)	045305
David Sánchez	
Spin-polarized two-dimensional electron gas embedded in a semimagnetic quantum well: Ground state, spin responses, spin excitations, and Raman spectrum (16 pages)	045306
Florent Perez	
 Electrically controllable g tensors in quantum dot molecules (7 pages)	045307
Till Andlauer and Peter Vogl	
 Non-Abelian adiabatic statistics and Hall viscosity in quantum Hall states and p_x+ip_y paired superfluids (41 pages)	045308
N. Read	
Ferromagnetic ordering in Mn induced by thermal strain (5 pages)	045309
Younghun Hwang, Jeongyong Choi, Soon Cheol Hong, Sunglae Cho, Suk-Hee Han, Kyung-Ho Shin, and Myung-Wha Jung	
Tuning the exciton g factor in single InAs/InP quantum dots (6 pages)	045310
Danny Kim, Weidong Sheng, Philip J. Poole, Dan Dalacu, Jacques Lefebvre, Jean Lapointe, Michael E. Reimer, Geoff C. Aers, and Robin L. Williams	
Size-dependent exciton g factor in self-assembled InAs/InP quantum dots (7 pages)	045311
N. A. J. M. Kleemans, J. van Bree, M. Bozkurt, P. J. van Veldhoven, P. A. Nouwens, R. Nötzel, A. Yu. Silov, P. M. Koenraad, and M. E. Flatté	
Optical spectra and microscopic structure of the oxidized Si(100) surface: Combined <i>in situ</i> optical experiments and first principles calculations (10 pages)	045312
Katalin Gaál-Nagy, Andrei Incze, Giovanni Onida, Yves Borensztein, Nadine Witkowski, Olivier Pluchery, Frank Fuchs, Friedhelm Bechstedt, and Rodolfo Del Sole	
Interface two-dimensional metallicity but lack of superconductivity in heterobonded semiconductors: ZnS/Si and GaP/Si (5 pages)	045313
S. H. Rhim, R. Saniz, and A. J. Freeman	
Spintronic single-qubit gate based on a Π -shaped lateral quantum dot with spin-orbit interaction (6 pages)	045314
S. Bellucci and P. Onorato	

(Continued)

	Spatial trends of noncollinear exchange coupling mediated by itinerant carriers with different Fermi surfaces (9 pages)	045315
	Hsin-Hua Lai, Wen-Min Huang, and Hsiu-Hau Lin	
	Condensate-induced transitions between topologically ordered phases (27 pages)	045316
	F. A. Bais and J. K. Slingerland	
	Electric-field-induced long-lived spin excitations in two-dimensional spin-orbit coupled systems (10 pages)	045317
	P. Kleinert and V. V. Bryksin	
	SiC/Ti ₃ SiC ₂ interface: Atomic structure, energetics, and bonding (10 pages)	045318
	Zhongchang Wang, Susumu Tsukimoto, Mitsuhiro Saito, and Yuichi Ikuhara	
	Enhancement of microcavity polariton relaxation under confinement (9 pages)	045319
	T. K. Paraíso, D. Sarchi, G. Nardin, R. Cerna, Y. Leger, B. Pietka, M. Richard, O. El Daïf, F. Morier-Genoud, V. Savona, and B. Deveaud-Plédran	
	Transient terahertz spectroscopy of excitons and unbound carriers in quasi-two-dimensional electron-hole gases (13 pages)	045320
	R. A. Kaindl, D. Hägele, M. A. Carnahan, and D. S. Chemla	
	Effects of disorder in three-dimensional Z ₂ quantum spin Hall systems (29 pages)	045321
	Ryuichi Shindou and Shuichi Murakami	
	Surface physics, nanoscale physics, low-dimensional systems	
	Tuning and monitoring of quantum dot growth by an <i>in situ</i> cantilever (7 pages)	045401
	Yan Wang, Jörg Weissmüller, and Huiling Duan	
	Coordination motifs and large-scale structural organization in atomic clusters (5 pages)	045402
	Zhu Yang and Lei-Han Tang	
	Potential-energy surfaces of adsorbates on periodic substrates: Application of the Morse theory (5 pages) ...	045403
	Štěpán Pick	
	Recovery of local density of states using scanning tunneling spectroscopy (11 pages)	045404
	M. Passoni, F. Donati, A. Li Bassi, C. S. Casari, and C. E. Bottani	
	Magnetotransport through graphene spin valves (7 pages)	045405
	Kai-He Ding, Zhen-Gang Zhu, and Jamal Berakdar	
	Addition spectra of Wigner islands of electrons on superfluid helium (10 pages)	045406
	Emmanuel Rousseau, Dmitri Ponarin, Likourgos Hristakos, Olivier Avenel, Eric Varoquaux, and Yuri Mukharsky	
	Comparison of electronic structure and template function of single-layer graphene and a hexagonal boron nitride nanomesh on Ru(0001) (6 pages)	045407
	Thomas Brugger, Sebastian Günther, Bin Wang, J. Hugo Dil, Marie-Laure Bocquet, Jürg Osterwalder, Joost Wintterlin, and Thomas Greber	
	Surface effects in zinc oxide nanoparticles (9 pages)	045408
	Nicolas Combe, Pierre-Marie Chassaing, and François Demangeot	
	Entanglement signatures of quantum Hall phase transitions (8 pages)	045409
	O. S. Zozulya, Masudul Haque, and Nicolas Regnault	

