

# CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 80, NUMBER 3

JULY 2009-15(I)

|                                                                                                                                                                             |        |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|
| Existence of an upper limit on the density of excitons in carbon nanotubes by diffusion-limited exciton-exciton annihilation: Experiment and theory (10 pages) . . . . .    | 035432 |
| Yoichi Murakami and Junichiro Kono                                                                                                                                          |        |
| High-resolution scanning tunneling microscopy investigation of the (12110) and (10000) two-fold symmetric <i>d</i> -Al-Ni-Co quasicrystalline surfaces (15 pages) . . . . . | 035433 |
| R. Mäder, R. Widmer, P. Gröning, S. Deloudi, W. Steurer, M. Heggen, P. Schall, M. Feuerbacher, and O. Gröning                                                               |        |
| Probing the average size of self-assembled metal nanoparticles using x-ray standing waves (5 pages) . . . . .                                                               | 035434 |
| M. K. Tiwari, K. J. S. Sawhney, Tien-Lin Lee, S. G. Alcock, and G. S. Lodha                                                                                                 |        |
| Surface electron band structure and very low-energy electron diffraction reflectivity for Al(111) (7 pages) . . . .                                                         | 035435 |
| M. N. Read                                                                                                                                                                  |        |
| Interface states in carbon nanotube junctions: Rolling up graphene (5 pages) . . . . .                                                                                      | 035436 |
| H. Santos, A. Ayuela, W. Jaskólski, M. Pelc, and L. Chico                                                                                                                   |        |
| Graphene grown on Co(0001) films and islands: Electronic structure and its precise magnetization dependence (6 pages) . . . . .                                             | 035437 |
| A. Varykhalov and O. Rader                                                                                                                                                  |        |
| Influence of the substrate on the spin-orbit splitting in surface alloys on (111) noble-metal surfaces (6 pages) . . . . .                                                  | 035438 |
| L. Moreschini, A. Bendounan, H. Bentmann, M. Assig, K. Kern, F. Reinert, J. Henk, C. R. Ast, and M. Grioni                                                                  |        |

## COMMENTS

|                                                                                                                                              |        |
|----------------------------------------------------------------------------------------------------------------------------------------------|--------|
| Comment on “Scaling behavior of classical wave transport in mesoscopic media at the localization transition” (2 pages) . . . . .             | 037101 |
| N. Cherroret, S. E. Skipetrov, and B. A. van Tiggelen                                                                                        |        |
| Reply to “Comment on ‘Scaling behavior of classical wave transport in mesoscopic media at the localization transition’ ” (2 pages) . . . . . | 037102 |
| S. K. Cheung and Z. Q. Zhang                                                                                                                 |        |

## ERRATA

|                                                                                                                                                                                                                                                                                                                      |           |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| Erratum: Fluctuating stripes in strongly correlated electron systems and the nematic-smectic quantum phase transition [Phys. Rev. B <b>78</b> , 085124 (2008)] (1 page) . . . . .                                                                                                                                    | 039901(E) |
| Kai Sun, Benjamin M. Fregoso, Michael J. Lawler, and Eduardo Fradkin                                                                                                                                                                                                                                                 |           |
| Erratum: Coating of a layer of Au on Al <sub>13</sub> : The findings of icosahedral Al@Al <sub>12</sub> Au <sub>20</sub> <sup>-</sup> and Al <sub>12</sub> Au <sub>20</sub> <sup>2-</sup> fullerenes using <i>ab initio</i> pseudopotential calculations [Phys. Rev. B <b>79</b> , 085423 (2009)] (1 page) . . . . . | 039902(E) |
| Vijay Kumar                                                                                                                                                                                                                                                                                                          |           |
| Erratum: Characterization of the torsional piezoelectriclike response of tantalum trisulfide associated with charge-density-wave depinning [Phys. Rev. B <b>79</b> , 241110(R) (2009)] (1 page) . . . . .                                                                                                            | 039903(E) |
| J. Nichols, D. Dominko, L. Ladino, J. Zhou, and J. W. Brill                                                                                                                                                                                                                                                          |           |
| Publisher’s Note: Upconversion-induced fluorescence in multicomponent systems: Steady-state excitation power threshold [Phys. Rev. B <b>78</b> , 195112 (2008)] (1 page) . . . . .                                                                                                                                   | 039904(E) |
| A. Monguzzi, J. Mezyk, F. Scotognella, R. Tubino, and F. Meinardi                                                                                                                                                                                                                                                    |           |

