

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 63, NUMBER 16

CONTENTS

15 APRIL 2001-II

Announcement: Electronic-First Publication and Article Numbers i

RAPID COMMUNICATIONS

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

- Large birefringence in two-dimensional silicon photonic crystals (*4 pages*) 161101(R)
F. Genereux, S. W. Leonard, H. M. van Driel, A. Birner, and U. Gösele
- Hall effect in single crystal $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ (*4 pages*) 161102(R)
L. M. Galvin, R. S. Perry, A. W. Tyler, A. P. Mackenzie, S. Nakatsuji, and Y. Maeno
- Transport properties in doped Mott insulator epitaxial $\text{La}_{1-y}\text{TiO}_{3+\delta}$ thin films (*4 pages*) 161103(R)
S. Gariglio, J. W. Seo, J. Fompeyrine, J.-P. Locquet, and J.-M. Triscone
- Photonic band-gap effect, localization, and waveguiding in the two-dimensional Penrose lattice (*4 pages*) 161104(R)
Mehmet Bayindir, E. Cubukcu, I. Bulu, and E. Ozbay

Semiconductors I: bulk

- Resonant donor defect as a cause of compensation in *p*-type ZnSe: Photoluminescence studies under hydrostatic pressure (*4 pages*) 161201(R)
Igor L. Kuskovsky, G. F. Neumark, J. G. Tischler, and B. A. Weinstein

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

- Electron-hole alignment in InAs/GaAs self-assembled quantum dots: Effects of chemical composition and dot shape (*4 pages*) 161301(R)
Weidong Sheng and Jean-Pierre Leburton
- Elementary excitations in modulation-doped Cd(Mn)Te quantum wells (*4 pages*) 161302(R)
Bernard Jusserand, Grzegorz Karczewski, Grzegorz Cywiński, Tomasz Wojtowicz, Aristide Lemaître, Christophe Testelin, and Claudette Rigaux
- Scaling of band-gap reduction in heavily nitrogen doped GaAs (*4 pages*) 161303(R)
Yong Zhang, A. Mascarenhas, H. P. Xin, and C. W. Tu
- Coherent confined LO phonons in $^{70}\text{Ge}/^{74}\text{Ge}$ isotope superlattices generated by ultrafast laser pulses (*4 pages*) 161304(R)
M. Nakajima, H. Harima, K. Morita, K. M. Itoh, K. Mizoguchi, and E. E. Haller
- Observation of multicharged excitons and biexcitons in a single InGaAs quantum dot (*4 pages*) 161305(R)
J. J. Finley, P. W. Fry, A. D. Ashmore, A. Lemaître, A. I. Tartakovskii, R. Oulton, D. J. Mowbray, M. S. Skolnick, M. Hopkinson, P. D. Buckle, and P. A. Maksym



Strain-induced change of surface reconstructions for InAs(001) (<i>4 pages</i>)	161306(R)
C. Ratsch	
Ballistic spin-filter transistor (<i>4 pages</i>)	161307(R)
Dirk Grundler	
Homogeneous broadening and excitation-induced dephasing of intersubband transitions in a quasi-two-dimensional electron gas (<i>4 pages</i>)	161308(R)
Robert A. Kaindl, Klaus Reimann, Michael Woerner, Thomas Elsaesser, R. Hey, and K. H. Ploog	
Enhanced phonon-assisted absorption in single InAs/GaAs quantum dots (<i>4 pages</i>)	161309(R)
A. Lemaître, A. D. Ashmore, J. J. Finley, D. J. Mowbray, M. S. Skolnick, M. Hopkinson, and T. F. Krauss	