(Continued)

Influence of laser pulse characteristics on the hot electron contribution to the third-order nonlinear optical response of gold nanoparticles (<i>9 pages</i>)	045410
Yannick Guillet, Majid Rashidi-Huyeh, and Bruno Palpant	
Irradiation-induced densification of cluster-assembled thin films (<i>11 pages</i>)	045411
K. Meinander and K. Nordlund	
First-principles calculations of clean Au(110) surfaces and chemisorption of atomic oxygen (<i>9 pages</i>)	045412
M. Landmann, E. Rauls, and W. G. Schmidt	
Vibrational, electronic, and vibronic excitations of polar C ₆₀ F ₁₈ molecules: Experimental and theoretical study (<i>11 pages</i>)	045413
A. A. Popov, V. M. Senyavin, V. I. Korepanov, I. V. Goldt, A. M. Lebedev, V. G. Stankevich, K. A. Menshikov, N. Yu. Svechnikov, O. V. Boltalina, I. E. Kareev, S. Kimura, O. Sidorova, K. Kanno, and I. Akimoto	
Two-dimensional simulation of superlubricity on NaCl and highly oriented pyrolytic graphite (<i>9 pages</i>)	045414
Pascal Steiner, Raphael Roth, Enrico Gnecco, Alexis Baratoff, Sabine Maier, Thilo Glatzel, and Ernst Meyer	
Ultrafast electron dynamics in metals: Real-time analysis of a reflected light field using photoelectrons (<i>9 pages</i>)	045415
U. Bovensiepen, S. Declair, M. Lisowski, P. A. Loukakos, A. Hotzel, M. Richter, A. Knorr, and M. Wolf	
 Formation of an Au-Si eutectic on a clean silicon surface (<i>7 pages</i>)	045416
A. L. Pinardi, S. J. Leake, R. Felici, and I. K. Robinson	
Energy gap opening in submonolayer lithium on graphene: Local density functional and tight-binding calculations (<i>7 pages</i>)	045417
M. Farjam and H. Rafii-Tabar	
Electronic and transport properties of rectangular graphene macromolecules and zigzag carbon nanotubes of finite length (<i>6 pages</i>)	045418
A. V. Nikolaev, A. V. Bibikov, A. V. Avdeenko, I. V. Bodrenko, and E. V. Tkalya	
Surface diffusion of charged particles: Monte Carlo study (<i>10 pages</i>)	045419
Krzysztof Pawlikowski and Andrzej Pękalski	
Multiple magnetic barriers in graphene (<i>9 pages</i>)	045420
Luca Dell'Anna and Alessandro De Martino	
 Distortion of the perfect lattice structure in bilayer graphene (<i>8 pages</i>)	045421
Vitor M. Pereira, R. M. Ribeiro, N. M. R. Peres, and A. H. Castro Neto	
Energetics and fragmentation of single-doped tin and lead clusters (<i>4 pages</i>)	045422
B. Waldschmidt, S. Barman, C. Rajesh, C. Majumder, G. P. Das, and R. Schäfer	
Structure and spin polarization of outermost surface of the Co ₂ FeAl _{0.5} Si _{0.5} full-Heusler alloy studied by spin-polarized ion-scattering spectroscopy (<i>6 pages</i>)	045423
T. T. Suzuki, H. Sukegawa, and K. Inomata	
 Theory of direct scattering, trapping, and desorption in atom-surface collisions (<i>14 pages</i>)	045424
Guoqing Fan and J. R. Manson	

(Continued)

Polymerized sp^2 - sp^3 hybrid metallic phase of C_{60} as obtained via constant-pressure molecular dynamics (7 pages)	045425
Yuichiro Yamagami and Susumu Saito	
Probing collective electronic excitations in as-deposited and modified Ag thin films grown on Cu(111) (7 pages)	045426
A. Politano, V. Formoso, E. Colavita, and G. Chiarello	
 Semiclassical framework for the calculation of transport anisotropies (12 pages)	045427
Karel Vybírný, Alexey A. Kovalev, Jairo Sinova, and T. Jungwirth	
Imaging perylene derivatives on rutile $TiO_2(110)$ by noncontact atomic force microscopy (8 pages)	045428
J. Schütte, R. Bechstein, P. Rahe, M. Rohlfing, A. Kühnle, and H. Langhals	
Dirac fermion quantization on graphene edges: Isospin-orbit coupling, zero modes, and spontaneous valley polarization (9 pages)	045429
Grigory Tkachov	
Temperature dependence of the surface free energy and surface stress: An atomistic calculation for Cu(110) (10 pages)	045430
T. Frolov and Y. Mishin	

ERRATA

Erratum: Analytic solution for electrons and holes in graphene under electromagnetic waves: Gap appearance and nonlinear effects [Phys. Rev. B 78 , 201406 (2008)] (1 page)	049901(E)
F. J. López-Rodríguez and G. G. Naumis	
Publisher's Note: Coordination motifs and large-scale structural organization in atomic clusters [Phys. Rev. B 79 , 045402 (2009)] (1 page)	049902(E)
Zhu Yang and Lei-Han Tang	