PHYSICAL REVIEW B **THIRD SERIES, VOLUME 77, NUMBER 11** **MARCH 2008-15(I)**

Experimental verification of surface plasmon amplification on a metallic transmission grating *(4 pages)* 115451
D. J. Park, S. B. Choi, K. J. Ahn, D. S. Kim, J. H. Kang, Q-Han Park, M. S. Jeong, and D.-K. Ko

Static dielectric response of icosahedral fullerenes from C_{60} to C_{2160} characterized by an all-electron density functional theory *(5 pages)* 115452
Rajendra R. Zope, Tunna Baruah, Mark R. Pederson, and B. I. Dunlap

Effect of atomic-scale defects on the low-energy electronic structure of graphene: Perturbation theory and local-density-functional calculations *(9 pages)* 115453
Joongoo Kang, Junhyeok Bang, Byungki Ryu, and K. J. Chang

ERRATA

Erratum: Photoionization cross section and intersublevel transitions in a one- and two-electron spherical quantum dot with a hydrogenic impurity [Phys. Rev. B **77**, 045317 (2008)] *(1 page)* . . . . . 119901(E)
Mehmet Şahin

Publisher's Note: High-fidelity all-optical control of quantum dot spins: Detailed study of the adiabatic approach [Phys. Rev. B **77**, 115322 (2008)] *(1 page)* . . . . . 119902(E)
Erik M. Gauger, Simon C. Benjamin, Ahsan Nazir, and Brendon W. Lovett

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 77, NUMBER 11** **MARCH 2008-15(I)**

Indium adlayer kinetics on the gallium nitride (0001) surface: Monitoring indium segregation and precursor-mediated adsorption *(7 pages)* 115435
Soojeong Choi, Tong-Ho Kim, Scott Wolter, April Brown, Henry O. Everitt, Maria Losurdo, and Giovanni Bruno

Boltzmann transport and residual conductivity in bilayer graphene *(6 pages)* 115436
Shaffique Adam and S. Das Sarma

Observation of coupling between surface plasmons in index-matched hole arrays *(5 pages)* 115437
Michiel J. A. de Dood, Eduard F. C. Driessen, Daniël Stolwijk, and Martin P. van Exter

Singlet-triplet relaxation in two-electron silicon quantum dots *(5 pages)* 115438
M. Prada, R. H. Blick, and R. Joynt

Optical field control of charge transmission through a molecular wire. I. Generalized master equation description *(12 pages)* 115439
Volkhard May and Oliver Kühn

Optical field control of charge transmission through a molecular wire. II. Photoinduced removal of the Franck-Condon blockade *(11 pages)* 115440
Volkhard May and Oliver Kühn

Exciton spectra in vertical stacks of triple and quadruple quantum dots in an electric field *(17 pages)* 115441
B. Szafran, E. Barczyk, F. M. Peeters, and S. Bednarek

Quasiparticle propagation in quantum Hall systems *(16 pages)* 115442
Diptiman Sen, Michael Stone, and Smitha Vishveshwara

Simple model of van der Waals interactions between two radially deformed single-wall carbon nanotubes *(10 pages)* 115443
A. Popescu, L. M. Woods, and I. V. Bondarev

Combinatorial high-energy x-ray microbeam study of the size-dependent oxidation of Pd nanoparticles on MgO(100) *(7 pages)* 115444
P. Nolte, A. Stierle, N. Kasper, N. Y. Jin-Phillipp, H. Reichert, A. Rühm, J. Okasinski, H. Dosch, and S. Schöder

Vibronic interactions in the visible and near-infrared spectra of C_{60}^- anions *(5 pages)* 115445
Ian D. Hands, Janette L. Dunn, Colin A. Bates, Michael J. Hope, Steve R. Meech, and David L. Andrews

Dirac and Klein-Gordon particles in one-dimensional periodic potentials *(9 pages)* 115446
Michaël Barbier, F. M. Peeters, P. Vasilopoulos, and J. Milton Pereira, Jr.

Ab initio study of evolution of mechanical and transport properties of clean and contaminated Au nanowires along the deformation path *(12 pages)* 115447
Pavel Jelínek, Rubén Pérez, José Ortega, and Fernando Flores

Electronic structure of a Co-decorated vicinal Cu(775) surface: High-resolution photoemission spectroscopy *(7 pages)* 115448
S.-C. Wang, M. B. Yilmaz, K. R. Knox, N. Zaki, J. I. Dadap, T. Valla, P. D. Johnson, and R. M. Osgood, Jr.

