

PHYSICAL REVIEW B

CONDENSED MATTER AND MATERIALS PHYSICS

THIRD SERIES, VOLUME 57, NUMBER 11

CONTENTS

15 MARCH 1998-I

BRIEF REPORTS

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

First-principles study of Zn-Sb thermoelectrics	6199
Seong-Gon Kim, I. I. Mazin, and D. J. Singh	
Temperature dependence of resistivity of quasi-one-dimensional conductors with nested electronic spectra	6204
Lev. P. Gor'kov and Mogus Mochena	
Lagrange-multiplier method in correlated-electron systems: Exact diagonalization study	6208
Takashi Yanagisawa	
Temperature-dependent electronic structure and ferromagnetism in the $d=\infty$ Hubbard model studied by a modified perturbation theory	6211
T. Wegner, M. Potthoff, and W. Nolting	
Positron-electron correlation energy in an electron gas according to the perturbed-hypernetted-chain approximation	6215
E. Boron'ski and H. Stachowiak	
Bonding of Au^+ in AuI from Mössbauer spectroscopy	6219
Jan Stanek, S. S. Hafner, and Barbara Miczko	
Spin and interaction effects on charge distribution and currents in one-dimensional conductors and rings within the Hartree-Fock approximation	6223
Avraham Cohen, Klaus Richter, and Richard Berkovits	
Electrical resistivity of single-crystal graphite under pressure: An anisotropic three-dimensional semimetal	6227
L. Edman, B. Sundqvist, E. McRae, and E. Litvin-Staszewska	
Photoinduced electronic transport in $\text{K}_{1-x}\text{Li}_x\text{TaO}_3$	6231
P. Sangalli, E. Giulotto, L. Rollandi, P. Calvi, P. Camagni, and G. Samoggia	
Scanning tunneling microscope study of charge-density-wave modulations in NbTe_4	6235
A. Prodan, S. W. Hla, V. Marinković, H. Böhm, F. W. Boswell, and J. C. Bennett	

Semiconductors I: bulk

Atomic model for the donor compensation in Cl-doped ZnTe	6239
Sun-Ghil Lee and K. J. Chang	
Antisites in silicon carbide	6243
L. Torpo, S. Pöykkö, and R. M. Nieminen	
Correlation between atomic structure and localized gap states in silicon grain boundaries	6247
Fabrizio Cleri, Pawel Koblinski, Luciano Colombo, Simon R. Phillpot, and Dieter Wolf	
Modulation instability of electromagnetic radiation in narrow-gap semiconductors	6251
V. I. Berezhiani, V. Skarka, and R. Miklaszewski	

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

First-principles calculations of the $\text{Si}(111)\text{-c}(2\times 8)$ surface	6255
Noboru Takeuchi	
$\text{Au}/\text{H}/\text{Si}(111)\text{-(}1\times 1\text{)}$ interface versus $\text{Au}/\text{Si}(111)\text{-(}7\times 7\text{)}$	6258
C. Grupp and A. Taleb-Ibrahimi	
Effect of hydrogen on the surface-energy anisotropy of diamond and silicon	6262
Suklyun Hong and M. Y. Chou	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 11

15 MARCH 1998-I

Random-cluster calculation of bond lengths in strained-semiconductor alloys	6266
J. C. Woicik	
Electric-field effects on excitons in quantum dots	6270
W. Heller, U. Bockelmann, and G. Abstreiter	
Scanning tunneling spectroscopy of a two-dimensional electron gas on the surface of ZnO	6274
M. Wolovelsky, Y. Goldstein, and O. Millo	
Magnetoluminescence study of a two-dimensional electron gas confined in diluted-magnetic-semiconductor quantum wells	6278
M. S. Salib, G. Kioseoglou, H. C. Chang, H. Luo, A. Petrou, M. Dobrowolska, J. K. Furdyna, and A. Twardowski	
$h/2e$ oscillations and quantum chaos in ballistic Aharonov-Bohm billiards	6282
Shiro Kawabata and Katsuhiko Nakamura	
Thomas-Fermi approximation in p -type δ -doped quantum wells of GaAs and Si	6286
L. M. Gaggero-Sager, M. E. Mora-Ramos, and D. A. Contreras-Solorio	
Photoluminescence spectroscopy of intersubband population inversion in a GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ triple-barrier tunneling structure	6290
Y. B. Li, J. W. Cockburn, J. P. Duck, M. J. Birkett, M. S. Skolnick, I. A. Larkin, M. Hopkinson, R. Grey, and G. Hill	
Real-time measurements of Si $2p$ core level during dry oxidation of Si(100)	6294
Y. Enta, Y. Miyanishi, H. Irimachi, M. Niwano, M. Suemitsu, N. Miyamoto, E. Shigemasa, and H. Kato	
Current-voltage instability in free-standing semiconductor quantum wires	6297
Lev G. Mouroukh	
Ga-atom-induced As rearrangement during GaAs epitaxial growth: Self-surfactant effect	6301
Kenji Shiraishi and Tomonori Ito	