Surface physics, low-dimensional systems, and related topics

Condensed phases of all-pentagon C_{20} cages as possible superconductors (<i>4 pages</i>)	161401(R)
Yoshiyuki Miyamoto and Mineo Saito	
Light absorption of silica nanoparticles (<i>4 pages</i>)	161402(R)
I. S. Altman, D. Lee, J. D. Chung, J. Song, and M. Choi	
Contact resistance between carbon nanotubes (<i>4 pages</i>)	161403(R)
Alper Buldum and Jian Ping Lu	
Electrical transport in doped multiwalled carbon nanotubes (<i>4 pages</i>)	161404(R)
K. Liu, Ph. Avouris, R. Martel, and W. K. Hsu	
Micro-Raman investigation of aligned single-wall carbon nanotubes (<i>4 pages</i>)	161405(R)
C. Fantini, M. A. Pimenta, M. S. S. Dantas, D. Ugarte, A. M. Rao, A. Jorio, G. Dresselhaus, and M. S. Dresselhaus	

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

Electronic structure and magnetism of $Sr_3Ru_2O_7$ (<i>7 pages</i>)	165101
D. J. Singh and I. I. Mazin	
Near-infrared-to-visible photon upconversion process induced by exchange interactions in Yb^{3+} -doped $RbMnCl_3$ (<i>11 pages</i>)	165102
Rafael Valiente, Oliver S. Wenger, and Hans U. Güdel	
Electromagnetic modes in metal-insulator-metal structures (<i>4 pages</i>)	165103
F. Villa, T. Lopez-Rios, and L. E. Regalado	
Electronic structure of K-intercalated 8-tris-hydroxyquinoline aluminum studied by photoemission spectroscopy (<i>5 pages</i>)	165104
T. Schwieger, H. Peisert, M. Knupfer, M. S. Golden, and J. Fink	
Optical studies of gap, hopping energies, and the Anderson-Hubbard parameter in the zigzag-chain compound $SrCuO_2$ (<i>11 pages</i>)	165105
Z. V. Popović, V. A. Ivanov, M. J. Konstantinović, A. Cantarero, J. Martínez-Pastor, D. Olguín, M. I. Alonso, M. Garriga, O. P. Khuong, A. Vietkin, and V. V. Moshchalkov	
Parametrization of modified embedded-atom-method potentials for Rh, Pd, Ir, and Pt based on density functional theory calculations, with applications to surface properties (<i>13 pages</i>)	165106
P. van Beurden and G. J. Kramer	
Self-interaction-corrected description of the electronic properties of americium monochalcogenides and monpnictides (<i>7 pages</i>)	165107
L. Petit, A. Svane, W. M. Temmerman, and Z. Szotek	
Eigenvalues in the non-Hermitian Anderson model (<i>6 pages</i>)	165108
J. Heinrichs	

