

PHYSICAL REVIEW B

CONDENSED MATTER AND MATERIALS PHYSICS

THIRD SERIES, VOLUME 57, NUMBER 19

CONTENTS

15 MAY 1998-I

BRIEF REPORTS

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

Orthogonal polynomial projectors for the projector augmented wave method of electronic structure calculations	11 827
N. A. W. Holzwarth, G. E. Matthews, A. R. Tackett, and R. B. Dunning	
Real-space renormalization-group study of the Hubbard model: A modified scheme	11 831
Bibhas Bhattacharyya and Shreekantha Sil	
Gaussian-basis LDA and GGA calculations for alkali-metal equations of state	11 834
John E. Jaffe, Zijong Lin, and Anthony C. Hess	
Mott-Peierls transition in the extended Peierls-Hubbard model	11 838
Eric Jeckelmann	
Anderson transitions in three-dimensional disordered systems with randomly varying magnetic flux	11 842
Tohru Kawarabayashi, Bernhard Kramer, and Tomi Ohtsuki	
Temperature-dependent core-level x-ray photoemission spectroscopy of the organic conductors (MeCl-DCNQI) ₂ Cu, (MeBr-DCNQI) ₂ Cu, and (DI-DCNQI) ₂ Cu	11 846
O. Akaki, A. Chainani, T. Takahashi, Y. Kashimura, and R. Kato	
Hall effect in crystalline Ni-Fe-Cr alloys showing resistivity minima	11 850
S. Chakraborty and A. K. Majumdar	
Violation of Kohler's rule by the magnetoresistance of a quasi-two-dimensional organic metal	11 854
Ross H. McKenzie, J. S. Qualls, S. Y. Han, and J. S. Brooks	
Variable-range-hopping conduction and dielectric relaxation in disordered Sr _{0.97} (Ti _{1-x} Fe _x)O _{3-δ}	11 858
Chen Ang, J. R. Jurado, Zhi Yu, M. T. Colomer, J. R. Frade, and J. L. Baptista	
Ensemble properties in quantum steady-state nonequilibrium theories	11 862
Carsten Heide and Nikolai F. Schwabe	

Semiconductors I: bulk

Acceleration fluctuation scheme for diffusion noise sources within a generalized impedance field method	11 866
P. Shiktorov, E. Starikov, V. Gružinskis, L. Reggiani, T. González, J. Mateos, D. Pardo, and L. Varani	
Angular dependence of impurity scattering in nonparabolic semiconductors	11 870
A. Dutta, P. S. Mallick, and D. Mukhopadhyay	
High-magnetic-field effects on the terahertz mobility of hot electrons in <i>n</i> -type InSb	11 872
E. W. S. Caetano, E. A. Mendes, V. N. Freire, J. A. P. da Costa, and X. L. Lei	
Transverse electric-field-induced magnetophonon resonance in <i>n</i> -type germanium	11 875
S. C. Lee, Y. B. Kang, G. Y. Hu, J. Y. Ryu, and S. D. Choi	

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

Suppression of Ostwald ripening in In _{0.5} Ga _{0.5} As quantum dots on a vicinal (100) substrate	11 879
Byung Don Min, Yong Kim, Eun Kyu Kim, Suk-Ki Min, and Mann Jang Park	
Surface structure of cesium adsorption on the Si(001) 2×1 surface	11 883
H. Hamamatsu, H. W. Yeom, T. Yokoyama, T. Kayama, and T. Ohta	
Excited Wannier-Stark states in the optical absorption of a superlattice in an electric field	11 887
S. Glutsch and F. Bechstedt	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 19

15 MAY 1998-I

Transport through an interacting quantum dot coupled to two superconducting leads	11 891
Kicheon Kang	
Change of Hall conductance induced by band crossing	11 895
Ming-Yi Lee, Ming-Che Chang, and Tzay-Ming Hong	
Tunneling spectrum of a strongly driven double-well diode	11 899
Mathias Wagner	
Discontinuity in the phase evolution of electron transport in a quantum channel with attached quantum dots	11 903
Hongqi Xu and Weidong Sheng	
Magnetoconductance of a quantum wire with several antidots: A transfer-matrix study	11 907
C. C. Wan, Tiago De Jesus, and Hong Guo	
Spin-orbit interaction in a two-dimensional electron gas in a InAs/AlSb quantum well with gate-controlled electron density	11 911
J. P. Heida, B. J. van Wees, J. J. Kuipers, T. M. Klapwijk, and G. Borghs	
Resistance resonance induced by electron-hole hybridization in a strongly coupled InAs/GaSb/AlSb heterostructure	11 915
L. J. Cooper, N. K. Patel, V. Drouot, E. H. Linfield, D. A. Ritchie, and M. Pepper	
Raman study of the nitrided GaAs thin layers	11 919
Eui Kwan Koh, Young Ju Park, Eun Kyu Kim, Suk-Ki Min, and Sung Ho Choh	