|                                                                                                                                                                                                       |        |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|
|  Breaking of phase symmetry in nonequilibrium Aharonov-Bohm oscillations through a quantum dot<br>(7 pages) .....    | 035416 |
| Vadim Puller, Yigal Meir, Martin Sigrist, Klaus Ensslin, and Thomas Ihn                                                                                                                               |        |
| Voltage-induced singularities in transport through molecular junctions (13 pages) .....                                                                                                               | 035417 |
| O. Entin-Wohlman, Y. Imry, and A. Aharony                                                                                                                                                             |        |
| Lithium adsorption on MgO(100) and its defects: Charge transfer, structure, and energetics (8 pages) .....                                                                                            | 035418 |
| J. A. Farmer, N. Ruzycki, J. F. Zhu, and Charles T. Campbell                                                                                                                                          |        |
| Raman spectroscopy study of heat-treated and boron-doped double wall carbon nanotubes (14 pages) .....                                                                                                | 035419 |
| F. Villalpando-Paez, H. Son, S. G. Chou, Ge. G. Samsonidze, Y. A. Kim, H. Muramatsu, T. Hayashi, M. Endo, M. Terrones, and M. S. Dresselhaus                                                          |        |
| Spectroscopic evidence of the existence of substantial Ca 3d derived states at the Fermi level in the Ca-intercalated graphite superconductor CaC <sub>6</sub> (5 pages) .....                        | 035420 |
| H. Okazaki, R. Yoshida, K. Iwai, K. Noami, T. Muro, T. Nakamura, T. Wakita, Y. Muraoka, M. Hirai, F. Tomioka, Y. Takano, A. Takenaka, M. Toyoda, T. Oguchi, and T. Yokoya                             |        |
| Liquid n-hexane condensed in silica nanochannels: A combined optical birefringence and vapor sorption isotherm study (6 pages) .....                                                                  | 035421 |
| Andriy V. Kityk, Klaus Knorr, and Patrick Huber                                                                                                                                                       |        |
| Modification of TiO <sub>2</sub> (001) surface electronic structure by Au impurity investigated with density functional theory (9 pages) .....                                                        | 035422 |
| E. Mete, O. Gülseren, and Ş. Ellialtıoğlu                                                                                                                                                             |        |
| Density dependence of valley polarization energy for composite fermions (5 pages) .....                                                                                                               | 035423 |
| Medini Padmanabhan, T. Gokmen, and M. Shayegan                                                                                                                                                        |        |
| Pb on Mo(110) studied by scanning tunneling microscopy (5 pages) .....                                                                                                                                | 035424 |
| A. Krupski                                                                                                                                                                                            |        |
| Computational study of stripe alloy formation on stepped surfaces (6 pages) .....                                                                                                                     | 035425 |
| Michail Michailov                                                                                                                                                                                     |        |
| Initial stages of nickel oxide growth on Ag(001) by pulsed laser deposition (8 pages) .....                                                                                                           | 035426 |
| S. H. Phark, Young Jun Chang, T. W. Noh, and J.-S. Kim                                                                                                                                                |        |
| Electronic transport properties of fullerene functionalized carbon nanotubes: <i>Ab initio</i> and tight-binding calculations (4 pages) .....                                                         | 035427 |
| J. A. Fürst, J. Hashemi, T. Markussen, M. Brandbyge, A. P. Jauho, and R. M. Nieminen                                                                                                                  |        |
| Thickness dependence of Shockley-type surface states of Ag(111) ultrathin films on Si(111)7×7 substrates (5 pages) .....                                                                              | 035428 |
| Keiichi Sawa, Yuki Aoki, and Hiroyuki Hirayama                                                                                                                                                        |        |
| Stoner ferromagnetic phase of graphene in the presence of an in-plane magnetic field (6 pages) .....                                                                                                  | 035429 |
| A. Qaiumzadeh and R. Asgari                                                                                                                                                                           |        |
| Photoinduced coherent adsorbate dynamics on a metal surface: Nuclear wave-packet simulation with quasi-diabatic potential energy curves using an open-boundary cluster model approach (8 pages) ..... | 035430 |
| Tomokazu Yasuike and Katsuyuki Nobusada                                                                                                                                                               |        |
| Dye adsorbates BrPDI, BrGly, and BrAsp on anatase TiO <sub>2</sub> (001) for dye-sensitized solar cell applications (6 pages) .....                                                                   | 035431 |
| D. Çakır, O. Gülseren, E. Mete, and Ş. Ellialtıoğlu                                                                                                                                                   |        |