Acoustic phonon scattering limited carrier mobility in two-dimensional extrinsic graphene *(6 pages)* 115449
E. H. Hwang and S. Das Sarma

Computational study of the thermal behavior of iron clusters on a porous substrate *(6 pages)* 115450
Anders Börjesson, Stefano Curtarolo, Avetik R. Harutyunyan, and Kim Bolton

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 77, NUMBER 11** **MARCH 2008-15(I)**

Low-energy structures of K atoms in expanded K_3C_{60} monolayers: *Ab initio* pseudopotential density-functional calculations *(5 pages)* 115418
Young-Moo Byun, Hyoung Joon Choi, Steven G. Louie, and Marvin L. Cohen

Electrodynamic effects in plasmonic nanolenses *(5 pages)* 115419
Jianhua Dai, Frantisek Čajko, Igor Tsukerman, and Mark I. Stockman

Slow-plasmon resonant-nanostrip antennas: Analysis and demonstration *(5 pages)* 115420
Thomas Søndergaard, Jonas Beermann, Alexandra Boltasseva, and Sergey I. Bozhevolnyi

Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface *(16 pages)* 115421
Jörg Behler, Karsten Reuter, and Matthias Scheffler

Effect of weak disorder on the density of states in graphene *(6 pages)* 115422
Balázs Dóra, Klaus Ziegler, and Peter Thalmeier

Quasibound states of quantum dots in single and bilayer graphene *(7 pages)* 115423
A. Matulis and F. M. Peeters

Step line tension and step morphological evolution on the Si(111) (1×1) surface *(12 pages)* 115424
A. B. Pang, K. L. Man, M. S. Altman, T. J. Stasevich, F. Szalma, and T. L. Einstein

Plasmonic band gaps of structured metallic thin films evaluated for a surface plasmon laser using the coupled-wave approach *(8 pages)* 115425
Takayuki Okamoto, Janne Simonen, and Satoshi Kawata

Simulation of refrigeration by electron emission across nanometer-scale gaps *(9 pages)* 115426
Tyler L. Westover and Timothy S. Fisher

Scaling behavior of the surface roughness of platinum films grown by oblique angle deposition *(5 pages)* 115427
A. Dolatshahi-Pirouz, M. B. Hovgaard, K. Rechendorff, J. Chevallier, M. Foss, and F. Besenbacher

Theoretical study of the lineshape of inelastic electron tunneling spectroscopy *(10 pages)* 115428
Tomomi Shimazaki and Yoshihiro Asai

Pulling the C_{60} molecule on a Si(001) surface with an STM tip: A theoretical study *(9 pages)* 115429
N. Martsinovich and L. Kantorovich

Electronic structure of Ag-adsorbed nanowire-like stripes on Si(110)-(16×2) surfaces. I. An *in situ* STM and STS experiment *(7 pages)* 115430
K. Bhattacharjee, A. Roy, K. Kundu, and B. N. Dev

Electronic structure of Ag-adsorbed nanowire-like stripes on Si(110)-(16×2) surfaces. II. A one-dimensional tight-binding model with Green's function approach *(15 pages)* 115431
K. Bhattacharjee, A. Roy, K. Kundu, and B. N. Dev

First principles study of three-dimensional polymers of C_{60}: Structure, electronic properties, and Raman spectra *(8 pages)* 115432
F. Zipoli and M. Bernasconi

Signature of chirality in scanning-probe imaging of charge flow in graphene *(5 pages)* 115433
Matthias Braun, Luca Chirolli, and Guido Burkard

Orientation of individual C_{60} molecules adsorbed on Cu(111): Low-temperature scanning tunneling microscopy and density functional calculations *(9 pages)* 115434
J. Andreas Larsson, Simon D. Elliott, James C. Greer, Jascha Repp, Gerhard Meyer, and Rolf Allenspach

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 77, NUMBER 11 MARCH 2008-15(I)

Surface physics, nanoscale physics, low-dimensional systems

Theory of the Auger decay in one-dimensional metals: Tomonaga-Luttinger model *(6 pages)* 115401
E. Perfetto

High-symmetry low-energy structures of $C_{60}H_{60}$ and related fullerenes and nanotubes *(5 pages)* 115402
Aristides D. Zdetsis

Strong coupling between a metallic nanoparticle and a single molecule *(6 pages)* 115403
Andreas Trügler and Ulrich Hohenester

Resonant two-photon photoemission study of electronically excited states at the lead phthalocyanine/graphite interface *(6 pages)* 115404
I. Yamamoto, M. Mikamori, R. Yamamoto, T. Yamada, K. Miyakubo, N. Ueno, and T. Munakata

Time-varying tip-sample force measurements and steady-state dynamics in tapping-mode atomic force microscopy *(6 pages)* 115405
Ozgur Sahin

Spin transport in proximity-induced ferromagnetic graphene *(8 pages)* 115406
Håvard Haugen, Daniel Huertas-Hernando, and Arne Brataas

Effect of rare-gas adsorption on the spin-orbit split bands of a surface alloy: Xe on Ag(111)-($\sqrt{3}\times\sqrt{3}$)$R30°$-Bi *(5 pages)* 115407
L. Moreschini, A. Bendounan, C. R. Ast, F. Reinert, M. Falub, and M. Grioni

Electronic states and magnetotransport in unipolar and bipolar graphene ribbons *(9 pages)* 115408
Alessandro Cresti, Giuseppe Grosso, and Giuseppe Pastori Parravicini