Physical properties of Heusler-like Fe_2VAl (12 pages)	165109
Ye Feng, J. Y. Rhee, T. A. Wiener, D. W. Lynch, B. E. Hubbard, A. J. Sievers, D. L. Schlagel, T. A. Lograsso, and L. L. Miller	
Weakly coupled Hubbard chains at half-filling and confinement (11 pages)	165110
Karyn Le Hur	
Higher period ordered phases on the Bethe lattice (11 pages)	165111
Ch. Gruber, N. Macris, Ph. Royer, and J. K. Freericks	
Interfacial structures and energetics of basal twins in $\alpha\text{-Al}_2\text{O}_3$: First-principles density-functional and empirical calculations (9 pages)	165112
A. G. Marinopoulos, S. Nufer, and C. Elsässer	
One-dimensional dynamics of the d electrons in $\alpha'\text{-NaV}_2\text{O}_5$ (13 pages)	165113
S. Atzkern, M. Knupfer, M. S. Golden, J. Fink, A. N. Yaresko, V. N. Antonov, A. Hübsch, C. Waidacher, K. W. Becker, W. von der Linden, G. Obermeier, and S. Horn	
Unusual behavior of the Kondo temperature of $\text{La}_{1-x}\text{Yb}_x\text{Cu}_3\text{Al}_2$ (6 pages)	165114
D. P. Rojas, L. P. Cardoso, A. A. Coelho, F. G. Gandra, and A. N. Medina	
Nonlocal effects in the electron-positron interaction in metals (13 pages)	165115
A. Rubaszek, Z. Szotek, and W. M. Temmerman	
Phase stabilities and structural relaxations in substoichiometric TiC_{1-x} (8 pages)	165116
Håkan W. Hugosson, Pavel Korzhavyi, Ulf Jansson, Börje Johansson, and Olle Eriksson	
Nonlocal dynamical correlations in the Hubbard model: A noncrossing approximation study (8 pages)	165117
Tran Minh-Tien	
Electron-correlation effects in appearance-potential spectra of Ni (6 pages)	165118
M. Potthoff, T. Wegner, W. Nolting, T. Schlathölder, M. Vonbank, K. Ertl, J. Braun, and M. Donath	
Semiconductors I: bulk	
Electric field gradient antishielding for HD and D_2 (4 pages)	165201
P. A. Fedders	
Positron thermalization in Si and GaAs (12 pages)	165202
J. Nissilä, K. Saarinen, and P. Hautojärvi	
Strongly confined polaron excitations in charged organic semiconductors (4 pages)	165203
M. Knupfer, J. Fink, and D. Fichou	
g values of effective mass donors in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys (10 pages)	165204
M. W. Bayerl, M. S. Brandt, T. Graf, O. Ambacher, J. A. Majewski, M. Stutzmann, D. J. As, and K. Lischka	
Electric-field-induced charge-density variations in covalently bonded binary compounds (10 pages)	165205
J. Stahn, U. Pietsch, P. Blaha, and K. Schwarz	
First-principles study of the origin and nature of ferromagnetism in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ (13 pages)	165206
Stefano Sanvito, Pablo Ordejón, and Nicola A. Hill	
Nanosecond dynamics of a gallium mirror's light-induced reflectivity change (4 pages)	165207
V. Albanis, S. Dhanjal, V. A. Fedotov, K. F. MacDonald, N. I. Zheludev, P. Petropoulos, D. J. Richardson, and V. I. Emel'yanov	
Collective free-carrier scattering in semiconductors (4 pages)	165208
G. R. M. Robb, B. W. J. McNeil, I. Galbraith, and D. A. Jaroszynski	
Quantum Monte Carlo treatment of elastic exciton-exciton scattering (7 pages)	165209
J. Shumway and D. M. Ceperley	
Structural, electronic, and effective-mass properties of silicon and zinc-blende group-III nitride semiconductor compounds (10 pages)	165210
L. E. Ramos, L. K. Teles, L. M. R. Scolfaro, J. L. P. Castineira, A. L. Rosa, and J. R. Leite	

