

RAPID COMMUNICATIONS

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

- Strongly correlated electron systems: Photoemission and the single-impurity model R7041
A. J. Arko, J. J. Joyce, A. B. Andrews, J. D. Thompson, J. L. Smith, D. Mandrus, M. F. Hundley,
A. L. Cornelius, E. Moshopoulou, Z. Fisk, P. C. Canfield, and Alois Menovsky
- Global quantum fluctuations in metallic particles R7045
J. A. Vergés, E. Cuevas, E. Louis, and M. Ortuño
- Nature of the insulating state in LaH_3 R7049
X. W. Wang and Changfeng Chen
- Metal-insulator transition in the mixed-valence manganites R7053
L. Sheng, D. Y. Xing, D. N. Sheng, and C. S. Ting
- Metal-insulator transition in layered manganites: $(\text{La}_{1-z}\text{Nd}_z)_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$ R7057
Y. Moritomo, Y. Maruyama, T. Akimoto, and A. Nakamura
- Observation of a gap opening in FeSi with photoelectron spectroscopy R7061
K. Breuer, S. Messerli, D. Purdie, M. Garnier, M. Hengsberger, Y. Baer, and M. Mihalik

Semiconductors I: bulk

- Quasiparticle calculations of semicore states in Si, Ge, and CdS R7065
Michael Rohlfing, Peter Krüger, and Johannes Pollmann
- Stranski-Krastanov growth mode during the molecular beam epitaxy of highly strained GaN R7069
B. Daudin, F. Widmann, G. Feuillet, Y. Samson, M. Arlery, and J. L. Rouvière

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

- Ab initio* modeling of a diffusion mode for a Si ad-dimer on the Si(001) surface R7073
C. M. Goringe and D. R. Bowler
- Manifestation of coherent spin precession in stimulated semiconductor emission dynamics R7076
S. Hallstein, J. D. Berger, M. Hilpert, H. C. Schneider, W. W. Rühle, F. Jahnke, S. W. Koch, H. M. Gibbs,
G. Khitrova, and M. Oestreich
- Long-range behavior of the layer-by-layer growth in Si/Si(111)-7×7 homoepitaxy R7080
D. Y. Noh, Y. Hwu, and K. S. Liang
- Magneto-oscillations in the electroluminescence intensity of resonantly coupled GaAs-AlAs superlattices: The
magnetoexciton resonance R7084
D. Bertram, K. v. Klitzing, O. Kuhn, D. K. Maude, J. C. Portal, H. T. Grahn, and K. H. Ploog
- Addition energies of a quantum dot with harmonic electron-electron interactions R7088
Antimo Angelucci and Arturo Tagliacozzo
- One-component to two-component transition of the $\nu=2/3$ fractional quantum Hall effect in a wide quantum well
induced by an in-plane magnetic field R7092
T. S. Lay, T. Jungwirth, L. Smrčka, and M. Shayegan
- Carrier quantum confinement in self-ordered $\text{Al}_x\text{Ga}_{1-x}\text{As}$ V-groove quantum wells R7096
E. Martinet, A. Gustafsson, G. Biasiol, F. Reinhardt, E. Kapon, and K. Leifer
- Quantum Hall effect of interacting electrons in a periodic potential R7100
Daniela Pfannkuche and A. H. MacDonald



Skyrmion spin distribution and states of orbital and spin symmetry in the $\nu=1$ quantum Hall effect	R7104
E. H. Rezayi	
Zeeman splittings of excitonic transitions at the Γ point in wurtzite GaN: A magnetorefectance investigation	R7108
J. Campo, M. Julier, D. Coquillat, J. P. Lascaray, D. Scalbert, and O. Briot	
Optical observation of twinning patterns characteristic of CuPt_B atomic ordering in $\text{Ga}_{1-x}\text{InP}$	R7112
J. Sapriel and A. Hassine	

Surface physics, low-dimensional systems, and related topics

Derivative relation for thermopower in the quantum Hall regime	R7116
Steven H. Simon and Nigel R. Cooper	
Perpendicular magnetization in ultrathin electrodeposited cobalt films	R7120
J. L. Bubendorff, E. Beaurepaire, C. Mény, P. Panissod, and J. P. Bucher	

