

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 1N01
2 Huntington Quadrangle
Melville, NY 11747-4502

THIRD SERIES, VOLUME 69, NUMBER 7

CONTENTS

FEBRUARY 2004-15(I)

BRIEF REPORTS

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

- Small adiabatic polaron with a long-range electron-phonon interaction (*4 pages*) 073101
A. S. Alexandrov and B. Ya. Yavidov
- Dephasing rate in metals versus diffusion constant (*3 pages*) 073102
Y. M. Galperin, V. I. Kozub, and V. M. Vinokur
- Ground states of the Falicov-Kimball model with hybridization (*4 pages*) 073103
L. G. Sarasua and M. A. Continentino
- Exciton formation and stability in semiconductor heterostructures (*3 pages*) 073104
S. Siggelkow, W. Hoyer, M. Kira, and S. W. Koch
- Crossover from two-dimensional to one-dimensional collective pinning in NbSe₃ (*4 pages*) 073105
E. Slot, H. S. J. van der Zant, K. O'Neill, and R. E. Thorne
- Spin magnetization of a strongly correlated electron gas confined in a two-dimensional finite lattice
(*4 pages*) 073106
M. Niță, V. Dinu, A. Aldea, and B. Tanatar

Semiconductors I: bulk

- Hall effect in cobalt-doped TiO_{2-δ} (*4 pages*) 073201
J. S. Higgins, S. R. Shinde, S. B. Ogale, T. Venkatesan, and R. L. Greene

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

- Intersublevel optical transitions in InAs nanocrystals probed by photoinduced absorption spectroscopy: The
role of thermal activation (*4 pages*) 073301
D. Krapf, S.-H. Kan, U. Banin, O. Millo, and A. Sa'ar
- Nuclear spin relaxation probed by a single quantum dot (*4 pages*) 073302
A. K. Hüttel, J. Weber, A. W. Holleitner, D. Weinmann, K. Eberl, and R. H. Blick
- From GaAs:N to oversaturated GaAsN: Analysis of the band-gap reduction (*4 pages*) 073303
T. Taliercio, R. Intartaglia, B. Gil, P. Lefebvre, T. Bretagnon, U. Tisch, E. Finkman, J. Salzman,
M.-A. Pinault, M. Laügt, and E. Tournié
- Coherently induced one-dimensional photonic band gap (*4 pages*) 073304
S. M. Sadeghi, W. Li, and H. M. van Driel
- Spin detection in quantum dots by electric currents (*4 pages*) 073305
Eugene G. Mishchenko, Arne Brataas, and Yaroslav Tserkovnyak
- Probing the ladder spectrum arising from motion in a two-dimensional lattice driven by in-plane constant
forces (*4 pages*) 073306
W. X. Yan, F. Claro, B. H. Xie, X. G. Zhao, X. P. Li, and J. Q. Liang



Copyright 2004 by The American Physical Society

(Continued)



0163-1829(20040215)69:7;1-A

Molecular-dynamics simulations of nucleation and crystallization in supercooled liquid silicon: Temperature-gradient effects (3 pages)	073307
Teruaki Motooka and Shinji Munetoh	
Imaging a two-dimensional electron system with a scanning charged probe (4 pages)	073308
Subhasish Chakraborty, I. J. Maasilta, S. H. Tessmer, and M. R. Melloch	
Optical modes in mesoscopic quantum cascade ring lasers (3 pages)	073309
S. Anders, V. Tamosiunas, W. Schrenk, and G. Strasser	
Slow spin relaxation in two-dimensional electron systems with antidots (4 pages)	073310
Yuriy V. Pershin and Vladimir Privman	
From localization to Landau quantization in a two-dimensional GaAs electron system containing self-assembled InAs quantum dots (4 pages)	073311
Gil-Ho Kim, C.-T. Liang, C. F. Huang, J. T. Nicholls, D. A. Ritchie, P. S. Kim, C. H. Oh, J. R. Juang, and Y. H. Chang	