Local atomic strain in $\text{ZnSe}_{1-x}\text{Te}_x$ from high real-space resolution neutron pair distribution function measurements (7 pages)	165211
P. F. Peterson, Th. Proffen, I.-K. Jeong, S. J. L. Billinge, K.-S. Choi, M. G. Kanatzidis, and P. G. Radaelli	
Second-harmonic generation of I-III-VI ₂ chalcopyrite semiconductors: Effects of chemical substitutions (12 pages)	165212
Sergey N. Rashkeev and Walter R. L. Lambrecht	
Exciton dissociation mechanisms in the polymeric semiconductors poly(9,9-dioctylfluorene) and poly(9,9-dioctylfluorene-co-benzothiadiazole) (18 pages)	165213
Mark A. Stevens, Carlos Silva, David M. Russell, and Richard H. Friend	
Semiconductors II: surfaces, interfaces, microstructures, and related topics	
Electron-electron interactions in square quantum dots (6 pages)	165301
S. Akbar and In-Ho Lee	
Bound polaron in a spherical quantum dot: Strong electron-phonon coupling case (8 pages)	165302
Dmitriy V. Melnikov and W. Beall Fowler	
In-plane anisotropy of the optical properties of $(\text{In}_{0.5}\text{Ga}_{0.5}\text{As})_n/(\text{InP})_n$ superlattices (9 pages)	165303
Rita Magri and Stefano Ossicini	
Optical properties of tilted II-VI superlattices grown on vicinal surfaces (10 pages)	165304
L. Marsal, A. Wasiela, G. Fishman, H. Mariette, F. Michelini, S. Nagahara, and T. Kita	
Leaky interface phonons in $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ structures (11 pages)	165305
I. V. Ponomarev and A. L. Efros	
Spin-orbit splitting in semiconductor quantum dots with a parabolic confinement potential (6 pages)	165306
O. Voskoboinikov, C. P. Lee, and O. Tretyak	
Vertical longitudinal magnetoresistance of semiconductor superlattices (6 pages)	165307
Yu. A. Pusep, G. M. Gusev, A. J. Chiquito, S. S. Sokolov, A. K. Bakarov, A. I. Toropov, and J. R. Leite	
Generation of coherent confined LO phonons under the drift of two-dimensional electrons (10 pages)	165308
S. M. Komirenko, K. W. Kim, V. A. Kochelap, I. Fedorov, and M. A. Strosio	
Symmetry and spin polarization in single and coupled quantum dots (12 pages)	165309
I. I. Yakimenko, A. M. Bychkov, and K.-F. Berggren	
Repulsive trap for two electrons in a magnetic field (5 pages)	165310
A. D. Chepelianskii and D. L. Shepelyansky	
Biexciton states in semiconductor microcavities (5 pages)	165311
T. Baars, G. Dasbach, M. Bayer, and A. Forchel	
Zero-point fluctuations in the ground state of a mesoscopic normal ring (12 pages)	165312
Pascal Cedraschi and Markus Büttiker	
Coherent and incoherent pumping of electrons in double quantum dots (10 pages)	165313
B. L. Hazelzet, M. R. Wegewijs, T. H. Stoof, and Yu. V. Nazarov	
Andreev tunneling, Coulomb blockade, and resonant transport of nonlocal spin-entangled electrons (11 pages)	165314
Patrik Recher, Eugene V. Sukhorukov, and Daniel Loss	
Observation of solvatochromism in CdSe colloidal quantum dots (6 pages)	165315
C. A. Leatherdale and M. G. Bawendi	
Kondo and mixed-valence regimes in multilevel quantum dots (5 pages)	165316
A. L. Chudnovskiy and S. E. Ulloa	
Resistance effects due to magnetic guiding orbits (8 pages)	165317
J. Reijniers and F. M. Peeters	