Thermodynamic Casimir effects involving interacting field theories with zero modes *(22 pages)* 115409
Daniel Grüneberg and H. W. Diehl

Effect of electron-electron interaction on the Fermi surface topology of doped graphene *(9 pages)* 115410
R. Roldán, M. P. López-Sancho, and F. Guinea

Quantitative determination of optical transmission through subwavelength slit arrays in Ag films: Role of surface wave interference and local coupling between adjacent slits *(5 pages)* 115411
D. Pacifici, H. J. Lezec, Harry A. Atwater, and J. Weiner

Density functional theory study of mercury adsorption on metal surfaces *(13 pages)* 115412
Janice A. Steckel

Dissociative adsorption of O_2 on Pt and Au surfaces: Potential-energy surfaces and electronic states *(6 pages)* 115413
Satoshi Yotsuhashi, Yuka Yamada, Tomoya Kishi, Wilson Agerico Diño, Hiroshi Nakanishi, and Hideaki Kasai

Stochastic theory for lineshape broadening in quasielastic He atom scattering with interacting adsorbates *(5 pages)* 115414
R. Martínez-Casado, J. L. Vega, A. S. Sanz, and S. Miret-Artés

Calculation of binary and ternary metallic immiscible clusters with icosahedral structures *(9 pages)* 115415
Abdiravuf A. Dzhurakhalov, Ivailo Atanasov, and Marc Hou

Raman spectroscopy of epitaxial graphene on a SiC substrate *(6 pages)* 115416
Z. H. Ni, W. Chen, X. F. Fan, J. L. Kuo, T. Yu, A. T. S. Wee, and Z. X. Shen

Defect evolution in oxide nanophases: The case of a zigzag-like TiO_x phase on Pt(111) *(8 pages)* 115417
Francesco Sedona, Gaetano Granozzi, Giovanni Barcaro, and Alessandro Fortunelli

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 77, NUMBER 11** **MARCH 2008-15(I)**

Dependence of multiple Mn^{2+} spin-flip Raman scattering in quantum wells on the magnetic field direction *(6 pages)* 115341
L. C. Smith, J. J. Davies, D. Wolverson, M. Lentze, J. Geurts, T. Wojtowicz, and G. Karczewski

Fe-induced spin-polarized electronic states in a realistic semiconductor tunnel barrier *(6 pages)* 115342
Massimiliano Marangolo and Fabio Finocchi

Femtosecond transient absorption spectroscopy of silanized silicon quantum dots *(8 pages)* 115343
Volker Kuntermann, Carla Cimpean, Georg Brehm, Guido Sauer, Carola Kryschi, and Hartmut Wiggers

Asymmetry of acceptor wave functions caused by surface-related strain and electric field in InAs *(8 pages)* 115344
S. Loth, M. Wenderoth, and R. G. Ulbrich

Hysteretic response of the electron-nuclear spin system in single $In_{0.75}Al_{0.25}As$ quantum dots: Dependences on excitation power and polarization *(5 pages)* 115345
R. Kaji, S. Adachi, H. Sasakura, and S. Muto

Influence of dephasing on the quantum Hall effect and the spin Hall effect *(7 pages)* 115346
Yanxia Xing, Qing-feng Sun, and Jian Wang

Model for the coherent optical manipulation of a single spin state in a charged quantum dot *(10 pages)* 115347
G. Slavcheva

Temperature dependence of the photoluminescence of self-assembled InAs/GaAs quantum dots in pulsed magnetic fields *(5 pages)* 115348
T. Nuytten, M. Hayne, M. Henini, and V. V. Moshchalkov

Geometry and diameter dependence of the electronic and physical properties of GaN nanowires from first principles *(12 pages)* 115349
Damien J. Carter, Julian D. Gale, Bernard Delley, and Catherine Stampfl

Origin of metallicity of $LaTiO_3/SrTiO_3$ heterostructures *(5 pages)* 115350
H. Ishida and A. Liebsch

Theory of shot noise in high-current space-charge-limited field emission *(6 pages)* 115351
L. Wu, L. K. Ang, and W. S. Koh

Anisotropic conductivity of disordered two-dimensional electron gases due to spin-orbit interactions *(7 pages)* 115352
Oleg Chalaev and Daniel Loss

Interaction effects in a two-dimensional electron gas in a random magnetic field: Implications for composite fermions and the quantum critical point *(28 pages)* 115353
T. A. Sedrakyan and M. E. Raikh

Dynamics of capillary condensation in bistable optical superlattices *(6 pages)* 115354
Zeno Gaburro, Mher Ghulinyan, Lorenzo Pavesi, Pierre Barthelemy, Costanza Toninelli, and Diederik Wiersma

Dielectric constant reduction in silicon nanostructures *(5 pages)* 115355
Han G. Yoo and Philippe M. Fauchet

Impact of oxidation-induced strain on microscopic processes related to oxidation reaction at the $SiO_2/Si(100)$ interface *(5 pages)* 115356
Toru Akiyama, Tomonori Ito, Hiroyuki Kageshima, and Masashi Uematsu

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 77, NUMBER 11** **MARCH 2008-15(I)**

Chemisorption of acetic acid on Si(100)-2×1 at room temperature *(4 pages)* 115324
Han-Koo Lee, Ki-jeong Kim, Jin-hee Han, Tai-Hee Kang, J. W. Chung, and Bongsoo Kim

Atomistic simulation of the interface structure of Si nanocrystals embedded in amorphous silica *(7 pages)* 115325
Flyura Djurabekova and Kai Nordlund

Contact dependence of the conductance of H_2 molecular junctions from first principles *(6 pages)* 115326
K. H. Khoo, J. B. Neaton, Hyoung Joon Choi, and Steven G. Louie

Signature of plasmon excitations in the stopping ratio of fast hydrogen clusters *(6 pages)* 115327
S. M. Shubeita, M. A. Sortica, P. L. Grande, J. F. Dias, and N. R. Arista

Electron tunneling spectroscopy of a quantum antidot in the integer quantum Hall regime *(10 pages)* 115328
V. J. Goldman, Jun Liu, and A. Zaslavsky

Dehydrogenation of 1,4-cyclohexadiene on Si(001): A first-principles study *(6 pages)* 115329
Jae-Kwon Ko and Jun-Hyung Cho

Crosshatching on $La_{0.5}Ca_{0.5}MnO_3$ ultrathin films epitaxially grown on $SrTiO_3$(100) *(5 pages)* 115330
Zhi-Hong Wang, O. I. Lebedev, G. Van Tendeloo, G. Cristiani, and H.-U. Habermeier

Resonant spin orientation at the exciton level anticrossing in InP quantum dots *(5 pages)* 115331
Yasuaki Masumoto, Ken Toshiyuki, Tsukasa Suzuki, and Michio Ikezawa

Wave localization in one-dimensional random structures composed of single-negative metamaterials *(8 pages)* 115332
P. Han, C. T. Chan, and Z. Q. Zhang

Conserving *GW* scheme for nonequilibrium quantum transport in molecular contacts *(22 pages)* 115333
Kristian S. Thygesen and Angel Rubio

Identification of shallow Al donors in Al-doped ZnO nanocrystals: EPR and ENDOR spectroscopy *(6 pages)* 115334
Serguei B. Orlinskii, Jan Schmidt, Pavel G. Baranov, Volker Lorrmann, Ingo Riedel, Daniel Rauh, and Vladimir Dyakonov

Dielectric mismatch effect on shallow impurity states in a semiconductor nanowire *(10 pages)* 115335
Bin Li, A. F. Slachmuylders, B. Partoens, W. Magnus, and F. M. Peeters

Self-organization of multiple polariton-polariton scattering in semiconductor microcavities *(6 pages)* 115336
D. N. Krizhanovskii, S. S. Gavrilov, A. P. D. Love, D. Sanvitto, N. A. Gippius, S. G. Tikhodeev, V. D. Kulakovskii, D. M. Whittaker, M. S. Skolnick, and J. S. Roberts

Perturbation of the magneto-optical properties of nanocrystalline CdSSe *(6 pages)* 115337
Donny Magana, Xing Wei, and Geoffrey F. Strouse

Polarization anisotropy dynamics for thin films of a conjugated polymer aligned by nanoimprinting *(8 pages)* 115338
S. A. Schmid, K. H. Yim, M. H. Chang, Z. Zheng, W. T. S. Huck, R. H. Friend, J. S. Kim, and L. M. Herz

Electron-photon interaction associated with uncertainty-based tunneling in a parallel double quantum dot *(15 pages)* 115339
Kao-Chin Lin and Der-San Chuu

Spatial and spectral shape of inhomogeneous nonequilibrium exciton-polariton condensates *(7 pages)* 115340
Michiel Wouters, Iacopo Carusotto, and Cristiano Ciuti

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 77, NUMBER 11** **MARCH 2008-15(I)**

Effects of hydrostatic pressure and aluminum concentration on the conduction-electron g factor in GaAs-(Ga,Al)As quantum wells under in-plane magnetic fields *(6 pages)* 115308
E. Reyes-Gómez, N. Raigoza, and L. E. Oliveira

Manifestation of spin-orbit interaction in tunneling between two-dimensional electron layers *(7 pages)* 115309
I. V. Rozhansky and N. S. Averkiev

Theory of magnetism in diluted magnetic semiconductor nanocrystals *(8 pages)* 115310
Shun-Jen Cheng

Five- and six-electron quantum rings in a magnetic field *(4 pages)* 115311
Y. M. Liu, G. M. Huang, and T. Y. Shi

Electronic band structure of pentacene: An experimental and theoretical study *(5 pages)* 115312
S. Berkebile, P. Puschnig, G. Koller, M. Oehzelt, F. P. Netzer, C. Ambrosch-Draxl, and M. G. Ramsey