Surface physics, low-dimensional systems, and related topics

Magnetic-nonmagnetic transition in fcc $4d$ -transition-metal clusters	6305
R. Guirado-López, D. Spanjaard, and M. C. Desjonquères	
Phase of RHEED oscillations	6309
Z. Mitura, S. L. Dudarev, and M. J. Whelan	
Atom transfer in the STM double-well potential during a voltage pulse	6313
P. Budau and M. Grigorescu	
Structure of the InSb(111)A- $(2\sqrt{3}\times 2\sqrt{3})$ -R30° surface and its dynamical formation processes	6317
Masayasu Nishizawa, Toyooki Eguchi, Tetsuya Misima, Jun Nakamura, and Toshiaki Osaka	
Rotational order in CO-intercalated C_{60} crystals	6321
Sander van Smaalen, Robert Dinnebier, Iwan Holleman, Gert von Helden, and Gerard Meijer	
Determination of scaling exponents in Ag(100) homoepitaxy with x-ray diffraction profiles	6325
J. Alvarez, E. Lundgren, X. Torrelles, and S. Ferrer	
Surface energy of a bounded electron gas: Analysis of the accuracy of the local-density approximation via <i>ab initio</i> self-consistent-field calculations	6329
J. M. Pitarke and A. G. Eguiluz	

ARTICLES

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

Spectral momentum density of electrons in copper	6333
X. Guo, Z. Fang, A. S. Kheifets, S. A. Canney, M. Vos, I. E. McCarthy, and E. Weigold	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 11

15 MARCH 1998-I

Hall effect in a quasi-one-dimensional system	6342
A. V. Lopatin	
Electronic structure of FeS ₂ : The crucial role of electron-lattice interaction	6350
V. Eyert, K.-H. Höck, S. Fiechter, and H. Tributsch	
Universal scaling behavior of coupled chains of interacting fermions	6360
S. Capponi, D. Poilblanc, and E. Arrigoni	
Systematic numerical study of spin-charge separation in one dimension	6370
M. G. Zacher, E. Arrigoni, W. Hanke, and J. R. Schrieffer	
Density-matrix renormalization-group study of the polaron problem in the Holstein model	6376
Eric Jeckelmann and Steven R. White	
Model of transient photoinduced absorption with an exciton polaron in conjugated polymers	6386
V. A. Shakin, S. Abe, and Y. Shimoi	
Order- <i>N</i> projection method for first-principles computations of electronic quantities and Wannier functions	6391
Uwe Stephan and David A. Drabold	
Electronic structure of <i>X</i> ₂ ZrSn- and <i>X</i> ZrSn-type Heusler alloys with <i>X</i> =Co or Ni	6408
A. Slebarski, A. Jezierski, S. Lütkehoff, and M. Neumann	
Spin polaron in a magnetic field	6413
D. Veberič, P. Prelovšek, and I. Sega	
Resonant Pd <i>L</i> ₃ - <i>M</i> _{4,5} <i>M</i> _{4,5} and <i>L</i> ₃ - <i>N</i> _{4,5} <i>N</i> _{4,5} Auger transitions	6422
T. M. Grehk, W. Drube, R. Treusch, and G. Materlik	
Cu-Au, Ag-Au, Cu-Ag, and Ni-Au intermetallics: First-principles study of temperature-composition phase diagrams and structures	6427
V. Ozoliņš, C. Wolverton, and Alex Zunger	
Theory of hole propagation in one-dimensional insulators and superconductors	6444
S. Sorella and A. Parola	
Exact ground state in an orbitally degenerate Hubbard model	6474
Shun-Qing Shen	

Semiconductors I: bulk

Luminescence properties of transition-metal-doped GaSb	6479
P. Hidalgo, B. Méndez, P. S. Dutta, J. Piqueras, and E. Dieguez	
Role of semicore <i>d</i> electrons in quasiparticle band-structure calculations	6485
Michael Rohlfing, Peter Krüger, and Johannes Pollmann	
Empirical <i>spds</i> * tight-binding calculation for cubic semiconductors: General method and material parameters	6493
Jean-Marc Jancu, Reinhard Scholz, Fabio Beltram, and Franco Bassani	
Theory of surface spin waves in ferromagnetic semiconductors	6508
J. M. Wesselinowa, E. Kroumova, N. Teofilov, and W. Nolting	
Optical spectra of silicon nanostructures from the random-matrix model	6514
V. M. Akulin, E. Borsella, G. Onida, O. Pulci, and A. Sarfati	
<i>Ab initio</i> second-harmonic susceptibilities of semiconductors: Generalized tetrahedron method and quasiparticle effects	6519
B. Adolph and F. Bechstedt	