(Continued)

|                                                                                                                                                                   |        |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|
| Mobility dependent efficiencies of organic bulk heterojunction solar cells: Surface recombination and charge transfer state distribution ( <i>6 pages</i> ) ..... | 035334 |
| Thomas Kirchartz, Bart E. Pieters, Kurt Taretto, and Uwe Rau                                                                                                      |        |
| Phonon-assisted tunneling in a superlattice in an applied magnetic field ( <i>5 pages</i> ) .....                                                                 | 035335 |
| R. N. Kini, A. J. Kent, and M. Henini                                                                                                                             |        |
| <b>Surface physics, nanoscale physics, low-dimensional systems</b>                                                                                                |        |
| Lenosky's energy and the phonon dispersion of graphene ( <i>5 pages</i> ) .....                                                                                   | 035401 |
| S. Viola Kusminskiy, D. K. Campbell, and A. H. Castro Neto                                                                                                        |        |
| Defective to fully coordinated crossover in complex directionally bonded nanoclusters ( <i>6 pages</i> ) .....                                                    | 035402 |
| E. Flikkema and Stefan T. Bromley                                                                                                                                 |        |
| Electronic properties of H on vicinal Pt surfaces: First-principles study ( <i>7 pages</i> ) .....                                                                | 035403 |
| T. Vehviläinen, P. Salo, T. Ala-Nissila, and S. C. Ying                                                                                                           |        |
| First-principles-based embedded atom method for PdAu nanoparticles ( <i>8 pages</i> ) .....                                                                       | 035404 |
| Bin Shan, Ligen Wang, Sang Yang, Jangsuk Hyun, Neeti Kapur, Yujun Zhao, John B. Nicholas, and Kyeongjae Cho                                                       |        |
| <i>Ab initio</i> calculation of phonons for bulk TiC and TiC(001)(1×1) ( <i>9 pages</i> ) .....                                                                   | 035405 |
| S. Bağcı, T. Kamlı, H. M. Tütüncü, and G. P. Srivastava                                                                                                           |        |
| Linear response and the Thomas-Fermi approximation in undoped graphene ( <i>6 pages</i> ) .....                                                                   | 035406 |
| L. Brey and H. A. Fertig                                                                                                                                          |        |
| Asymmetrical excitation of surface plasmon polaritons on blazed gratings at normal incidence ( <i>11 pages</i> ) ....                                             | 035407 |
| Benfeng Bai, Xiangfeng Meng, Janne Laukkanen, Tristan Sfez, Libo Yu, Wataru Nakagawa, Hans Peter Herzig, Lifeng Li, and Jari Turunen                              |        |
| Magnetoresistive junctions based on epitaxial graphene and hexagonal boron nitride ( <i>5 pages</i> ) .....                                                       | 035408 |
| Oleg V. Yazyev and Alfredo Pasquarello                                                                                                                            |        |
| Temperature dependence of magnetic coupling in ultrathin NiO/Fe <sub>3</sub> O <sub>4</sub> (001) films ( <i>9 pages</i> ) .....                                  | 035409 |
| C. Boeglin, O. Ersen, M. Pilard, V. Speisser, and F. Kronast                                                                                                      |        |
| Degree of polarization of the thermal near field generated by arrays of metallic nanoparticles ( <i>4 pages</i> ) .....                                           | 035410 |
| Vassilios Yannopapas and Nikolay V. Vitanov                                                                                                                       |        |
| Acoustic modes in metallic nanoparticles: Atomistic versus elasticity modeling ( <i>7 pages</i> ) .....                                                           | 035411 |
| Nicolas Combe and Lucien Saviot                                                                                                                                   |        |
| Exchange effects in spin-polarized transport through carbon nanotube quantum dots ( <i>13 pages</i> ) .....                                                       | 035412 |
| Christoph Schenke, Sonja Koller, Leonhard Mayrhofer, and Milena Grifoni                                                                                           |        |
| Electronic structure of titania-based nanotubes investigated by EELS spectroscopy ( <i>6 pages</i> ) .....                                                        | 035413 |
| Alexandre Gloter, Christopher Ewels, Polona Umek, Denis Arcon, and Christian Colliex                                                                              |        |
| Stabilizing a molecular switch at solid surfaces: A density functional theory study of azobenzene on Cu(111), Ag(111), and Au(111) ( <i>10 pages</i> ) .....      | 035414 |
| Erik McNellis, Jörg Meyer, Abbas Dehghan Baghi, and Karsten Reuter                                                                                                |        |
| Influence of electronic effects on the surface erosion of tungsten ( <i>11 pages</i> ) .....                                                                      | 035415 |
| S. Khakshouri and D. M. Duffy                                                                                                                                     |        |

(Continued)

# CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 80, NUMBER 3

JULY 2009-15(I)

|                                                                                                                                                                                     |        |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|
| Ground state and excitations of quantum dots with magnetic impurities (15 pages) . . . . .                                                                                          | 035318 |
| Ribhu K. Kaul, Denis Ullmo, Gergely Zaránd, Shailesh Chandrasekharan, and Harold U. Baranger                                                                                        |        |
| Long tunneling contact as a probe of fractional quantum Hall neutral edge modes (5 pages) . . . . .                                                                                 | 035319 |
| B. J. Overbosch and Claudio Chamon                                                                                                                                                  |        |
| Dynamical correlations in electronic transport through a system of coupled quantum dots (14 pages) . . . . .                                                                        | 035320 |
| Grzegorz Michałek and Bogdan R. Bułka                                                                                                                                               |        |
| Tunable electron counting statistics in a quantum dot at thermal equilibrium (6 pages) . . . . .                                                                                    | 035321 |
| X. C. Zhang, G. Mazzeo, A. Brataas, M. Xiao, E. Yablonovitch, and H. W. Jiang                                                                                                       |        |
| Effect of nonuniform continuum density of states on a Fano resonance in semiconductor quantum wells (5 pages) . . . . .                                                             | 035322 |
| Jongseok Lim, W.-R. Lee, H.-S. Sim, R. D. Averitt, J. M. O. Zide, A. C. Gossard, and Jaewook Ahn                                                                                    |        |
| Probing formally forbidden optical transitions in PbSe nanocrystals by time- and energy-resolved transient absorption spectroscopy (6 pages) . . . . .                              | 035323 |
| Juleon M. Schins, M. Tuan Trinh, Arjan J. Houtepen, and Laurens D. A. Siebbeles                                                                                                     |        |
| Atomic processes in molecular beam epitaxy on strained InAs(137): A density-functional theory study (7 pages) . . . . .                                                             | 035324 |
| P. Kratzer and T. Hammerschmidt                                                                                                                                                     |        |
| Gate control of low-temperature spin dynamics in two-dimensional hole systems (7 pages) . . . . .                                                                                   | 035325 |
| M. Kugler, T. Andlauer, T. Korn, A. Wagner, S. Fehrer, R. Schulz, M. Kubová, C. Gerl, D. Schuh, W. Wegscheider, P. Vogl, and C. Schüller                                            |        |
| Dynamics of the nuclear spin polarization by optically oriented electrons in a (In,Ga)As/GaAs quantum dot ensemble (8 pages) . . . . .                                              | 035326 |
| Roman V. Cherbunin, Sergey Yu. Verbin, Thomas Auer, Dmitri R. Yakovlev, Dirk Reuter, Andreas D. Wieck, Ilya Ya. Gerlovin, Ivan V. Ignatiev, Dmitry V. Vishnevsky, and Manfred Bayer |        |
| Quantum walk on the line with quantum rings (8 pages) . . . . .                                                                                                                     | 035327 |
| Orsolya Kálmán, Tamás Kiss, and Péter Földi                                                                                                                                         |        |
| Spectral barcoding of quantum dots: Deciphering structural motifs from the excitonic spectra (7 pages) . . . . .                                                                    | 035328 |
| Vladan Mlinar and Alex Zunger                                                                                                                                                       |        |
| Shallow donor states near a semiconductor-insulator-metal interface (10 pages) . . . . .                                                                                            | 035329 |
| Y. L. Hao, A. P. Djotyan, A. A. Avetisyan, and F. M. Peeters                                                                                                                        |        |
| Multiexponential photoluminescence decay of blinking nanocrystal ensembles (9 pages) . . . . .                                                                                      | 035330 |
| K. Dunn, J. Derr, T. Johnston, M. Chaker, and F. Rosei                                                                                                                              |        |
| Defect-induced magnetic order in pure ZnO films (5 pages) . . . . .                                                                                                                 | 035331 |
| M. Khalid, M. Ziese, A. Setzer, P. Esquinazi, M. Lorenz, H. Hochmuth, M. Grundmann, D. Spemann, T. Butz, G. Brauer, W. Anwand, G. Fischer, W. A. Adeagbo, W. Hergert, and A. Ernst  |        |
| Charge relaxation resistance in the Coulomb blockade problem (20 pages) . . . . .                                                                                                   | 035332 |
| Ya. I. Rodionov, I. S. Burmistrov, and A. S. Ioselevich                                                                                                                             |        |
| Quantum efficiency of stimulated emission in colloidal semiconductor nanocrystal quantum dots (6 pages) . . . . .                                                                   | 035333 |
| Chunfeng Zhang, Jian Xu, Ting Zhu, Fan Zhang, Zhanao Tan, Steven J. Schiff, Huaipeng Su, Shuai Gao, and Andrew Y. Wang                                                              |        |

(Continued)

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

|                                                                                                                                                                                 |        |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|
| Magnetoconductance switching in an array of oval quantum dots (9 pages) . . . . .                                                                                               | 035301 |
| C. Morfonios, D. Buchholz, and P. Schmelcher                                                                                                                                    |        |
| Atomistic simulations of adiabatic coherent electron transport in triple donor systems (7 pages) . . . . .                                                                      | 035302 |
| Rajib Rahman, Seung H. Park, Jared H. Cole, Andrew D. Greentree, Richard P. Muller,<br>Gerhard Klimeck, and Lloyd C. L. Hollenberg                                              |        |
| Spin states in InAs/AlSb/GaSb semiconductor quantum wells (11 pages) . . . . .                                                                                                  | 035303 |
| Jun Li, Wen Yang, and Kai Chang                                                                                                                                                 |        |
| Full-band envelope-function approach for type-II broken-gap superlattices (7 pages) . . . . .                                                                                   | 035304 |
| Till Andlauer and Peter Vogl                                                                                                                                                    |        |
| Spin-orbit-induced anisotropic conductivity of a disordered two-dimensional electron gas (19 pages) . . . . .                                                                   | 035305 |
| Oleg Chalaev and Daniel Loss                                                                                                                                                    |        |
| Experimental and theoretical study of cross-phase modulation in InGaAs/AlAsSb coupled double quantum wells with a AlGaAs coupling barrier (10 pages) . . . . .                  | 035306 |
| G. W. Cong, R. Akimoto, K. Akita, S. Gozu, T. Mozume, T. Hasama, and H. Ishikawa                                                                                                |        |
| Emission spectrum of a two-electron quantum dot molecule driven by a strong electromagnetic field (7 pages) . . . . .                                                           | 035307 |
| Andreas F. Terzis and Emmanuel Paspalakis                                                                                                                                       |        |
| Nonequilibrium transport through a singlet-triplet Anderson impurity (5 pages) . . . . .                                                                                        | 035308 |
| P. Roura Bas and A. A. Aligia                                                                                                                                                   |        |
| Modulation of electrical conduction through individual molecules on silicon by the electrostatic fields of nearby polar molecules: Theory and experiment (21 pages) . . . . .   | 035309 |
| George Kirczenow, Paul G. Piva, and Robert A. Wolkow                                                                                                                            |        |
| Role of background impurities in the single-particle relaxation lifetime of a two-dimensional electron gas (7 pages) . . . . .                                                  | 035310 |
| S. J. MacLeod, K. Chan, T. P. Martin, A. R. Hamilton, A. See, A. P. Micolich, M. Aagesen, and<br>P. E. Lindelof                                                                 |        |
| Full counting statistics of Andreev reflection: Signatures of a quantum transition (8 pages) . . . . .                                                                          | 035311 |
| G. C. Duarte-Filho and A. M. S. Macêdo                                                                                                                                          |        |
| Effect of interdot Coulomb repulsion on tunneling current through a double quantum dot system in the weak tunneling limit: Strong electron-phonon coupling (15 pages) . . . . . | 035312 |
| Igor G. Medvedev                                                                                                                                                                |        |
| Spin relaxation in submonolayer and monolayer InAs structures grown in a GaAs matrix (5 pages) . . . . .                                                                        | 035313 |
| Chunlei Yang, Xiaodong Cui, Shun-Qing Shen, Zhongying Xu, and Weikun Ge                                                                                                         |        |
| Saturation and self-lensing in self-assembled quantum dots with constant-wave driving (6 pages) . . . . .                                                                       | 035314 |
| A. Tierno, T. Ackemann, T. Maggipinto, and M. Brambilla                                                                                                                         |        |
| Spin ordering in semiconductor heterostructures with ferromagnetic $\delta$ layers (15 pages) . . . . .                                                                         | 035315 |
| V. N. Men'shov, V. V. Tugushev, S. Caprara, P. M. Echenique, and E. V. Chulkov                                                                                                  |        |
| Band structure of segmented semiconductor nanowires (14 pages) . . . . .                                                                                                        | 035316 |
| M.-E. Pistol and C. E. Pryor                                                                                                                                                    |        |
| High-order fractional microwave-induced resistance oscillations in two-dimensional systems (5 pages) . . . . .                                                                  | 035317 |
| S. Wiedmann, G. M. Gusev, O. E. Raichev, A. K. Bakarov, and J. C. Portal                                                                                                        |        |

(Continued)

# CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 80, NUMBER 3

JULY 2009-15(I)

|                                                                                                                                                                |        |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|
| <i>Ab initio</i> study of pressure-induced metal-insulator transition in cubic FeGe (8 pages) . . . . .                                                        | 035122 |
| Matthias Neef, Klaus Doll, and Gertrud Zwicknagl                                                                                                               |        |
| Minimization of out-of-plane losses of photonic crystal membranes (8 pages) . . . . .                                                                          | 035123 |
| Rumen Iliew, Christoph Etrich, Thomas Pertsch, and Falk Lederer                                                                                                |        |
| Theory of tunneling transport in periodic chains (12 pages) . . . . .                                                                                          | 035124 |
| Emil Prodan and Roberto Car                                                                                                                                    |        |
| Exchange-correlation energy functional based on the Airy-gas reference system (10 pages) . . . . .                                                             | 035125 |
| Lucian A. Constantin, Adrienn Ruzsinszky, and John P. Perdew                                                                                                   |        |
| Density-functional theory study of polarization saturation in strained ferroelectrics (6 pages) . . . . .                                                      | 035126 |
| Yanpeng Yao and Huaxiang Fu                                                                                                                                    |        |
| Nonclassical properties of electronic states of aperiodic chains in a homogeneous electric field (7 pages) . . . .                                             | 035127 |
| B. J. Spisak and M. Wołoszyn                                                                                                                                   |        |
| Soliton wall superlattice charge-density-wave phase in the quasi-one-dimensional conductor (Per) <sub>2</sub> Pt(mnt) <sub>2</sub> (7 pages) . . . . .         | 035128 |
| Si Wu and A. G. Lebed                                                                                                                                          |        |
| Asymmetry between the electron- and hole-doped Mott transition in the periodic Anderson model (15 pages) . . . . .                                             | 035129 |
| G. Sordi, A. Amaricci, and M. J. Rozenberg                                                                                                                     |        |
| Numerical simulations of localization of electromagnetic waves in two- and three-dimensional disordered media (8 pages) . . . . .                              | 035130 |
| Ameneh Sheikhan, M. Reza Rahimi Tabar, and Muhammad Sahimi                                                                                                     |        |
| Pseudo-Jahn–Teller instability in the axial Fe <sup>+</sup> center in KTaO <sub>3</sub> (7 pages) . . . . .                                                    | 035131 |
| A. Trueba, P. García-Fernández, M. T. Barriuso, M. Moreno, and J. A. Aramburu                                                                                  |        |
| <b>Semiconductors I: bulk</b>                                                                                                                                  |        |
| Density-dependent exciton kinetics in synthetic diamond crystals (7 pages) . . . . .                                                                           | 035201 |
| N. Naka, J. Omachi, H. Sumiya, K. Tamasaku, T. Ishikawa, and M. Kuwata-Gonokami                                                                                |        |
| Dilute-defect magnetism: Origin of magnetism in nanocrystalline CeO <sub>2</sub> (7 pages) . . . . .                                                           | 035202 |
| V. Fernandes, R. J. O. Mossaneck, P. Schio, J. J. Klein, A. J. A. de Oliveira, W. A. Ortiz, N. Mattoso, J. Valada, W. H. Schreiner, M. Abbate, and D. H. Mosca |        |
| Accurate band structures and effective masses for InP, InAs, and InSb using hybrid functionals (9 pages) . . . .                                               | 035203 |
| Yoon-Suk Kim, Kerstin Hummer, and Georg Kresse                                                                                                                 |        |
| Percolation versus cluster models for multimode vibration spectra of mixed crystals: GaAsP as a case study (12 pages) . . . . .                                | 035204 |
| O. Pagès, J. Souhaby, A. V. Postnikov, and A. Chafi                                                                                                            |        |
| Group-IIIA versus IIIB delafossites: Electronic structure study (7 pages) . . . . .                                                                            | 035205 |
| Muhammad N. Huda, Yanfa Yan, Aron Walsh, Su-Huai Wei, and Mowafak M. Al-Jassim                                                                                 |        |
| Growth and band gap determination of the ZrS <sub>x</sub> Se <sub>2-x</sub> single crystal series (6 pages) . . . . .                                          | 035206 |
| Mohamed Moustafa, Thorsten Zandt, Christoph Janowitz, and Recardo Manzke                                                                                       |        |
| Molecular hydrogen in silicon: A path-integral simulation (8 pages) . . . . .                                                                                  | 035207 |
| Carlos P. Herrero and Rafael Ramírez                                                                                                                           |        |

(Continued)

# CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 80, NUMBER 3

JULY 2009-15(I)

|                                                                                                                                                                                          |        |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|
| Resistive switching and resonant tunneling in epitaxial perovskite tunnel barriers (4 pages) . . . . .                                                                                   | 035105 |
| Junwoo Son and Susanne Stemmer                                                                                                                                                           |        |
| Evolution of the electronic structure of a ferromagnetic metal: Case of SrRuO <sub>3</sub> (4 pages) . . . . .                                                                           | 035106 |
| Priya Mahadevan, F. Aryasetiawan, A. Janotti, and T. Sasaki                                                                                                                              |        |
| Evidence for strongly coupled charge-density-wave ordering in three-dimensional R <sub>5</sub> Ir <sub>4</sub> Si <sub>10</sub> compounds from optical measurements (11 pages) . . . . . | 035107 |
| Riccardo Tediosi, Fabrizio Carbone, A. B. Kuzmenko, J. Teyssier, D. van der Marel, and J. A. Mydosh                                                                                      |        |
| In-plane coupling and field enhancement in infrared metamaterial surfaces (6 pages) . . . . .                                                                                            | 035108 |
| Boubacar Kanté, André de Lustrac, and Jean Michel Lourtioz                                                                                                                               |        |
| Negative refractive index response of weakly and strongly coupled optical metamaterials (6 pages) . . . . .                                                                              | 035109 |
| Jiangfeng Zhou, Thomas Koschny, Maria Kafesaki, and Costas M. Soukoulis                                                                                                                  |        |
| Charge and spin transport in strongly correlated one-dimensional quantum systems driven far from equilibrium (18 pages) . . . . .                                                        | 035110 |
| Giuliano Benenti, Giulio Casati, Tomaž Prosen, Davide Rossini, and Marko Žnidarič                                                                                                        |        |
| Localized optical orbital approach to study localized states of light in photonic crystals (6 pages) . . . . .                                                                           | 035111 |
| Zhuo Ye, Xinhua Hu, Ming Li, Kai-Ming Ho, Jiangrong Cao, and Mamoru Miyawaki                                                                                                             |        |
| Optical and energy-loss spectra of MgO, ZnO, and CdO from <i>ab initio</i> many-body calculations (10 pages) . . .                                                                       | 035112 |
| A. Schleife, C. Rödl, F. Fuchs, J. Furthmüller, and F. Bechstedt                                                                                                                         |        |
| Suppression of the mass enhancement in CaCu <sub>3</sub> Ru <sub>4</sub> O <sub>12</sub> (5 pages) . . . . .                                                                             | 035113 |
| Soutarou Tanaka, