

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 62, NUMBER 3

CONTENTS

15 JULY 2000-I

Subject Matter Categories for Physical Review B	iii
Physical Review B Editorial Policies and Practices	iv
Physical Review B Information for Contributors	viii
Guidelines for Estimating Length for Physical Review B	xi

BRIEF REPORTS

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

Laser frequency stabilization using regenerative spectral hole burning	1473
N. M. Strickland, P. B. Sellin, Y. Sun, J. L. Carlsten, and R. L. Cone	
Splitting of triply degenerate refractive indices by photonic crystals	1477
Hideo Kosaka, Akihisa Tomita, Takayuki Kawashima, Takashi Sato, and Shojiro Kawakami	
Fermi surface of composite fermions and one-particle excitations at $\nu = \frac{1}{2}$: Effect of band-mass anisotropy	1481
D. B. Balagurov and Yu. E. Lozovik	
Specific heat of the periodic Anderson model at finite U	1485
Hong-Gang Luo and Shun-Jin Wang	
Measuring the size of excitons on isolated phenylene-vinylene chains: From dimers to polymers	1489
Gerwin H. Gelinck, Jacob J. Piet, Bas R. Wegewijs, Klaus Müllen, Jurjen Wildeman, Georges Hadzioannou, and John M. Warman	
Electron-hole liquid in the hexaborides	1492
M. E. Zhitomirsky and T. M. Rice	
Polaron features of the one-dimensional Holstein molecular crystal model	1496
V. Cataudella, G. De Filippis, and G. Iadonisi	
Role of occupied d states in the relaxation of hot electrons in Au	1500
I. Campillo, J. M. Pitarke, A. Rubio, and P. M. Echenique	
Temperature dependence of the structural parameters of the host lattice in blue bronze $K_{0.3}MoO_3$	1504
Mingliang Tian, Lin Chen, and Yuheng Zhang	
Lithium trapping by excess oxygen in WO_3 : A first-principles study	1508
G. A. de Wijs and R. A. de Groot	
Electronic structure of the superconducting layered ternary nitrides $CaTaN_2$ and $CaNbN_2$	1512
Josep M. Oliva, Ruben Weht, Pablo Ordejón, and Enric Canadell	
Fragility of photonic band gaps in inverse-opal photonic crystals	1516
Zhi-Yuan Li and Zhao-Qing Zhang	
Giant low-temperature enhancement of magneto-optic Kerr effects in $PtMnSb$	1520
R. Carey, D. M. Newman, and M. L. Wears	



Semiconductors I: bulk

First-principles study of aluminum and sodium complexes with hydrogen in silicon dioxide	1524
Marco Magagnini	
Self-interstitial in diamond	1528
Gordon Davies, Hannah Smith, and H. Kanda	
Time-resolved photoluminescence study of hydrogenated amorphous silicon nitride	1532
Kwang Soo Seol, Takashi Watanabe, Makoto Fujimaki, Hiromitsu Kato, Yoshimichi Ohki, and Makoto Takiyama	
Resonant Raman scattering in spontaneously ordered GaInP ₂	1536
Hyeonsik M. Cheong, Angelo Mascarenhas, John F. Geisz, and Jerry M. Olson	