Surface physics, low-dimensional systems, and related topics

Edge-driven transition in the surface structure of nanoscale silicon	11 923
Sohrab Ismail-Beigi and Tomás Arias	
Surface flatness and structure of the <i>bc</i> -cleaved plane of spin-Peierls material CuGeO ₃	11 927
I. Tsukada, N. Koide, Y. Sasago, and K. Uchinokura	
Adsorption of water on MgO(100): A singular behavior	11 931
C. Girardet, P. N. M. Hoang, A. Marmier, and S. Picaud	
In-plane magnetic anisotropy of bcc Co on GaAs(001)	11 935
Y. Z. Wu, H. F. Ding, C. Jing, D. Wu, G. L. Liu, V. Gordon, G. S. Dong, X. F. Jin, S. Zhu, and K. Sun	
Charge transfer and doping-dependent hybridization of C ₆₀ on noble metals	11 939
B. W. Hoogenboom, R. Hesper, L. H. Tjeng, and G. A. Sawatzky	
Electronic-momentum distribution in deformed sodium clusters	11 943
A. Rigo, M. Casas, F. Garcias, E. Moya de Guerra, and P. Sarriuren	
Quasiclassical approach to the weak levitation of extended states in the quantum Hall effect	11 947
M. M. Fogler	
Femtosecond dynamics of adsorbate charge-transfer processes as probed by high-resolution core-level spectroscopy	11 951
C. Keller, M. Stichler, G. Comelli, F. Esch, S. Lizzit, D. Menzel, and W. Wurth	

ARTICLES

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

Charge-transfer metal-insulator transitions in the spin- $\frac{1}{2}$ Falicov-Kimball model	11 955
Woonki Chung and J. K. Freericks	
First-order corrections to random-phase approximation <i>GW</i> calculations in silicon and diamond	11 962
R. T. M. Ummels, P. A. Bobbert, and W. van Haeringen	
Multiple-excited-state absorption of V ²⁺ in low-field crystals: An <i>ab initio</i> model-potential embedded-cluster study	11 974
Sara López-Moraza, Luis Seijo, and Zoila Barandiarán	
Quantum Monte Carlo study of hole binding and pairing correlations in the three-band Hubbard model	11 980
M. Guerrero, J. E. Gubernatis, and Shiwei Zhang	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 19

15 MAY 1998-I

Interplay between Hund coupling and Hubbard interaction in Sr_2RuO_4	11 989
Mario Cuoco, Canio Noce, and Alfonso Romano	
Density-functional crystal orbital study on the structures and energetics of polyacetylene isomers	11 994
So Hirata, Hajime Torii, and Mitsuo Tasumi	
Potential role of silanones in the photoluminescence-excitation, visible-photoluminescence-emission, and infrared spectra of porous silicon	12 002
James L. Gole and David A. Dixon	
Total energy differences between SiC polytypes revisited	12 017
Sukit Limpijumnong and Walter R. L. Lambrecht	
Systematic study of the electronic state in θ -type BEDT-TTF organic conductors by changing the electronic correlation	12 023
Hatsumi Mori, Shoji Tanaka, and Takehiko Mori	
Electronic structure of CeSe probed by resonant photoemission spectroscopy: A test case for the single-impurity Anderson Hamiltonian	12 030
G. Chiaia, L. Duò, O. Tjernberg, M. Göthelid, M. Björkqvist, H. Kumigashira, S.-H. Yang, T. Takahashi, T. Suzuki, and I. Lindau	
Electrical transport properties of stoichiometric YbP single crystal	12 036
D. X. Li, K. Sumiyama, K. Suzuki, A. Oyamada, K. Hashi, and T. Suzuki	
Simple treatment of the metal-insulator transition: Effects of degeneracy, temperature, and applied magnetic field	12 041
Andrzej Klejnberg and Jozef Spałek	
Local-field correction for the ferromagnetic electron gas	12 056
Jener J. S. Brito	
Resonant electron-exchange excitations in transition-metal oxides	12 069
B. Fromme, M. Möller, C. Bethke, U. Brunokowski, and E. Kisker	
Three-point bounds and other estimates for strongly nonlinear composites	12 077
P. Ponte Castañeda	
Dissipation of core-hole momentum by phonons in soft-x-ray radiation processes from valence band to core level of wide-gap insulators	12 084
Tatsuya Minami and Keiichiro Nasu	
Photoluminescence studies of Sm^{2+} in the stimuable phosphor SrS:Eu,Sm	12 094
Lawrence H. Robins and J. Ari Tuchman	
Multichannel impurity scattering in a Tomonaga-Luttinger liquid	12 104
Yu-Liang Liu	
Electron distribution in MgO probed by x-ray emission	12 111
P. Jonnard, F. Vergand, C. Bonnelle, E. Orgaz, and M. Gupta	
Correlation effects in the quasi-one-dimensional charged Bose condensate	12 119
A. Gold and L. Calmels	
Impurity bands in photonic insulators	12 127
N. Stefanou and A. Modinos	
Ternary transition-metal aluminide alloy formation: The BiF_3 structure	12 134
R. E. Watson, M. Weinert, and M. Alatalo	