Surface physics, low-dimensional systems, and related topics

Elastic properties of single-walled carbon nanotubes in transverse directions (3 pages)	073401
Chunyu Li and Tsu-Wei Chou	
Adsorption and migration of carbon adatoms on carbon nanotubes: Density-functional <i>ab initio</i> and tight-binding studies (4 pages)	073402
A. V. Krashennnikov, K. Nordlund, P. O. Lehtinen, A. S. Foster, A. Ayuela, and R. M. Nieminen	
<i>Ab initio</i> calculation of graphite surface-bulk core-level splitting (4 pages)	073403
Antonín Šimůnek and Jiří Vackář	
Computer simulation study of the ground-state structures of singly ionized clusters of C ₆₀ molecules (3 pages)	073404
C. Rey, J. García-Rodeja, and L. J. Gallego	
Magnetophonon resonance in high-density high-mobility quantum well systems (4 pages)	073405
C. Faugeras, D. K. Maude, G. Martinez, L. B. Rigal, C. Proust, K. J. Friedland, R. Hey, and K. H. Ploog	
Interface intermixing in metal heteroepitaxy on the atomic scale (4 pages)	073406
R. C. Longo, V. S. Stepanyuk, W. Hergert, A. Vega, L. J. Gallego, and J. Kirschner	
Thermal conductivity of zigzag single-walled carbon nanotubes: Role of the umklapp process (4 pages)	073407
J. X. Cao, X. H. Yan, Y. Xiao, and J. W. Ding	

ARTICLES

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

Real-space pseudopotential method for computing the electronic properties of periodic systems (6 pages)	075101
M. M. G. Alemany, Manish Jain, Leeor Kronik, and James R. Chelikowsky	
Tests of a ladder of density functionals for bulk solids and surfaces (11 pages)	075102
Viktor N. Staroverov, Gustavo E. Scuseria, Jianmin Tao, and John P. Perdew	
$2k_F$ transitions in a series of (DMET) ₂ (X ₁ X ₂ TCNQ) (X ₁ , X ₂ =Br, Cl, F, CH ₃ , H): Subsidiary lattice effect by anion radicals (5 pages)	075103
T. Sato, T. Hasegawa, T. Akutagawa, T. Nakamura, and R. Kondo	
Magnetic oscillations in planar systems with the Dirac-like spectrum of quasiparticle excitations (22 pages) ..	075104
S. G. Sharapov, V. P. Gusynin, and H. Beck	
Effective nonlinear optical properties of composite media of graded spherical particles (8 pages)	075105
L. Gao, J. P. Huang, and K. W. Yu	
Competing density-wave orders in a one-dimensional hard-boson model (15 pages)	075106
Paul Fendley, K. Sengupta, and Subir Sachdev	

Phase-dependent decoherence of optical transitions in $\text{Pr}^{3+}:\text{LaF}_3$ in the presence of a driving field (4 pages) ..	075107
G. J. Pryde, M. J. Sellars, and N. B. Manson	
Reflectivity of metallodielectric photonic glasses (5 pages)	075108
Krassimir P. Velikov, Willem L. Vos, Alexander Moroz, and Alfons van Blaaderen	
Path integral approach to the Anderson-Holstein model (11 pages)	075109
Hyun C. Lee and Han-Yong Choi	
Structural, electronic, and magneto-optical properties of YVO_3 (11 pages)	075110
A. A. Tsvetkov, F. P. Mena, P. H. M. van Loosdrecht, D. van der Marel, Y. Ren, A. A. Nugroho, A. A. Menovsky, I. S. Elfimov, and G. A. Sawatzky	
Many-body density matrices for free fermions (12 pages)	075111
Siew-Ann Cheong and Christopher L. Henley	
Operator-based truncation scheme based on the many-body fermion density matrix (20 pages)	075112
Siew-Ann Cheong and Christopher L. Henley	
Electronic origin of structural trends across early transition-metal disilicides: Anomalous behavior of CrSi_2 (9 pages)	075113
D. A. Pankhurst, D. Nguyen-Manh, and D. G. Pettifor	
Fermi-surface analysis of a quasi-two-dimensional monophosphate tungsten bronze (8 pages)	075114
L. Roca, A. Mascaraque, J. Avila, S. Drouard, H. Guyot, and M. C. Asensio	
Ferroelectric phase transition, ionicity condensation, and multicriticality in charge-transfer organic complexes (5 pages)	075115
Jun-ichiro Kishine, Tadeusz Luty, and Kenji Yonemitsu	
Ultrafast four-wave mixing in strongly correlated electron systems (7 pages)	075116
Akira Takahashi, Hiroki Gomi, and Masaki Aihara	
First-principles electronic structure of spinel LiCr_2O_4 : A possible half-metal (8 pages)	075117
Markus Lauer, Roser Valenti, H. C. Kandpal, and Ram Seshadri	
Orbital wave and its observation in orbital-ordered titanates and vanadates (9 pages)	075118
Sumio Ishihara	
Weak localization of electrons in an external electric field (10 pages)	075119
O. Bleibaum and D. Belitz	