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

High-density ultrasmall epitaxial Ge islands on Si(111) surfaces with a SiO ₂ coverage	1540
Alexander A. Shklyae, Motoshi Shibata, and Masakazu Ichikawa	
Thermodynamics of half-filled Landau levels: A study of the composite fermion mass	1544
Luis G. C. Rego	
From spatially indirect excitons to momentum-space indirect excitons by an in-plane magnetic field	1548
L. V. Butov, A. V. Mintsev, Yu. E. Lozovik, K. L. Campman, and A. C. Gossard	
Asymmetric photoluminescence spectra from excitons in a coupled microcavity	1552
M. Emam-Ismael, V. N. Astratov, M. S. Skolnick, D. M. Whittaker, and J. S. Roberts	
Structural and electronic properties of the Sn/Si(111) $\sqrt{3}\times\sqrt{3}$ R30° surface	1556
G. Profeta, A. Continenza, L. Ottaviano, W. Mannstadt, and A. J. Freeman	
Peak position of the intersubband absorption spectrum of quantum wells with controlled electron concentrations	1560
S. Tsujino, M. Rüfenacht, H. Nakajima, T. Noda, C. Metzner, and H. Sakaki	
Single-electron acoustic charge transport on shallow-etched channels in a perpendicular magnetic field	1564
J. Cunningham, V. I. Talyanskii, J. M. Shilton, M. Pepper, A. Kristensen, and P. E. Lindelof	
Dynamics of carrier tunneling between vertically aligned double quantum dots	1568
Atsushi Tackeuchi, Takamasa Kuroda, Kazuo Mase, Yoshiaki Nakata, and Naoki Yokoyama	
Frictional drag between coupled two-dimensional hole gases in GaAs/Al _{0.3} Ga _{0.7} As heterostructures	1572
C. Jörger, S. J. Cheng, H. Rubel, W. Dietsche, R. Gerhardts, P. Specht, K. Eberl, and K. v. Klitzing	
Shot noise of Coulomb drag current	1576
V. L. Gurevich and M. I. Muradov	
Transport through a coupled quantum dot system: Role of interdot interactions	1580
Sushil Lamba and S. K. Joshi	
Quantum confinement of quasi-two-dimensional E_1 excitons in Ge nanocrystals studied by resonant Raman scattering	1584
K. L. Teo, S. H. Kwok, P. Y. Yu, and Soumyendu Guha	
Transfer of coherent dynamics between discrete excitons and exciton Fano continua in quantum wells	1588
S. Arlt, J. Kunde, F. Morier-Genoud, U. Keller, and U. Siegner	
Effects of few-particle interaction on the atomiclike levels of a single strain-induced quantum dot	1592
Ross Rinaldi, Salvatore Antonaci, Massimo DeVittorio, Roberto Cingolani, Ulrich Hohenester, Elisa Molinari, Harri Lipsanen, and Jukka Tulkki	
Adsorption of benzene on Si(100) from first principles	1596
Pier Luigi Silvestrelli, Francesco Ancilotto, and Flavio Toigo	

Surface physics, low-dimensional systems, and related topics

Structures and electronic properties of small carbon nanotube tori	1600
Dong-Hwa Oh, Jung Mee Park, and Kwang S. Kim	
Unambiguous assignment of the ground state of a nearly degenerate cluster	1604
G. L. Gutsev, S. N. Khanna, and P. Jena	
Hydrogen-bonded array of NH ₂ on the Si(100) surface	1607
Jun-Hyung Cho and Kwang S. Kim	
Energetics and many-particle mechanisms of two-dimensional cluster diffusion on Cu(100) surfaces	1611
O. S. Trushin, P. Salo, and T. Ala-Nissila	
In-induced surface reconstruction on GaSb(001)	1615
Fumihiko Maeda, Munehiro Sugiyama, and Yoshio Watanabe	
Kinetic roughening during rare-gas homoepitaxy	1619
E. Nabighian, M. C. Bartelt, and X. D. Zhu	
Bilayer growth in the initial stages of Mg epitaxy on Mo(001)	1623
D. F. Droppo, C. D. Storey, and M. C. Gallagher	
Fine-structure analysis of Gd M_{45} near-edge EELS on the valence state of Gd@C ₈₂ microcrystals	1627
K. Suenaga, S. Iijima, H. Kato, and H. Shinohara	
Natural linewidth of the Ag(111) L -gap surface state as determined by photoemission spectroscopy	1631
G. Nicolay, F. Reinert, S. Schmidt, D. Ehm, P. Steiner, and S. Hüfner	
Determination of the lattice relaxation at the Yb(111) surface using chemical-shift photoelectron diffraction	1635
M. E. Dávila, S. L. Molodtsov, M. C. Asensio, and C. Laubschat	
Coherent radiation scattering by resonant nanostructures	1639
V. V. Klimov and V. S. Letokhov	
Pressure dependence of the optical absorption spectra of single-walled carbon nanotube films	1643
S. Kazaoui, N. Minami, H. Yamawaki, K. Aoki, H. Kataura, and Y. Achiba	
Pattern evolution of NiSi ₂ grown on a Si surface upon high-current pulsed Ni-ion implantation	1647
H. N. Zhu, K. Y. Gao, and B. X. Liu	
Covalent interaction of H with the d electrons at the (111) surface of Ag	1651
Geunseop Lee and E. W. Plummer	

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

Anderson-Mott transition in a magnetic field: Corrections to scaling	1655
D. Belitz and T. R. Kirkpatrick	
LDA and GGA calculations for high-pressure phase transitions in ZnO and MgO	1660
John E. Jaffe, James A. Snyder, Zijing Lin, and Anthony C. Hess	
Polarization and localization in insulators: Generating function approach	1666
Ivo Souza, Tim Wilkens, and Richard M. Martin	
Limits on phase separation for two-dimensional strongly correlated electrons	1684
W. O. Putikka and M. U. Luchini	
Bound-state instability of the chiral Luttinger liquid in one dimension	1688
A. F. Ho and P. Coleman	
Slabs of stabilized jellium: Quantum-size and self-compression effects	1699
I. Sarria, C. Henriques, C. Fiolhais, and J. M. Pitarke	
Influence of crystal structure and quasiparticle effects on second-harmonic generation: Silicon carbide polytypes	1706
B. Adolph and F. Bechstedt	