Magneto-optical properties of multilayer graphene *(8 pages)* 115313
Mikito Koshino and Tsuneya Ando

Pseudopotential calculations of band gaps and band edges of short-period $(InAs)_n/(GaSb)_m$ superlattices with different substrates, layer orientations, and interfacial bonds *(16 pages)* 115314
Paulo Piquini, Alex Zunger, and Rita Magri

Stimulated Raman spin coherence and spin-flip induced hole burning in charged GaAs quantum dots *(5 pages)* 115315
Jun Cheng, Wang Yao, Xiaodong Xu, D. G. Steel, A. S. Bracker, D. Gammon, and L. J. Sham

Quantum dots and tunnel barriers in InAs/InP nanowire heterostructures: Electronic and optical properties *(12 pages)* 115316
Yann-Michel Niquet and Dulce Camacho Mojica

Crystal truncation planes revealed by three-dimensional reconstruction of reciprocal space *(9 pages)* 115317
I. A. Vartanyants, A. V. Zozulya, K. Mundboth, O. M. Yefanov, M.-I. Richard, E. Wintersberger, J. Stangl, A. Diaz, C. Mocuta, T. H. Metzger, G. Bauer, T. Boeck, and M. Schmidbauer

Effect of charge manipulation on scanning tunneling spectra of single Mn acceptors in InAs *(7 pages)* 115318
Felix Marczinowski, Jens Wiebe, Focko Meier, Katsushi Hashimoto, and Roland Wiesendanger

Spin resonance of electrons localized on Ge/Si quantum dots *(6 pages)* 115319
A. F. Zinovieva, A. V. Dvurechenskii, N. P. Stepina, A. S. Deryabin, A. I. Nikiforov, R. M. Rubinger, N. A. Sobolev, J. P. Leitão, and M. C. Carmo

Quantum dot defined in a two-dimensional electron gas at a n-AlGaAs/GaAs heterojunction: Simulation of electrostatic potential and charging properties *(9 pages)* 115320
S. Bednarek, K. Lis, and B. Szafran

Interaction strength and molecular orientation of a single layer of pentacene in organic-metal interface and organic-organic heterostructure *(7 pages)* 115321
Mirco Chiodi, Luca Gavioli, Marco Beccari, Valeria Di Castro, Albano Cossaro, Luca Floreano, Alberto Morgante, Aloke Kanjilal, Carlo Mariani, and Maria Grazia Betti

High-fidelity all-optical control of quantum dot spins: Detailed study of the adiabatic approach *(6 pages)* 115322
Erik M. Gauger, Simon C. Benjamin, Ahsan Nazir, and Brendon W. Lovett

Finite-temperature Bell test for quasiparticle entanglement in the Fermi sea *(6 pages)* 115323
W.-R. Hannes and M. Titov

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 77, NUMBER 11** **MARCH 2008-15(I)**

Large-scale density-functional calculations on silicon divacancies *(9 pages)* 115208
Jun-ichi Iwata, Kenji Shiraishi, and Atsushi Oshiyama

Elastic constants of silicon materials calculated as a function of temperature using a parametrization of the second-generation reactive empirical bond-order potential *(19 pages)* 115209
J. David Schall, Guangtu Gao, and Judith A. Harrison

Electronic polarization effects on charge carriers in anthracene: A valence bond study *(14 pages)* 115210
Frédéric Castet, Philippe Aurel, Alain Fritsch, Laurent Ducasse, Daniel Liotard, Mathieu Linares, Jérôme Cornil, and David Beljonne

Transport in the metallic regime of Mn-doped III-V semiconductors *(13 pages)* 115211
Louis-François Arsenault, B. Movaghar, P. Desjardins, and A. Yelon

Terahertz Zeeman spectroscopy of boron in germanium to high magnetic fields *(7 pages)* 115212
R. E. M. Vickers, R. A. Lewis, P. Fisher, and Y.-J. Wang

Valence band density of states of zinc-blende and wurtzite InN from x-ray photoemission spectroscopy and first-principles calculations *(7 pages)* 115213
P. D. C. King, T. D. Veal, C. F. McConville, F. Fuchs, J. Furthmüller, F. Bechstedt, J. Schörmann, D. J. As, K. Lischka, Hai Lu, and W. J. Schaff

All-optical octave-broad ultrafast switching of Si woodpile photonic band gap crystals *(6 pages)* 115214
Tijmen G. Euser, Adriaan J. Molenaar, J. G. Fleming, Boris Gralak, Albert Polman, and Willem L. Vos

General mobility and carrier concentration relationship in transparent amorphous indium zinc oxide films *(5 pages)* 115215
Andrew J. Leenheer, John D. Perkins, Maikel F. A. M. van Hest, Joseph J. Berry, Ryan P. O'Hayre, and David S. Ginley

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

Comparative study of screened interlayer interactions in the Coulomb drag effect in bilayer electron systems *(10 pages)* 115301
R. Asgari, B. Tanatar, and B. Davoudi