Semiconductors I: bulk

Disorder controlled hole transport in MEH-PPV (8 pages)	075201
Anto Regis Inigo, Hsiang-Chih Chiu, Wunshain Fann, Ying-Sheng Huang, U-Ser Jeng, Tsang-Lang Lin, Chia-Hung Hsu, Kang-Yung Peng, and Show-An Chen	
Resonant photoemission of $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ at the Mn L edge (7 pages)	075202
O. Rader, C. Pampuch, A. M. Shikin, W. Gudat, J. Okabayashi, T. Mizokawa, A. Fujimori, T. Hayashi, M. Tanaka, A. Tanaka, and A. Kimura	
Optical polarization of nuclear spins in GaAs (8 pages)	075203
Anant K. Paravastu, Sophia E. Hayes, Birgit E. Schwickert, Long N. Dinh, Mehdi Balooch, and Jeffrey A. Reimer	
Raman investigation of anharmonicity and disorder-induced effects in $\text{Zn}_{1-x}\text{Be}_x\text{Se}$ epilayers (6 pages)	075204
L. Y. Lin, C. W. Chang, W. H. Chen, Y. F. Chen, S. P. Guo, and M. C. Tamargo	
Band-gap engineering with $\text{HfS}_x\text{Se}_{2-x}$ (5 pages)	075205
Christof Gaiser, Thorsten Zandt, Alica Krapf, Ralf Serverin, Christoph Janowitz, and Recardo Mancke	
Influence of defects on the lattice constant of GaMnAs (5 pages)	075206
J. Sadowski and J. Z. Domagala	
Density-functional-based tight-binding calculation of excitons in conjugated polymers (8 pages)	075207
Thomas G. Pedersen	
Site preference for Mn substitution in spintronic $\text{CuM}^{\text{III}}\text{X}_2^{\text{VI}}$ chalcopyrite semiconductors (7 pages)	075208
Yu-Jun Zhao and Alex Zunger	

Linewise kinetic Monte Carlo study of silicon dislocation dynamics (9 pages)	075209
S. Scarle, C. P. Ewels, M. I. Heggie, and N. Martsinovich	
Isoelectronic oxygen-related defect in CdTe crystals investigated using thermoelectric effect spectroscopy (4 pages)	075210
Salah A. Awadalla, Alan W. Hunt, Kelvin G. Lynn, Howard Glass, Csaba Szeles, and Su-Huai Wei	
Theory of polaron bandwidth narrowing in organic molecular crystals (7 pages)	075211
K. Hannewald, V. M. Stojanović, J. M. T. Schellekens, P. A. Bobbert, G. Kresse, and J. Hafner	
Anisotropy effects in phonon-assisted charge-carrier transport in organic molecular crystals (12 pages)	075212
K. Hannewald and P. A. Bobbert	
Phonon modes in Si [111] nanowires (5 pages)	075213
T. Thonhauser and G. D. Mahan	
High-field transport of electrons and radiative effects using coupled force-balance and Fokker-Planck equations beyond the relaxation-time approximation (12 pages)	075214
Danhong Huang, T. Apostolova, P. M. Alsing, and D. A. Cardimona	
Optical pumping NMR in the compensated semiconductor InP:Fe (7 pages)	075215
Atsushi Goto, Kenjiro Hashi, Tadashi Shimizu, Ryo Miyabe, Xiaogang Wen, Shinobu Ohki, Susumu Machida, Takahiro Iijima, and Giyuu Kido	
Semiconductors II: surfaces, interfaces, microstructures, and related topics	
Atomic-scale model of <i>c</i> -Si/ <i>a</i> -Si:H interfaces (7 pages)	075301
M. Tosolini, L. Colombo, and M. Peressi	
Symmetry of anisotropic exchange interactions in semiconductor nanostructures (5 pages)	075302
K. V. Kavokin	
Adsorption kinetics of acetylene and ethylene on Si(001) (6 pages)	075303
Jun-Hyung Cho and Leonard Kleinman	
Luminescence emission originating from nitrogen doping of β -Ga ₂ O ₃ nanowires (7 pages)	075304
Y. P. Song, H. Z. Zhang, C. Lin, Y. W. Zhu, G. H. Li, F. H. Yang, and D. P. Yu	
Power-law dependence of the angular momentum transition fields in few-electron quantum dots (6 pages)	075305
E. Anisimovas, A. Matulis, M. B. Tavernier, and F. M. Peeters	
Two-dimensional electron gas near full polarization (16 pages)	075306
G. Zala, B. N. Narozhny, I. L. Aleiner, and Vladimir I. Fal'ko	
Impact of phonons on quantum phase transitions in nanorings of coupled quantum dots (13 pages)	075307
Ioan Bâldea, Horst Köppel, and Lorenz S. Cederbaum	
Effects of inhomogeneous broadening on reflection spectra of Bragg multiple quantum well structures with a defect (11 pages)	075308
L. I. Deych, M. V. Erementchouk, and A. A. Lisyansky	
First-principles calculations of strontium on Si(001) (13 pages)	075309
Christopher R. Ashman, Clemens J. Först, Karlheinz Schwarz, and Peter E. Blöchl	
Effects of electron-electron and electron-phonon interactions in weakly disordered conductors and heterostructures (11 pages)	075310
A. Sergeev, M. Yu. Reizer, and V. Mitin	
Orbital magnetic properties of quantum dots: The role of electron-electron interactions (8 pages)	075311
L. G. G. V. Dias da Silva, Caio H. Lewenkopf, and Nelson Studart	
Radiative corrections to the excitonic molecule state in GaAs microcavities (15 pages)	075312
A. L. Ivanov, P. Borri, W. Langbein, and U. Woggon	
Mobility in V-shaped quantum wires due to interface roughness and alloy scattering (8 pages)	075313
M. Tsetseri and G. P. Triberis	

Direct observation of LO phonon-plasmon coupled modes in the infrared transmission spectra of n -GaAs and n -In _x Ga _{1-x} As epilayers (8 pages)	075314
J. Ibáñez, Enver Tarhan, A. K. Ramdas, S. Hernández, R. Cuscó, L. Artús, M. R. Melloch, and M. Hopkinson	
Split gate nanoscale Coulomb driven stochastic resonance mechanism for separating like-charged impurities in semiconductors (7 pages)	075315
V. Narayan and S. Stafström	
Masking by weak localization of metallic behavior in a two-dimensional electron system in strong parallel magnetic fields (6 pages)	075316
A. Lewalle, M. Pepper, C. J. B. Ford, D. J. Paul, and G. Redmond	
SiGe/Si(001) Stranski-Krastanow islands by liquid-phase epitaxy: Diffuse x-ray scattering versus growth observations (7 pages)	075317
M. Hanke, M. Schmidbauer, D. Grigoriev, H. Raidt, P. Schäfer, R. Köhler, A.-K. Gerlitzke, and H. Wawra	
Electron transport through interacting quantum dots in the metallic regime (22 pages)	075318
Dmitri S. Golubev and Andrei D. Zaikin	
Spin precession and oscillations in mesoscopic systems (8 pages)	075319
Martin Y. Veillette, Cristina Bena, and Leon Balents	
Theory of quantum optical control of a single spin in a quantum dot (8 pages)	075320
Pochung Chen, C. Piermarocchi, L. J. Sham, D. Gammon, and D. G. Steel	
Solvable regime of disorder and interactions in ballistic nanostructures: Consequences for Coulomb blockade (33 pages)	075321
Ganpathy Murthy, R. Shankar, Damir Herman, and Harsh Mathur	
Surface physics, low-dimensional systems, and related topics	
Surface properties of CeO ₂ from first principles (8 pages)	075401
N. V. Skorodumova, M. Baudin, and K. Hermansson	
Electronic states and quantum transport in double-wall carbon nanotubes (10 pages)	075402
Seiji Uryu	
Photoluminescence from an individual single-walled carbon nanotube (5 pages)	075403
J. Lefebvre, J. M. Fraser, P. Finnie, and Y. Homma	
Growth and properties of strained VO _x thin films with controlled stoichiometry (11 pages)	075404
A. D. Rata, A. R. Chezan, M. W. Haverkort, H. H. Hsieh, H.-J. Lin, C. T. Chen, L. H. Tjeng, and T. Hibma	
Theoretical modeling of photon- and electron-stimulated Na and K desorption from SiO ₂ (7 pages)	075405
D. Domínguez-Ariza, N. Lopez, F. Illas, G. Pacchioni, and T. E. Madey	
Coarsening of multicomponent thin films (13 pages)	075406
David N. Brunelli and Rex T. Skodje	
Discrete-event analytic technique for surface growth problems (5 pages)	075407
A. Kolakowska and M. A. Novotny	
Structural evolution of pentacene on a Ag(110) surface (5 pages)	075408
Y. L. Wang, W. Ji, D. X. Shi, S. X. Du, C. Seidel, Y. G. Ma, H.-J. Gao, L. F. Chi, and H. Fuchs	
First-principles study of H ₂ O diffusion on a metal surface: H ₂ O on Al{100} (4 pages)	075409
A. Michaelides, V. A. Ranea, P. L. de Andres, and D. A. King	
Low-energy electron diffraction study of Xe adsorption on the ten-fold decagonal Al-Ni-Co quasicrystal surface (6 pages)	075410
N. Ferralis, R. D. Diehl, K. Pussi, M. Lindroos, I. Fisher, and C. J. Jenks	
Structure and energetics of polyhydroxylated carbon fullerenes (13 pages)	075411
J. G. Rodríguez-Zavala and R. A. Guirado-López	