ARTICLES

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

Magnetic susceptibility and heat-capacity studies of $\text{NiS}_{2-x}\text{Se}_x$ single crystals: A study of transitions at nonzero temperature	7129
X. Yao, Y.-K. Kuo, D. K. Powell, J. W. Brill, and J. M. Honig	
Correlation effects for electron-positron momentum density in solids	7136
B. Barbiellini, M. Hakala, M. J. Puska, R. M. Nieminen, and A. A. Manuel	
Electronic-structure calculations of praseodymium metal by means of modified density-functional theory	7143
A. Svane, J. Trygg, B. Johansson, and O. Eriksson	
On-site correlation in valence and core states of ferromagnetic nickel	7149
F. Manghi, V. Bellini, and C. Arcangeli	
Enhanced $d_{x^2-y^2}$ pairing correlations in the two-leg Hubbard ladder	7162
R. M. Noack, N. Bulut, D. J. Scalapino, and M. G. Zacher	
Effects of disorder on two strongly correlated coupled chains	7167
E. Orignac and T. Giamarchi	
Electronic structure and properties of Cu_2O	7189
Eliseo Ruiz, Santiago Alvarez, Pere Alemany, and Robert A. Evarestov	
Applications of the generalized-gradient approximation to atoms, clusters, and solids	7197
In-Ho Lee and Richard M. Martin	
LDA simulations of pressure-induced anomalies in c/a and electric-field gradients for Zn and Cd	7206
D. L. Novikov, A. J. Freeman, N. E. Christensen, A. Svane, and C. O. Rodriguez	
Accurate valence band width of diamond	7215
I. Jiménez, L. J. Terminello, D. G. J. Sutherland, J. A. Carlisle, E. L. Shirley, and F. J. Himpsel	
Chemical trend of occupied and unoccupied Mn $3d$ states in MnY ($Y=\text{S,Se,Te}$)	7222
Hitoshi Sato, Takahiro Mihara, Akihito Furuta, Masamochi Tamura, Kojiro Mimura, Naohisa Happo, Masaki Taniguchi, and Yoshifumi Ueda	
Crossover between Luttinger and Fermi-liquid behavior in weakly coupled metallic chains	7232
Peter Kopietz, Volker Meden, and Kurt Schönhammer	
Electronic structure of $\text{CeNi}_{1-x}\text{Pd}_x\text{Sn}$ and LaMn ($M=\text{Ni,Cu,Pd}$)	7245
A. Slebarski, A. Jezierski, S. Mähl, M. Neumann, and G. Borstel	
Effect of lattice distortions on the competition between the double and superexchange mechanisms in LaMnO_3 ...	7255
O. N. Mryasov, R. F. Sabiryanov, A. J. Freeman, and S. S. Jaswal	
Renormalization-group approach to the metal-insulator transitions in $(\text{DCNQI})_2M$ (DCNQI is N,N' -dicyanoquinonediimine and $M=\text{Ag, Cu}$)	7262
K. Yonemitsu	
<i>Ab initio</i> calculations for the neutral and charged O vacancy in sapphire	7277
Yong-Nain Xu, Zhong-Quan Gu, Xue-Fu Zhong, and W. Y. Ching	

Theoretical analysis of the magnetic circular dichroism in the $2p3d$ and $2p4d$ x-ray emission of Gd	7285
F. M. F. de Groot, M. Nakazawa, A. Kotani, M. H. Krisch, and F. Sette	
Nonequilibrium linked cluster expansion for steady-state quantum transport	7293
Petr Král	
<i>Ab initio</i> formation energies of point defects in pure and Ge-doped SiO_2	7304
Gianfranco Pacchioni and Gianluigi Ieranò	
Symmetry reduction in group $4mm$ photonic crystals	7313
Cheryl M. Anderson and Konstantinos P. Giapis	
SiO_2 stishovite under high pressure: Dielectric and dynamical properties and the ferroelastic phase transition	7321
Changyol Lee and Xavier Gonze	

Semiconductors I: bulk

Helium in silicon: Thermal-desorption investigation of bubble precursors	7331
F. Corni, C. Nobili, G. Ottaviani, R. Tonini, G. Calzolari, G. F. Cerofolini, and G. Queirolo	
Correlated <i>ab initio</i> calculations for ground-state properties of II-VI semiconductors	7339
Martin Albrecht, Beate Paulus, and Hermann Stoll	
Hydrostatic-pressure coefficient of the indirect gap and fine structure of the valence band of $6H\text{-SiC}$	7348
F. Engelbrecht, J. Zeman, G. Wellenhofer, C. Peppermüller, R. Helbig, G. Martinez, and U. Rössler	
Electron-positron momentum distributions and positron lifetime in semiconductors in the generalized gradient approximation	7356
B. K. Panda, W. LiMing, S. Fung, and C. D. Beling	
Effective masses and valence-band splittings in GaN and AlN	7363
Kwiseon Kim, Walter R. L. Lambrecht, Benjamin Segall, and Mark van Schilfgaarde	
Cerium filling and doping of cobalt triantimonide	7376
Donald T. Morelli, Gregory P. Meisner, Baoxing Chen, Siqing Hu, and Ctirad Uher	
Negatively charged Si vacancy in $4H\text{ SiC}$: A comparison between theory and experiment	7384
T. Wimbauer, B. K. Meyer, A. Hofstaetter, A. Scharmann, and H. Overhof	
Electron-spin polarization in ferromagnetic semiconductors	7389
Masao Takahashi	
Dynamic band unblocking and leakage two-photon absorption in InSb	7395
M. P. Hasselbeck, E. W. Van Stryland, and M. Sheik-Bahae	
<i>Ab initio</i> lattice dynamics of BN and AlN: Covalent versus ionic forces	7404
Krystian Karch and Friedhelm Bechstedt	
Photocurrent enhancement in light-soaked chalcogenide glasses	7416
Naoko Toyosawa and Keiji Tanaka	
High-field spin resonance of weakly bound electrons in GaAs	7422
M. Seck, M. Potemski, and P. Wyder	
Platinum-enhanced oxidation of GaAs	7428
Tomohiro Kubota, Yoshihiro Nakato, Kenji Yoneda, and Hikaru Kobayashi	

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

Optimum widths of dimer vacancy lines on $\text{Si}(100)\text{-(}2\times 1\text{)}$	7435
M.-H. Tsai, Y.-S. Tsai, C. S. Chang, Y. Wei, and I. S. T. Tsong	
Vibrational properties and charge transfer of C_{60} adsorbed on $\text{Si}(111)\text{-(}7\times 7\text{)}$ and $\text{Si}(100)\text{-(}2\times 1\text{)}$ surfaces	7439
Shozo Suto, Kazuyuki Sakamoto, Takanori Wakita, Chang-Wu Hu, and Atsuo Kasuya	
Symmetric Sb dimers and the possibility of mixed Si-Ge layers in the $\text{Sb/Ge/Si}(100)$ surface	7446
Noboru Takeuchi	
STM tip-induced diffusion of In atoms on the $\text{Si}(111)\sqrt{3}\times\sqrt{3}\text{-In}$ surface	7449
A. A. Saranin, T. Numata, O. Kubo, H. Tani, M. Katayama, V. G. Lifshits, and K. Oura	