Semiconductors I: bulk

Diffusion quantum Monte Carlo calculations of the excited states of silicon	12 140
A. J. Williamson, Randolph Q. Hood, R. J. Needs, and G. Rajagopal	
Stochastic model of plasma waves for a simple band structure in semiconductors	12 145
M. Zakari	
Neutral-donor-bound-exciton complexes in ZnO crystals	12 151
D. C. Reynolds, D. C. Look, B. Jogai, C. W. Litton, T. C. Collins, W. Harsch, and G. Cantwell	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 19

15 MAY 1998-I

Resonant and nonresonant polarons in bulk InSb	12 156
P. Pfeffer	
Chlorine-impurity-related defects in ZnSe	12 164
S. Pöykkö, M. J. Puska, and R. M. Nieminen	
<i>DX</i> -center transformation of Te donors in GaSb under hydrostatic pressure	12 169
H. Navarro-Contreras, F. de Anda-Salazar, Leon Hsu, and E. E. Haller	
Nitrogen-impurity-native-defect complexes in ZnSe	12 174
S. Pöykkö, M. J. Puska, and R. M. Nieminen	
Band-gap states of Ti, V, and Cr in 4 <i>H</i> -SiC: Identification and characterization by elemental transmutation of radioactive isotopes	12 181
Norbert Achtziger and Wolfgang Witthuhn	
Raman-scattering study of photoexcited plasma in semiconducting and semi-insulating InP	12 197
R. Cuscó, J. Ibáñez, and L. Artús	
Ultrafast charge recombination in undoped amorphous hydrogenated silicon	12 207
Ilya A. Shkrob and Robert A. Crowell	
Electron momentum distributions in elemental semiconductors probed by positrons	12 219
Z. Tang, M. Hasegawa, T. Chiba, M. Saito, H. Sumiya, Y. Kawazoe, and S. Yamaguchi	
Phonon conductivity in As-, Sb-, and P-doped Ge for intermediate donor concentration	12 229
M. K. Roy and B. K. Deb	
Calculation of vibrational lifetimes in amorphous silicon using molecular dynamics simulations	12 234
S. R. Bickham and J. L. Feldman	
Giant magnetoresistance in zero-band-gap $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$	12 239
Tineke Thio, S. A. Solin, J. W. Bennett, D. R. Hines, M. Kawano, N. Oda, and M. Sano	

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

Electronic and optical properties of laterally composition-modulated $\text{Al}_x\text{In}_{1-x}\text{As}$, $\text{Ga}_x\text{In}_{1-x}\text{P}$, and $\text{Ga}_x\text{In}_{1-x}\text{As}$ alloys	12 245
Yong Zhang and A. Mascarenhas	
Influence of stress and defects on the silicon-terminated SiC(001) surface structure	12 255
Alessandra Catellani, Giulia Galli, François Gygi, and Fabio Pellacini	
Vertical correlations and anticorrelations in multisheet arrays of two-dimensional islands	12 262
V. A. Shchukin, D. Bimberg, V. G. Malyshkin, and N. N. Ledentsov	
Effects of interfacial charges on semiconductor films	12 275
A. M. Alencar, R. N. Costa Filho, V. N. Freire, and G. A. Farias	
Pair-tunneling states in semiconductor quantum dots: Ground-state behavior in a magnetic field	12 281
Ernestine Lee, Aaron Puzder, M. Y. Chou, T. Uzer, and David Farrelly	
Anharmonic decay of confined optical phonons in quantum dots	12 285
Xin-Qi Li and Yasuhiko Arakawa	
Exciton fine structure in CdSe nanoclusters	12 291
K. Leung, S. Pokrant, and K. B. Whaley	
Non-Abelian geometric phases and conductance of spin- $\frac{3}{2}$ holes	12 302
Daniel P. Arovas and Yuli Lyanda-Geller	
Classical and quantum dynamics of electrons in open equilateral triangular billiards	12 306
L. Christensson, H. Linke, P. Omling, P. E. Lindelof, I. V. Zozoulenko, and K.-F. Berggren	
Si intralayers at GaAs/AlAs and GaAs/GaAs junctions: Polar versus nonpolar interfaces	12 314
M. Moreno, H. Yang, M. Höricke, M. Alonso, J. A. Martín-Gago, R. Hey, K. Horn, J. L. Sacedón, and K. H. Ploog	
Andreev reflection in the fractional quantum Hall effect	12 324
Nancy P. Sandler, Claudio de C. Chamon, and Eduardo Fradkin	
Skyrmions in arbitrarily polarized quantum Hall states	12 333
Sudhansu S. Mandal and V. Ravishankar	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 19

15 MAY 1998-I

Electron-electron interaction effect on the conductivity and the Hall conductivity of weakly disordered electron systems	12 338
Michael Reizer	
Optical-phonon-induced frictional drag in coupled two-dimensional electron gases	12 345
Ben Yu-Kuang Hu	
Edge-induced modification of tunnel mixing and resistance resonance in double-quantum-well strips	12 350
O. E. Raichev and F. T. Vasko	
1/f noise in polycrystalline silicon thin films	12 360
Laurence Michelutti	
Size dependence of exciton-exciton scattering in semiconductor quantum wires	12 364
W. Braun, M. Bayer, A. Forchel, O. M. Schmitt, L. Bányai, H. Haug, and A. I. Filin	
Femtosecond relaxation kinetics of highly excited electronic wave packets in semiconductors	12 369
K. El Sayed, J. A. Kenrow, and C. J. Stanton	
Effect of lateral confinement on valence-band mixing and polarization anisotropy in quantum wires	12 378
F. Vouilloz, D. Y. Oberli, M.-A. Dupertuis, A. Gustafsson, F. Reinhardt, and E. Kapon	
Intrasubband and intersubband transitions in lightly and heavily doped GaAs/Al _x Ga _{1-x} As multiple quantum wells	12 388
Qin-Sheng Zhu, X. B. Wang, Z. T. Zhong, X. C. Zhou, Y. P. He, Z. P. Cao, G. Z. Zhang, J. Xiao, X. H. Sun, H. Z. Yang, and Q. G. Du	
High-resolution surface-sensitive C 1s core-level spectra of clean and hydrogen-terminated diamond (100) and (111) surfaces	12 397
R. Graupner, F. Maier, J. Ristein, L. Ley, and Ch. Jung	
Compositional ordering in SiGe alloy thin films	12 410
K. L. Whiteaker, I. K. Robinson, J. E. Van Nostrand, and D. G. Cahill	
Growth mode in Si(100)-(2×1) epitaxy by low-temperature chemical-vapor deposition	12 421
Perng-Hung Wu and Deng-Sung Lin	
Tunable polariton absorption of distributed feedback microcavities at room temperature	12 428
Tohru Fujita, Yoshihiro Sato, Tetsuya Kuitani, and Teruya Ishihara	
Oblique roughness replication in strained SiGe/Si multilayers	12 435
V. Holý, A. A. Darhuber, J. Stangl, G. Bauer, J. Nützel, and G. Abstreiter	
RHEED intensity oscillations observed during the growth of CaF ₂ on Si(111)	12 443
Andrzej Daniluk, Piotr Mazurek, Krzysztof Paprocki, and Paweł Mikołajczak	
Path-integral approach to the scattering theory of quantum transport	12 448
D. Endesfelder	