Metal-cluster nanoarrays on Si(111)7×7: Rate equations and kinetic Monte Carlo simulations (5 pages)	075412
E. Vasco	
Molecular adsorption on the surface of strongly correlated transition-metal oxides: A case study for CO/NiO(100) (13 pages)	075413
A. Rohrbach, J. Hafner, and G. Kresse	
Stable geometries and magnetic properties of single-walled carbon nanotubes doped with 3d transition metals: A first-principles study (9 pages)	075414
Yosuke Yagi, Tina M. Briere, Marcel H. F. Sluiter, Vijay Kumar, Amir A. Farajian, and Yoshiyuki Kawazoe	
Complete measurement of the surface second-harmonic magneto-optical Kerr effect for permalloy films (6 pages)	075415
Charles W. Teplin, Debra Krause, Drew Marcy, and Charles T. Rogers	
Analysis of the substrate influence on the ordering of epitaxial molecular layers: The special case of point-on-line coincidence (9 pages)	075416
S. C. B Mannsfeld and T. Fritz	
Electronic properties of potassium-intercalated C ₆₀ peapods (7 pages)	075417
X. Liu, T. Pichler, M. Knupfer, J. Fink, and H. Kataura	
Oxygen-dosage effect on the structure and composition of ultrathin NiO layers reactively grown on Ag(001) (7 pages)	075418
C. Giovanardi, A. di Bona, and S. Valeri	
Isomeric structures and electronic properties of A ₄ B ₄ (A,B=Na, Mg, Al, and Si) binary clusters (10 pages)	075419
Chiranjib Majumder and S. K. Kulshreshtha	
Friction mechanisms of graphite from a single-atomic tip to a large-area flake tip (9 pages)	075420
Kouji Miura, Naruo Sasaki, and Shu Kamiya	
Thermodynamic stability of PdO surfaces (8 pages)	075421
Jutta Rogal, Karsten Reuter, and Matthias Scheffler	
Chemical and thermal stability of carbyne-like structures in cluster-assembled carbon films (7 pages)	075422
C. S. Casari, A. Li Bassi, L. Ravagnan, F. Siviero, C. Lenardi, P. Piseri, G. Bongiorno, C. E. Bottani, and P. Milani	
Atomic-scale imaging and spectroscopy of the V ₂ O ₃ (0001) surface: Bulk versus surface effects (5 pages) . . .	075423
M. Preisinger, J. Moosburger-Will, M. Klemm, S. Klimm, and S. Horn	

ERRATA

Publisher's Note: Equation of state of an anisotropic three-dimensional C ₆₀ polymer: The most stable form of fullerene [Phys. Rev. B 68 , 193414 (2003)] (1 page)	079901(E)
M. Mezouar, L. Marques, J.-L. Hodeau, V. Pischedda, and M. Nunez-Regueiro	
Erratum: Effect of isotopic composition on the lattice parameter of germanium measured by x-ray backscattering [Phys. Rev. B 67 , 113306 (2003)] (1 page)	079902(E)
M. Y. Hu, H. Sinn, A. Alatas, W. Sturhahn, E. E. Alp, H.-C. Willie, Yu. V. Shvyd'ko, J. P. Sutter, J. Bandaru, E. E. Haller, V. I. Ozogin, S. Rodriguez, R. Colella, E. Kartheuser, and M. A. Villeret	

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