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

Electron injection into conduction bands of the diamond (100) surface by nitrogen impurities	6527
Yoshiyuki Miyamoto and Mineo Saito	
Correlation between atomic-scale structure and mobility anisotropy in InAs/Ga _{1-x} In _x Sb superlattices	6534
A. Y. Lew, S. L. Zuo, E. T. Yu, and R. H. Miles	
Spontaneous symmetry breaking of magnetic polarons in low-dimensional semimagnetic structures	6540
Yu. G. Semenov and C. Benoit à la Guillaume	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 11

15 MARCH 1998-I

Heavy-hole intersubband scattering by confined optical phonons in a Si/ZnS superlattice	6550
G. Sun, Y. Lu, L. Friedman, and R. A. Soref	
Negative electron-electron drag between narrow quantum Hall channels	6561
H. C. W. Tso, D. J. W. Geldart, and P. Vasilopoulos	
Observation of direct and phonon-assisted indirect transitions in GaAs/Ga _x Al _{1-x} As multiquantum wells under hydrostatic pressure	6566
N. Dai, D. Huang, X. Q. Liu, Y. M. Mu, W. Lu, and S. C. Shen	
Shallow-impurity states of semiconductor Fibonacci superlattices	6573
A. Bruno-Alfonso, M. de Dios-Leyva, and L. E. Oliveira	
Localized-state band induced by B δ -doping in Si/Si _{1-x} Ge _x /Si quantum wells	6579
K. Schmalz, I. N. Yassievich, K. L. Wang, and S. G. Thomas	
Exciton binding energies and diamagnetic shifts in semiconductor quantum wires and quantum dots	6584
M. Bayer, S. N. Walck, T. L. Reinecke, and A. Forchel	
Interaction energy for a pair of quantum wells	6592
Bo E. Sernelius and P. Björk	
Rate equations for quantum transport in multidot systems	6602
S. A. Gurvitz	
Mechanism for persistent current in mesoscopic normal rings based on quantum Luttinger solitons	6612
E. Ben-Jacob, F. Guinea, Z. Hermon, and A. Shnirman	
Scattering theory for spin waves in quantum Hall ferromagnets	6618
J. H. Oaknin, B. Paredes, L. Martín-Moreno, and C. Tejedor	
Ballistic-electron-emission-microscopy studies on Au/SiO ₂ / <i>n</i> -type Si(100) and Ir/SiO ₂ / <i>n</i> -type Si(100) structures with very thin oxides	6623
Lidia Quattropiani, Ivan Maggio-Aprile, Philippe Niedermann, and Øystein Fischer	
Exchange interaction in <i>p</i> -type GaAs/Al _x Ga _{1-x} As heterostructures studied by magnetotransport	6629
M. Kemerink, P. M. Koenraad, and J. H. Wolter	
C ₆₀ /Ge(100)-(2×1) interfacial structure	6636
R. D. Aburano, Hawoong Hong, K.-S. Chung, M. C. Nelson, P. Zschack, H. Chen, and T.-C. Chiang	
Localized states in a strong magnetic field: Resonant scattering and the Dicke effect	6642
T. V. Shahbazyan and S. E. Ulloa	
Noise in three-dimensional nanowires	6654
A. G. Scherbakov, E. N. Bogachek, and Uzi Landman	

Surface physics, low-dimensional systems, and related topics

Photoinduced plasmon excitations in alkali-metal overlayers	6662
S. R. Barman, K. Horn, P. Häberle, H. Ishida, and A. Liebsch	
Optical-absorption spectra of inorganic fullerenelike MS ₂ (<i>M</i> =Mo, W)	6666
G. L. Frey, S. Elani, M. Homyonfer, Y. Feldman, and R. Tenne	
Band effects on inelastic scattering of low-energy ions from metallic and ionic surfaces: A formalism beyond the adiabatic molecular-orbitals calculation	6672
Evelina A. García and E. C. Goldberg	
Molecular-dynamics study of transient-diffusion mechanisms in low-temperature epitaxial growth	6685
Y. Yue, Y. K. Ho, and Z. Y. Pan	
Lattice dynamics study of zigzag and armchair carbon nanotubes	6689
A. Charlier, E. McRae, M.-F. Charlier, A. Spire, and S. Forster	
Resistivity determination from small crystallites	6697
S. Hyun, M. F. Thorpe, M. D. Jaeger, B. Golding, and A. R. Day	
Two-sphere model of photon emission from the scanning tunneling microscope	6706
A. Downes, M. E. Taylor, and M. E. Welland	
Predicting nucleation and growth processes: Atomistic modeling of metal atoms on ionic substrates	6715
J. H. Harding, A. M. Stoneham, and J. A. Venables	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 11

15 MARCH 1998-I

Multilayer adsorption of deuterium hydride on graphite	6720
Hong Wu and G. B. Hess	
Persistent currents in toroidal carbon nanotubes	6731
M. F. Lin and D. S. Chuu	
Electronic structure of acetylene on Si(111)-7×7: X-ray photoelectron and x-ray absorption spectroscopy	6738
F. Rochet, G. Dufour, P. Prieto, F. Sirotti, and F. C. Stedile	
Cumulative Author Index	6749