Surface physics, low-dimensional systems, and related topics

Tunneling currents and boundary conditions in ballistic-electron-emission microscopy	12 456
Katsuyoshi Kobayashi	
Magnetic moments of Ni clusters	12 469
F. Aguilera-Granja, S. Bouarab, M. J. López, A. Vega, J. M. Montejano-Carrizales, M. P. Ñíguez, and J. A. Alonso	
Adsorption mechanisms, structures, and growth regimes of an archetypal self-assembling system: Decanethiol on Au(111)	12 476
F. Schreiber, A. Eberhardt, T. Y. B. Leung, P. Schwartz, S. M. Wetterer, D. J. Lavrich, L. Berman, P. Fenter, P. Eisenberger, and G. Scoles	
H-induced reconstructions on Pd(110)	12 482
V. Ledentu, W. Dong, P. Sautet, G. Kresse, and J. Hafner	
Structural model for the Si(100)4×3-In surface phase	12 492
A. V. Zotov, A. A. Saranin, V. G. Lifshits, J.-T. Ryu, O. Kubo, H. Tani, M. Katayama, and K. Oura	
Observation of domain structure and coarsening at Cu-Pd alloy vicinal surfaces	12 497
S. Goapper, L. Barbier, B. Salanon, A. Loiseau, and X. Torrelles	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 57, NUMBER 19

15 MAY 1998-I

Self-assembled islands on strained systems: Control of formation, evolution, and spatial distribution	12 501
C. A. C. Mendonça, M. A. Cotta, E. A. Meneses, and M. M. G. Carvalho	
Positron states and annihilation characteristics at the (100), (110), and (111) surfaces of alkali metals	12 506
N. G. Fazleev, J. L. Fry, and A. H. Weiss	
Bond-orientational structure and melting signature in krypton physisorbed onto graphite at complete coverage	12 520
M. W. Roth	
Epitaxial film growth of the charge-density-wave conductor $\text{Rb}_{0.30}\text{MoO}_3$ on $\text{SrTiO}_3(001)$	12 530
A. J. Steinfort, H. S. J. van der Zant, A. B. Smits, O. C. Mantel, P. M. L. O. Scholte, and C. Dekker	
Low-temperature growth morphology of singular and vicinal $\text{Ge}(001)$	12 536
Joseph E. Van Nostrand, S. Jay Chey, and David G. Cahill	
High-resolution LEED profile analysis and diffusion barrier estimation for submonolayer homoepitaxy of $\text{Ag}/\text{Ag}(100)$	12 544
L. Bardotti, C. R. Stoldt, C. J. Jenks, M. C. Bartelt, J. W. Evans, and P. A. Thiel	
Electronic excitations in alkali-metal overlayers. I. Unreconstructed low-temperature phase of Li/Al	12 550
H. Ishida and A. Liebsch	
Electronic excitations in alkali-metal overlayers. II. Effects of substitutional adsorption of $\text{Na}/\text{Al}(001)$	12 558
H. Ishida and A. Liebsch	
Sputtering of high-energy particles from the $\text{Ag}\{100\}$ surface	12 564
Che-Chen Chang and Jiin-Yun Hsieh	
Forward electron emission produced in grazing ion-surface collisions: Dependence on the surface topography	12 573
G. R. Gómez, E. A. Sánchez, and O. Grizzi	
O^- formation in grazing scattering from an $\text{Al}(111)$ surface	12 579
C. Auth, H. Winter, A. G. Borisov, B. Bahrim, D. Teillet-Billy, and J. P. Gauyacq	
Nanomechanical properties of Au (111), (001), and (110) surfaces	12 588
J. D. Kiely and J. E. Houston	
Orientational ordering in films of molecular hydrogen on boron nitride: Thick (12-layer) films and bilayer films	12 595
Kiho Kim and N. S. Sullivan	
Kinetic-energy functionals studied by surface calculations	12 611
L. Vitos, H. L. Skriver, and J. Kollár	

Errata

Erratum: Simple but efficient correlation functional from a model pair-correlation function [Phys. Rev. B 49 , 7874 (1994)]	12 616
Emil I. Proynov and Dennis R. Salahub	
Erratum: Self-diffusion of adatoms, dimers, and vacancies on $\text{Cu}(100)$ [Phys. Rev. B 56 , 7643 (1997)]	12 617
Ghyslain Boisvert and Laurent J. Lewis	
Erratum: Evidence for an enhanced magnetoresistance accompanying a continuous phase transition in semiconducting $\text{La}_{0.67}\text{Mg}_{0.33}\text{MnO}_3$ [Phys. Rev. B 56 , 12 714 (1997)]	12 617
X. Z. Zhou, H. P. Kunkel, J. H. Zhao, P. A. Stampe, and Gwyn Williams	
Erratum: Full nonlinear closure for a hydrodynamic model of transport in silicon [Phys. Rev. B 57 , 4456 (1998)]	12 617
M. Trovato and P. Falsaperla	

Cumulative Author Index	12 618
-------------------------------	--------