Faraday rotation in a study of charged excitons in $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ (7 pages)	165318
W. Małana, W. Mac, J. A. Gaj, P. Kossacki, A. Golnik, J. Cibert, S. Tatarenko, T. Wojtowicz, G. Karczewski, and J. Kossut	
Formation mechanism and energy levels of GaN six-bilayer periodic structures grown on GaAs(001) (7 pages)	165319
Mitsuru Funato, Shizuo Fujita, and Shigeo Fujita	
Trimer adatom structure of phosphorus on Ge(111) (7 pages)	165320
L. Vitali, M. G. Ramsey, and F. P. Netzer	
Electronic structure and vertical transport in random dimer GaAs- $\text{Al}_x\text{Ga}_{1-x}\text{As}$ superlattices (7 pages)	165321
A. Parisini, L. Tarricone, V. Bellani, G. B. Parravicini, E. Diez, F. Domínguez-Adame, and R. Hey	
Evolution of elementary excitations at a doped polar semiconductor surface in a depletion-layer formation process (20 pages)	165322
Takeshi Inaoka	
Giant tunability of exciton photoluminescence emission in antiferromagnetic EuTe (5 pages)	165323
W. Heiss, G. Prechtel, and G. Springholz	
Structure and stability of germanium nanoparticles (5 pages)	165324
Laurent Pizzagalli, Giulia Galli, John E. Klepeis, and François Gygi	
Optical second-harmonic spectra of Si(001) with H and Ge adatoms: First-principles theory and experiment (8 pages)	165325
V. I. Gavrilenko, R. Q. Wu, M. C. Downer, J. G. Ekerdt, D. Lim, and P. Parkinson	
Single-electron magnetoconductivity of a nondegenerate two-dimensional electron system in a quantizing magnetic field (14 pages)	165326
Frank Kuehnel, Leonid P. Pryadko, and M. I. Dykman	
Reconfiguration of charge density waves by surface nanostructures on TaS_2 (7 pages)	165327
R. Adelung, J. Brandt, L. Kipp, and M. Skibowski	
Dynamic correlations in double-layer electron systems (10 pages)	165328
B. Tanatar and B. Davoudi	
Energy dependence of quantum dot formation by ion sputtering (5 pages)	165329
S. Facsko, H. Kurz, and T. Dekorsy	
Fermi-edge singularities in photoluminescence spectra of <i>n</i> -type modulation-doped quantum wells with a lateral periodic potential (6 pages)	165330
Shintaro Nomura, Takeshi Nakanishi, and Yoshinobu Aoyagi	
Surface physics, low-dimensional systems, and related topics	
Interaction of charged particles with surface plasmons in cylindrical channels in solids (13 pages)	165401
Néstor R. Arista and Miguel A. Fuentes	
Thermovoltage mapping of standing electron waves on Au(111) surfaces at low temperatures (6 pages)	165402
K. J. Engel, M. Wenderoth, N. Quaas, T. C. G. Reusch, K. Sauthoff, and R. G. Ulbrich	
Observation of a one-dimensional state on stepped Cu(775) (8 pages)	165403
X. J. Shen, H. Kwak, D. Mocuta, A. M. Radojevic, S. Smadici, and R. M. Osgood, Jr.	
Fractional exclusion statistics and shot noise in ballistic conductors (6 pages)	165404
G. Gomila and L. Reggiani	
Wave-vector-dependent symmetry analysis of a photoemission matrix element: The quasi-one-dimensional model system Cu(110)(2×1)O (8 pages)	165405
F. Pforte, A. Gerlach, A. Goldmann, R. Matzdorf, J. Braun, and A. Postnikov	
Transmission electron microscopy and Monte Carlo simulations of ordering in Au-Cu clusters produced in a laser vaporization source (10 pages)	165406
B. Pauwels, G. Van Tendeloo, E. Zhurkin, M. Hou, G. Verschoren, L. Theil Kuhn, W. Bouwen, and P. Lievens	