Mean-field theory of Coulomb blockade distribution for a disordered ensemble of quantum dots *(7 pages)* 115302
Akashdeep Kamra, Praveen Pathak, and Vijay A. Singh

Dynamical matrix of two-dimensional electron crystals *(11 pages)* 115303
R. Côté, M.-A. Lemonde, C. B. Doiron, and A. M. Ettouhami

Quantum dynamics in electron-nuclei coupled spin system in quantum dots: Bunching, revival, and quantum correlation in electron-spin measurements *(16 pages)* 115304
Özgür Çakır and Toshihide Takagahara

Metal-organic-silicon nanoscale contacts *(6 pages)* 115305
Adam J. Dickie and Robert A. Wolkow

Sagnac rotational phase shifts in a mesoscopic electron interferometer with spin-orbit interactions *(8 pages)* 115306
Marko Zivkovic, Markku Jääskeläinen, Christopher P. Search, and Ivana Djuric

Tunable terahertz amplification in optically excited biased semiconductor superlattices: Influence of excited excitonic states *(10 pages)* 115307
Dawei Wang, Aizhen Zhang, Lijun Yang, and Marc M. Dignam

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 77, NUMBER 11 MARCH 2008-15(I)

Kondo-hole conduction in the La-doped Kondo insulator $Ce_3Bi_4Pt_3$ *(7 pages)* 115134
T. Pietrus, H. v. Löhneysen, and P. Schlottmann

Unconventional resistivity at the border of metallic antiferromagnetism in NiS_2 *(7 pages)* 115135
P. G. Niklowitz, P. L. Alireza, M. J. Steiner, G. G. Lonzarich, D. Braithwaite, G. Knebel, J. Flouquet, and J. A. Wilson

Photoluminescence modification by a high-order photonic band with abnormal dispersion in ZnO inverse opal *(9 pages)* 115136
Heeso Noh, Michael Scharrer, Mark A. Anderson, Robert P. H. Chang, and Hui Cao

Electronic structure of $PrCoO_3$ and its temperature evolution *(8 pages)* 115137
S. K. Pandey, Swapnil Patil, V. R. R. Medicherla, R. S. Singh, and Kalobaran Maiti

Induced noncollinear magnetic order of Nd^{3+} in $NdNiO_3$ observed by resonant soft x-ray diffraction *(6 pages)* 115138
V. Scagnoli, U. Staub, Y. Bodenthin, M. García-Fernández, A. M. Mulders, G. I. Meijer, and G. Hammerl

Electrostatics in periodic boundary conditions and real-space corrections *(13 pages)* 115139
Ismaila Dabo, Boris Kozinsky, Nicholas E. Singh-Miller, and Nicola Marzari

Impact of lattice-shape moduli on band structure of photonic crystals *(4 pages)* 115140
Arash Mafi

End-current injection contacts for anisotropic materials: Fabrication and application to the quasi-one-dimensional conductor $NbSe_3$ *(5 pages)* 115141
A. F. Isakovic, K. Cicak, and R. E. Thorne

Influence of point defects on the metal-insulator transition in $BaVS_3$ *(4 pages)* 115142
Ana Akrap, Aurore Rudolf, Florence Rullier-Albenque, Helmuth Berger, and László Forró

Semiconductors I: bulk

Bulk electronic properties of $FeSi_{1-x}Ge_x$ investigated by high-resolution x-ray spectroscopies *(7 pages)* 115201
H. Yamaoka, N. Tsujii, H. Oohashi, D. Nomoto, I. Jarrige, K. Takahiro, K. Ozaki, K. Kawatsura, and Y. Takahashi

Structure and band gaps of Ga-(V) semiconductors: The challenge of Ga pseudopotentials *(8 pages)* 115202
O. Anatole von Lilienfeld and Peter A. Schultz

Dynamics of electron-nuclear and heteronuclear polarization transfers in optically oriented semi-insulating InP:Fe *(7 pages)* 115203
Atsushi Goto, Kenjiro Hashi, Tadashi Shimizu, and Shinobu Ohki

Phase diagrams of a model diluted fcc magnet with arbitrary spin and modified RKKY interaction: Influence of external magnetic field and structural short-range order *(15 pages)* 115204
Karol Szałowski and Tadeusz Balcerzak

Bulk electrical properties of rubrene single crystals: Measurements and analysis *(7 pages)* 115205
D. Braga, N. Battaglini, A. Yassar, G. Horowitz, M. Campione, A. Sassella, and A. Borghesi

Exciton emission in PTCDA thin films under uniaxial pressure *(8 pages)* 115206
V. R. Gangilenka, A. DeSilva, H. P. Wagner, R. E. Tallman, B. A. Weinstein, and R. Scholz

Nitrogen vacancies in InN: Vacancy clustering and metallic bonding from first principles *(9 pages)* 115207
X. M. Duan and C. Stampfl