Electron-hole interactions in silicon nanocrystals	7455
Kevin Leung and K. B. Whaley	
Wire-width dependence of the LO-phonon splitting and photoluminescence energy in ZnSe/Cd _{0.35} Zn _{0.65} Se quantum wires	7469
G. Lermann, T. Bischof, A. Materny, W. Kiefer, T. Kümmell, G. Bacher, A. Forchel, and G. Landwehr	
Giant back-scattering resonances in edge-state transport through quantum dots	7477
J. P. Bird, M. Stopa, K. Connolly, D. P. Pivin, Jr., D. K. Ferry, Y. Aoyagi, and T. Sugano	
Effect of electron correlations and disorder on mobility and localization in quasi-one-dimensional wires	7485
J. S. Thakur and D. Neilson	
Exciton-phonon coupling in semiconductor quantum dots: Resonant Raman scattering	7491
A. V. Fedorov, A. V. Baranov, and K. Inoue	
Resonance patterns of an antidot cluster: From classical to quantum ballistics	7503
G. Kirczenow, B. L. Johnson, P. J. Kelly, C. Gould, A. S. Sachrajda, Y. Feng, and A. Delage	
Classical transport of electrons through magnetic barriers	7508
I. S. Ibrahim, V. A. Schweigert, and F. M. Peeters	
Virial expansions, exclusion statistics, and the fractional quantum Hall effect	7517
Kahren Tevosyan and A. H. MacDonald	
Spin-flip and spin-wave excitations in arbitrarily polarized quantum Hall states	7525
Sudhansu S. Mandal	
Coupled plasmon-phonon mode effects on the Coulomb drag in double-quantum-well systems	7535
K. Güven and B. Tanatar	
Magneto-optical spectroscopy of two-dimensional holes in GaAs/Al _x Ga _{1-x} As single heterojunctions	7541
O. V. Volkov, V. E. Zhitomirskii, I. V. Kukushkin, W. Dietsche, K. v. Klitzing, A. Fischer, and K. Eberl	
Phonon response of Al _x Ga _{1-x} Sb/GaSb epitaxial layers by Fourier-transform infrared-reflectance and Raman spectroscopies	7549
R. Ferrini, M. Galli, G. Guizzetti, M. Patrini, A. Bosacchi, S. Franchi, and R. Magnanini	
Bottleneck effects in the relaxation and photoluminescence of microcavity polaritons	7554
F. Tassone, C. Piermarocchi, V. Savona, A. Quattropani, and P. Schwendimann	
Stimulated emission, gain, and coherent oscillations in II-VI semiconductor microcavities	7564
P. V. Kelkar, V. G. Kozlov, A. V. Nurmikko, C.-C. Chu, J. Han, and R. L. Gunshor	
Optical spin resonance and transverse spin relaxation in magnetic semiconductor quantum wells	7574
S. A. Crooker, D. D. Awschalom, J. J. Baumberg, F. Flack, and N. Samarth	
Geometry-dependent scattering through Ballistic microstructures: Semiclassical theory beyond the stationary-phase approximation	7589
Ludger Wirtz, Jian-Zhi Tang, and Joachim Burgdörfer	
Tunneling in quantum wires: Exact solution of the spin isotropic case	7598
F. Lesage, H. Saleur, and P. Simonetti	
Surface physics, low-dimensional systems, and related topics	
Structural and electronic properties of small neutral (MgO) _n clusters	7607
E. de la Puente, A. Aguado, A. Ayuela, and J. M. López	
Sb doping of Si molecular-beam epitaxial layers: Influence of the substrate misorientation	7615
M. Ladevèze, F. Bassani, F. Arnaud d'Avitaya, G. Tréglia, C. Dubois, and R. Stuck	
Coupling effects in the excitations by an external electron beam near close particles	7623
N. Zabala, A. Rivacoba, and P. M. Echenique	
Removal of the clock reconstruction of Ni(100)-(2×2) <i>p4g</i> -N by coadsorption of K: A spot-profile-analysis low-energy-electron-diffraction and angle-resolved ultraviolet-photoemission-spectroscopy study	7636
P. Finetti, M. J. Scantlebury, J. R. Mercer, S. D'Addato, and R. McGrath	
Self-diffusion of adatoms, dimers, and vacancies on Cu(100)	7643
Ghyslain Boisvert and Laurent J. Lewis	

Local density of states from spectroscopic scanning-tunneling-microscope images: Ag(111)	7656
Jiutao Li, Wolf-Dieter Schneider, and Richard Berndt	
Surface electronic structure of the NdB ₆ (110) clean surface studied by angle-resolved photoemission spectroscopy	7660
Akinori Tanaka, Koji Tamura, Hiroshi Tsunematsu, Kazutoshi Takahashi, Masayuki Hatano, Shoji Suzuki, Shigeru Sato, Satoru Kunii, Ayumi Harasawa, Akio Kimura, and Akito Kakizaki	
Surface electron motion near monatomic steps: Two-photon photoemission studies on stepped Cu(111)	7665
X. Y. Wang, X. J. Shen, and R. M. Osgood, Jr.	
Modulation of the charge of a single-electron transistor by distant defects	7675
Neil M. Zimmerman, Jonathan L. Cobb, and Alan F. Clark	
Etching behavior of Si(001)-2×1 studied with optical anisotropy	7679
D. J. Wentink, M. Kuijper, H. Wormeester, and A. van Silfhout	
Linear and circular dichroism in photoemission angular distribution from the valence band of 1T-TaS ₂	7687
T. Matsushita, S. Imada, H. Daimon, T. Okuda, K. Yamaguchi, H. Miyagi, and S. Suga	
Tribological behavior of a polymer grafted on silanized silica probed with a nanotip	7694
T. Bouhacina, J. P. Aimé, S. Gauthier, D. Michel, and V. Heroguez	
Propagator theory of scanning tunneling microscopy	7704
C. Bracher, M. Riza, and M. Kleber	
Theoretical study of ultraviolet photoelectron spectra of carbonyl systems: CO, Cr(CO) ₆ , and CO/Cu(100)	7716
José Luis Pascual, Lars G. M. Pettersson, and Hans Ågren	
Surface-roughness fractality effects in electrical conductivity of single metallic and semiconducting films	7726
G. Palasantzas and J. Barnaś	
Cumulative Author Index	7732