Influence of d electrons on the dispersion relation of Ag surface plasmons for different single-crystal faces (12 pages)	165407
Catalina López Bastidas, Ansgar Liebsch, and W. Luis Mochán	
Electron energy-loss spectroscopy of electron states in isolated carbon nanostructures (4 pages)	165408
K. Suenaga, E. Sandré, C. Colliex, C. J. Pickard, H. Kataura, and S. Iijima	
Surface-embedded Green-function method: A formulation using a linearized-augmented-plane-wave basis set (10 pages)	165409
H. Ishida	
Theoretical study of chlorine adsorption on the Ag(111) surface (6 pages)	165410
K. Doll and N. M. Harrison	
Atomic-scale three-dimensional kinetic Monte Carlo simulation of organometallic vapor-phase epitaxy of ordered films (11 pages)	165411
C. S. Deo and D. J. Srolovitz	
Alternative to the Shuttleworth formulation of solid surface stress (5 pages)	165412
D. J. Bottomley and T. Ogino	
Multifractal behavior of crystallization on Au/Ge bilayer films (5 pages)	165413
Z. W. Chen, X. P. Wang, S. Tan, S. Y. Zhang, J. G. Hou, and Z. Q. Wu	
Growth of (110) diamond using pure dicarbon (9 pages)	165414
M. Sternberg, M. Kaukonen, R. M. Nieminen, and Th. Frauenheim	
Influence of alloying additions on grain boundary cohesion of transition metals: First-principles determination and its phenomenological extension (9 pages)	165415
W. T. Geng, A. J. Freeman, and G. B. Olson	
Adsorption sites and microstructures of CO ₂ on Fe(111) derived from specular and off-specular HREELS (7 pages)	165416
G. Heß, Ch. Baumgartner, and H. Froitzheim	
Fluctuations and critical phenomena in catalytic CO oxidation on nanoscale Pt facets (12 pages)	165417
Yu. Suchorski, J. Beben, R. Imbihl, E. W. James, Da-Jiang Liu, and J. W. Evans	
Classical dynamics of electrons in quantized-acoustoelectric-current devices (12 pages)	165418
A. M. Robinson and C. H. W. Barnes	
Coulomb interactions in carbon nanotubes (7 pages)	165419
M. P. López Sancho, M. C. Muñoz, and L. Chico	
Spatially resolved spectroscopy on superconducting proximity nanostructures (4 pages)	165420
M. Vinet, C. Chapelier, and F. Lefloch	
Surface electronic states of the partially hydrogenated diamond C(100)-(2×1):H surface (9 pages)	165421
Kirill Bobrov, Geneviève Comtet, Gérald Dujardin, Lucette Hellner, Philippe Bergonzo, and Christine Mer	
Near-field optical response of a two-dimensional grating of gold nanoparticles (6 pages)	165422
M. Salerno, N. Féridj, J. R. Krenn, A. Leitner, F. R. Aussenegg, and J. C. Weeber	
Thermodynamic properties of a system of interacting particles adsorbed on a lattice with two nonequivalent sites (11 pages)	165423
A. A. Tarasenko, Z. Chvoj, L. Jastrabík, F. Nieto, and C. Uebing	
Magnetic scanning tunneling microscopy with a two-terminal nonmagnetic tip: Quantitative results (5 pages)	165424
T. P. Pareek and Patrick Bruno	
Interaction between Cu atoms and isolated ¹¹¹ In probe atoms on a Cu(100) surface (10 pages)	165425
M. F. Roşu, F. Pleiter, and L. Niesen	
Nonequilibrium electronic transport and interaction in short metallic nanobridges (6 pages)	165426
H. B. Weber, R. Häußler, H. v. Löhneysen, and J. Kroha	
Structure and stability of hydrogen clusters up to H ₂₁ ⁺ (10 pages)	165427
H. Chermette and I. V. Ymmud	

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 63, NUMBER 16

15 APRIL 2001-II

Charge-density-wave STM observation in η -Mo ₄ O ₁₁ (4 pages)	165428
P. Mallet, H. Guyot, J. Y. Veuillen, and N. Motta	
Weight of zero-loss electrons and sum rules in extrinsic processes that can influence photoemission spectra (6 pages)	165429
K. Schulte, M. A. James, P. G. Steeneken, G. A. Sawatzky, R. Suryanarayanan, G. Dhalenne, and A. Revcolevschi	
Effects of confinement on the vibrational spectra of liquid water adsorbed in carbon nanotubes (5 pages)	165430
J. Martí and M. C. Gordillo	
Determination of buried dislocation structures by scanning tunneling microscopy (6 pages)	165431
J. de la Figuera, A. K. Schmid, N. C. Bartelt, K. Pohl, and R. Q. Hwang	
Electronic effects in scanning tunneling microscopy of dendritic, Cr-filled carbon nanotubes (5 pages)	165432
F.-X. Zha, D. L. Carroll, R. Czerw, A. Loiseau, H. Pascard, W. Clauss, and S. Roth	

ERRATA

Erratum: Effects of Rayleigh scattering on photovoltaic spectra associated with 1s orthoexcitons in Cu ₂ O [Phys. Rev. B 63 , 033202 (2001)] (1 page)	169901(E)
A. Mori, N. Naka, and N. Nagasawa	

Cumulative Author Index	iii
-------------------------------	-----