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 77, NUMBER 11** **MARCH 2008-15(I)**

Optical excitation of deep defect levels in insulators within many-body perturbation theory: The *F* center in calcium fluoride *(4 pages)* 115118
Yuchen Ma and Michael Rohlfing

Knitting algorithm for calculating Green functions in quantum systems *(7 pages)* 115119
K. Kazymyrenko and X. Waintal

GaN and InN conduction-band states studied by ellipsometry *(8 pages)* 115120
Munise Rakel, Christoph Cobet, Norbert Esser, Frank Fuchs, Friedhelm Bechstedt, Rüdiger Goldhahn, Wolf Gero Schmidt, and William Schaff

Electrodynamics of the vanadium oxides VO_2 and V_2O_3 *(10 pages)* 115121
M. M. Qazilbash, A. A. Schafgans, K. S. Burch, S. J. Yun, B. G. Chae, B. J. Kim, H. T. Kim, and D. N. Basov

Theory of core-hole effects in 1*s* core-level spectroscopy of the first-row elements *(7 pages)* 115122
Shang-Peng Gao, Chris J. Pickard, Mike C. Payne, Jing Zhu, and Jun Yuan

Fractional charge perspective on the band gap in density-functional theory *(6 pages)* 115123
Aron J. Cohen, Paula Mori-Sánchez, and Weitao Yang

Slow-light enhanced collinear second-harmonic generation in two-dimensional photonic crystals *(9 pages)* 115124
Rumen Iliew, Christoph Etrich, Thomas Pertsch, and Falk Lederer

Influence of disorder on the transport properties of heavy-fermion systems *(17 pages)* 115125
Claas Grenzebach, Frithjof B. Anders, Gerd Czycholl, and Thomas Pruschke

Magic angle in electron energy loss spectra: Relativistic and dielectric corrections *(10 pages)* 115126
A. P. Sorini, J. J. Rehr, and Z. H. Levine

Material metrics for laser cooling of solids *(15 pages)* 115127
Jedo Kim, Ankur Kapoor, and Massoud Kaviany

X-ray magnetic circular dichroism and photoemission studies of ferromagnetism in $CaMn_{1-x}Ru_xO_3$ thin films *(6 pages)* 115128
K. Terai, K. Yoshii, Y. Takeda, S. I. Fujimori, Y. Saitoh, K. Ohwada, T. Inami, T. Okane, M. Arita, K. Shimada, H. Namatame, M. Taniguchi, K. Kobayashi, M. Kobayashi, and A. Fujimori

Spectral functions of two-dimensional systems with coupling of electrons to collective or localized spin degrees of freedom *(12 pages)* 115129
A. A. Katanin and V. Yu. Irkhin

Electronic properties of $Sc_5M_4Si_{10}$ (M=Co, Rh, Ir) probed by NMR and first-principles calculations *(6 pages)* 115130
C. S. Lue, R. F. Liu, Y. F. Fu, C. Cheng, and H. D. Yang

Character of eigenstates of the three-dimensional disordered Hamiltonian *(7 pages)* 115131
J. Brndiar and P. Markoš

Spin-charge filtering through a spin-orbit coupled quantum dot controlled via an Aharonov-Bohm interferometer *(8 pages)* 115132
R. J. Heary, J. E. Han, and Lingyin Zhu

Orbital hybridization and spin polarization in the resonant 1*s* photoexcitations of α-Fe_2O_3 *(7 pages)* 115133
Pieter Glatzel, Alessandro Mirone, Sigrid G. Eeckhout, Marcin Sikora, and Gabriele Giuli

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 77, NUMBER 11 MARCH 2008-15(I)

Charge and spin excitation spectra in the one-dimensional Hubbard model with next-nearest-neighbor hopping *(6 pages)* 115102
S. Nishimoto, T. Shirakawa, and Y. Ohta

Electron energy-loss study of the electronic structure of atomic scale $SrTiO_3$-$SrMnO_3$-$LaMnO_3$ superlattices *(6 pages)* 115103
Amish B. Shah, Xiaofang Zhai, Bin Jiang, Jian-Guo Wen, James N. Eckstein, and Jian-Min Zuo

Optical absorption and electronic band structure first-principles calculations of α-glycine crystals *(7 pages)* 115104
M. Z. S. Flores, V. N. Freire, R. P. dos Santos, G. A. Farias, E. W. S. Caetano, M. C. F. de Oliveira, J. R. L. Fernandez, L. M. R. Scolfaro, M. J. B. Bezerra, T. M. Oliveira, G. A. Bezerra, B. S. Cavada, and H. W. Leite Alves

Transmission through nonlinear barriers *(10 pages)* 115105
Arthur R. McGurn

Electronic band structure and exchange coupling constants in ACr_2X_4 spinels (A=Zn, Cd, Hg; X=O, S, Se) *(15 pages)* 115106
A. N. Yaresko

Effect of the boundary shape in the effective theory of fractional quantum Hall edges *(10 pages)* 115107
D. C. Cabra and N. E. Grandi

Electron localization function for two-dimensional systems *(7 pages)* 115108
E. Räsänen, A. Castro, and E. K. U. Gross

Modeling disorder in graphene *(17 pages)* 115109
Vitor M. Pereira, J. M. B. Lopes dos Santos, and A. H. Castro Neto

Electronic structure of cation-deficient CoO from first principles *(6 pages)* 115110
U. D. Wdowik and K. Parlinski

Electronic structure and lattice vibrations of $Ca_2CuO_2Cl_2$: A hybrid density functional study *(6 pages)* 115111
C. H. Patterson

Pfaffian pairing and backflow wavefunctions for electronic structure quantum Monte Carlo methods *(13 pages)* 115112
M. Bajdich, L. Mitas, L. K. Wagner, and K. E. Schmidt

Charge disproportionation and dynamics in θ-$(BEDT\text{-}TTF)_2CsZn(SCN)_4$ *(10 pages)* 115113
R. Chiba, K. Hiraki, T. Takahashi, H. M. Yamamoto, and T. Nakamura

Tuning impurity states in bilayer graphene *(10 pages)* 115114
Hari P. Dahal, A. V. Balatsky, and Jian-Xin Zhu

Doping-driven Mott transition in $La_{1-x}Sr_xTiO_3$ via simultaneous electron and hole doping of t_{2g} subbands as predicted by LDA+DMFT calculations *(5 pages)* 115115
A. Liebsch

Tight-binding energy dispersions of armchair-edge graphene nanostrips *(6 pages)* 115116
D. Gunlycke and C. T. White

Temperature-pressure phase diagram of URu_2Si_2 from resistivity measurements and ac calorimetry: Hidden order and Fermi-surface nesting *(9 pages)* 115117
E. Hassinger, G. Knebel, K. Izawa, P. Lejay, B. Salce, and J. Flouquet

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 77, NUMBER 11 MARCH 2008-15(I)

Far-field second-harmonic fingerprint of twinning in single ZnO rods *(4 pages)* 113311
S. W. Liu, H. J. Zhou, A. Ricca, R. Tian, and Min Xiao

Polarization fields in (Zn,Cd)O/ZnO quantum well structures *(4 pages)* 113312
S. Kalusniak, S. Sadofev, J. Puls, H. J. Wünsche, and F. Henneberger

Manipulating the spin texture in a spin-orbit superlattice by terahertz radiation *(4 pages)* 113313
D. V. Khomitsky

Surface physics, nanoscale physics, low-dimensional systems

Dynamics of lines and grooves on vicinal crystals: Morphological instability and surface patterning *(4 pages)* 113401
Jérôme Colin

Structural, electronic, cohesive, and elastic properties of diamondlike allotropes of crystalline C_{40} *(4 pages)* 113402
Andrey N. Enyashin and Alexander L. Ivanovskii

Metal contacts in carbon nanotube field-effect transistors: Beyond the Schottky barrier paradigm *(4 pages)* 113403
J. J. Palacios, P. Tarakeshwar, and Dae M. Kim

Kinetics of island formation in organic film growth *(4 pages)* 113404
D. Y. Zhong, M. Hirtz, W. C. Wang, R. F. Dou, L. F. Chi, and H. Fuchs

Vibration-induced correction to the current through a single molecule *(4 pages)* 113405
R. Egger and A. O. Gogolin

Multichannel interaction mechanism in a molecule-metal interface *(4 pages)* 113406
Wei Ji, Zhong-Yi Lu, and Hong-Jun Gao

Electron energy spectrum and the Berry phase in a graphite bilayer *(4 pages)* 113407
G. P. Mikitik and Yu. V. Sharlai

Aharonov-Bohm effect in the magnetoresistance of a multiwalled carbon nanotube with tunneling contacts *(4 pages)* 113408
M.-G. Kang, T. Morimoto, N. Aoki, J.-U. Bae, Y. Ochiai, and J. P. Bird

Theory of huge tunneling magnetoresistance in graphene *(4 pages)* 113409
Feng Zhai and Kai Chang

Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene *(4 pages)* 113410
Cheol-Hwan Park, Feliciano Giustino, Jessica L. McChesney, Aaron Bostwick, Taisuke Ohta, Eli Rotenberg, Marvin L. Cohen, and Steven G. Louie

Surface plasmon mediated transmission of subwavelength slits at THz frequencies *(4 pages)* 113411
T. H. Isaac, J. Gómez Rivas, J. R. Sambles, W. L. Barnes, and E. Hendry

Hydrogen absorption in oxide-supported palladium nanocrystals *(4 pages)* 113412
M. Wilde, K. Fukutani, M. Naschitzki, and H.-J. Freund

ARTICLES

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

Half semimetallic antiferromagnetism in the $Sr_2Cr\mathcal{T}O_6$ system ($\mathcal{T}$=Os,Ru) *(6 pages)* 115101
K.-W. Lee and W. E. Pickett

(Continued)