Towards grid-based $O(N)$ density-functional theory methods: Optimized nonorthogonal orbitals and multigrid acceleration	1713
J.-L. Fattebert and J. Bernholc	
Multiple-scattering EXAFS and EXELFS of titanium aluminum alloys	1723
T. Sikora, G. Hug, M. Jaouen, and J. J. Rehr	
Electronic structure and optical properties of CdMoO_4 and CdWO_4	1733
Y. Abraham, N. A. W. Holzwarth, and R. T. Williams	
Electronic structure and optical spectra of LuInCu_4 and YbMCu_4 ($M = \text{Cu, Ag, Au, Pd, and In}$)	1742
V. N. Antonov, M. Galli, F. Marabelli, A. N. Yaresko, A. Ya. Perlov, and E. Bauer	
Dielectric response of the charge-induced correlated state in the quasi-one-dimensional conductor $(\text{TMTTF})_2\text{PF}_6$	1753
F. Nad, P. Monceau, C. Carcel, and J. M. Fabre	
Mechanism for linear and nonlinear optical effects in LiB_3O_5 , CsB_3O_5 , and $\text{CsLiB}_6\text{O}_{10}$ crystals	1757
Zheshuai Lin, Jiao Lin, Zhizhong Wang, Chuangtian Chen, and Ming-Hsien Lee	
Scaling properties of one-dimensional Anderson models in an electric field: Exponential versus factorial localization	1765
Matthias Weiss, Tsampikos Kottos, and T. Geisel	
Electronic structure of α - and δ -Pu from photoelectron spectroscopy	1773
A. J. Arko, J. J. Joyce, L. Morales, J. Wills, J. Lashley, F. Wastin, and J. Rebizant	
Emission spectrum of a dipole in a semi-infinite periodic dielectric structure: Effect of the boundary	1780
A. G. Galstyan, M. E. Raikh, and Z. V. Vardeny	
Many-body vertex corrections in a one-dimensional electron system interacting with a long-range Coulomb potential	1787
B. Tanatar and E. Demirel	
^7Li NMR studies of $\text{Li}_{1-x}\text{Zn}_x\text{V}_2\text{O}_4$ and $\text{Li}(\text{V}_{1-y}\text{Ti}_y)_2\text{O}_4$	1793
W. Trinkl, N. Büttgen, H. Kaps, A. Loidl, M. Klemm, and S. Horn	

Semiconductors I: bulk

Electrical resistivity of a -SiC:H as a function of temperature: Evidence for discontinuities	1801
R. Murri, N. Pinto, G. Ambrosone, and U. Coscia	
Role of NiAs phase in pressure-induced structural phase transitions in IIA-VI chalcogenides	1806
Aparna Chakrabarti	
Lattice-strain field induced by $\{311\}$ self-interstitial defects in silicon	1815
Paola Alippi and Luciano Colombo	
Fluorine atoms in AlAs, GaAs, and InAs: Stable state, diffusion, and carrier passivation	1821
Akihito Taguchi, Takahisa Ohno, and Taizo Sasaki	
Mechanisms of the semi-insulating conversion of InP by anelastic spectroscopy	1828
R. Cantelli, F. Cordero, O. Palumbo, G. Cannelli, F. Trequattrini, G. M. Guadalupi, and B. Molinas	
Cumulant expansion approach to stimulated emission in semiconductor lasers	1835
Witold Bardyszewski, David Yevick, and Mirosław Prywata	
Generalization of $k \cdot p$ theory for periodic perturbations	1843
R. Stubner, R. Winkler, and O. Pankratov	
First-principles calculation of the interaction between nitrogen atoms and vacancies in silicon	1851
H. Sawada and K. Kawakami	
Experimental study of negative differential conductivity in GaAs:Cr	1859
R. M. Rubinger, A. G. de Oliveira, J. C. Bezerra, G. M. Ribeiro, W. N. Rodrigues, and M. V. B. Moreira	
Role of electronegativity in semiconductors: Isoelectronic S, Se, and O in ZnTe	1866
M. J. Seong, H. Alawadhi, I. Miotkowski, A. K. Ramdas, and S. Miotkowska	
Inter-valence-band electronic Raman scattering due to photoexcited holes in $\text{Ge}_{1-x}\text{Si}_x$	1873
Elena Nazvanova, Tohru Suemoto, Shoichi Maruyama, and Yukio Takano	

Defect study of light-emitting HCl-treated porous silicon	1878
S. M. Prokes, W. E. Carlos, Lenward Seals, and James L. Gole	
Semiconductors II: surfaces, interfaces, microstructures, and related topics	
Local structure of $(\text{Ge}_4\text{Si}_4)_5$ monolayer strained-layer superlattice probed by fluorescence x-ray absorption fine structure	1883
Shiqiang Wei, Hiroyuki Oyanagi, K. Sakamoto, Y. Takeda, and T. P. Pearsall	
Absence of a step-edge barrier on a polar semiconductor surface with reconstruction	1889
Makoto Itoh and Takahisa Ohno	
Size, shape, and stability of InAs quantum dots on the GaAs(001) substrate	1897
L. G. Wang, P. Kratzer, N. Moll, and M. Scheffler	
Level quantization in the narrow-gap-semiconductor quantum well in a parallel magnetic field	1905
V. K. Dugaev, V. I. Litvinov, and W. Dobrowolski	
Coulomb coupling and the role of symmetries in quantum-dot arrays for cellular automata	1912
F. Ramírez, E. Cota, and S. E. Ulloa	
Transition between compressible and incompressible states in infinite-layer fractional quantum Hall systems	1921
Sei Suzuki and Yoshio Kuramoto	
Boundary condition for the interface between silicon and silicon oxide	1929
J. U. Kim and Hong H. Lee	
Interaction-induced magnetization of a two-dimensional electron gas	1935
Felix von Oppen, Denis Ullmo, and Harold U. Baranger	
Free harmonic oscillators, Jack polynomials, and Calogero-Sutherland systems	1943
N. Gurappa and Prasanta K. Panigrahi	
Modular recursive Green's function method for ballistic quantum transport	1950
Stefan Rotter, Jian-Zhi Tang, Ludger Wirtz, Johannes Trost, and Joachim Burgdörfer	
Transport through double quantum dots	1961
R. Ziegler, C. Bruder, and Herbert Schoeller	
Measurement of semiconductor local carrier concentration from displacement current-voltage curves with a scanning vibrating probe	1971
Yutaka Majima, Yutaka Oyama, and Mitsumasa Iwamoto	
Landauer-Büttiker formula for time-dependent transport through resonant-tunneling structures: A nonequilibrium Green's function approach	1978
J. Q. You, Chi-Hang Lam, and H. Z. Zheng	
Phonon-coupled electron tunneling in two- and three-dimensional tunneling configurations	1984
E. Pazy and B. Laikhtman	
Collective modes of quantum Hall stripes	1993
R. Côté and H. A. Fertig	
Liouvillian approach to the integer quantum Hall effect transition	2008
Jairo Sinova, V. Meden, and S. M. Girvin	
Optical study of thermally annealed Er-doped hydrogenated α -Si films	2016
A. R. Zanatta and F. L. Freire, Jr.	
Luminescence decay kinetics of Mn^{2+} -doped ZnS nanoclusters grown in reverse micelles	2021
Brian A. Smith, Jin Z. Zhang, Alan Joly, and Jun Liu	
Atomic structural changes of a Br-chemisorbed Si(111)- 7×7 surface under 10–150 eV electron impact	2029
Kozo Mochiji and Masakazu Ichikawa	
Capacitance of a molecular overlayer on the silicon surface measured by scanning tunneling microscopy	2034
Ryota Akiyama, Takuya Matsumoto, and Tomoji Kawai	
First-principles electron-ion dynamics of excited systems: H-terminated Si(111) surfaces	2039
Yoshiyuki Miyamoto and Osamu Sugino	

Exciton formation assisted by LO phonons in quantum wells	2045
I.-K. Oh, Jai Singh, A. Thilagam, and A. S. Vengurlekar	
Anisotropy of the electron g factor in lattice-matched and strained-layer III-V quantum wells	2051
A. Malinowski and R. T. Harley	
Effects of electron-electron scattering on electron-beam propagation in a two-dimensional electron gas	2057
H. Predel, H. Buhmann, L. W. Molenkamp, R. N. Gurzhi, A. N. Kalinenko, A. I. Kopeliovich, and A. V. Yanovsky	
Surface physics, low-dimensional systems, and related topics	
Role of tip shape in light emission from the scanning tunneling microscope	2065
J. Aizpurua, S. P. Apell, and R. Berndt	
Atomically resolved edges and kinks of NaCl islands on Cu(111): Experiment and theory	2074
R. Bennewitz, A. S. Foster, L. N. Kantorovich, M. Bammerlin, Ch. Loppacher, S. Schär, M. Guggisberg, E. Meyer, and A. L. Shluger	
Size effect in Mn^{2+} -doped BaTiO_3 nanopowders observed by electron paramagnetic resonance	2085
R. Böttcher, C. Klimm, D. Michel, H.-C. Semmelhack, G. Völkel, H.-J. Gläsel, and E. Hartmann	
Nanofaceting of vicinal Nb(011)	2096
C. P. Flynn, W. Swiech, R. S. Appleton, and M. Ondrejcek	
Determination of step-edge orientation by helium atom scattering	2108
M. Patting, D. Fariás, and K. H. Rieder	
Surface x-ray diffraction study of the $\text{Rh}(100)(2 \times 2)\text{-O}$ reconstruction	2113
A. G. Norris, F. Schedin, G. Thornton, V. R. Dhanak, T. S. Turner, and R. McGrath	
Surface roughening in shadowing growth and etching in $2+1$ dimensions	2118
Jason T. Drotar, Y.-P. Zhao, T.-M. Lu, and G.-C. Wang	
Surface energetics in a heteroepitaxial model system: $\text{Co}/\text{Cu}(111)$	2126
J. E. Prieto, J. de la Figuera, and R. Miranda	
Ordering and percolation transitions for hard squares: Equilibrium versus nonequilibrium models for adsorbed layers with $c(2 \times 2)$ superlattice ordering	2134
Da-Jiang Liu and J. W. Evans	
Dynamics near the surface reconstruction of $\text{W}(100)$	2146
M. R. Baldan, E. Granato, and S. C. Ying	
Distorted iron films on $\text{GaAs}(001)\text{-(}4 \times 6\text{)}$	2151
R. A. Gordon, E. D. Crozier, D.-T. Jiang, T. L. Monchesky, and B. Heinrich	
Growth kinetics of $\text{CaF}_2/\text{Si}(111)$ for a two-step deposition	2158
Andreas Klust, Robert Kayser, and Joachim Wollschläger	
<i>In situ</i> x-ray diffraction topography studies on the phase formation in thin yttrium hydride films	2164
A. Remhof, G. Song, C. Sutter, D. Labergerie, M. Hübener, H. Zabel, and J. Härtwig	
Uptake of gases in bundles of carbon nanotubes	2173
George Stan, Mary J. Bojan, Stefano Curtarolo, Silvina M. Gatica, and Milton W. Cole	
Wave spectrum of multilayers with finite thicknesses of interfaces	2181
V. A. Ignatchenko, Yu. I. Mankov, and A. A. Maradudin	
Stable two-dimensional soliton supported by a local nonlinearity	2185
Er'el Granot and Boris A. Malomed	
Fano resonances in electronic transport through a single-electron transistor	2188
J. Göres, D. Goldhaber-Gordon, S. Heemeyer, M. A. Kastner, Hadas Shtrikman, D. Mahalu, and U. Meirav	
Anomalous hopping exponents of ultrathin metal films	2195
N. Marković, C. Christiansen, D. E. Grupp, A. M. Mack, G. Martinez-Arizala, and A. M. Goldman	
Electrical properties of self-assembled carbon networks	2201
L. V. Govor, M. Goldbach, I. A. Bashmakov, I. B. Butylina, and J. Parisi	

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 62, NUMBER 3

15 JULY 2000-I

<i>Ab initio</i> studies of the $\text{CoSi}_2(100)/\text{Si}(100)$ interface	2209
R. Stadler and R. Podloucky	
<i>Ab initio</i> studies of 5-atom ring carbon and silicon amorphous clusters both pure and with group-V impurities	2220
R. M. Valladares, C. C. Díaz, M. Arroyo, M. A. Mc Nelis, and Ariel A. Valladares	

COMMENTS

Comment on “Correlation holes in a spin-polarized dense electron gas”	2227
Karla Schmidt, Stefan Kurth, Jianmin Tao, and John P. Perdew	
Reply to “Comment on ‘Correlation holes in a spin-polarized dense electron gas’ ”	2232
Vitaly A. Rassolov, John A. Pople, and Mark A. Ratner	
Comment on “Local dimer-adatom stacking fault structures from 3×3 to 13×13 along $\text{Si}(111)-7\times 7$ domain boundaries”	2236
Makoto Itoh	
Cumulative Author Index	2237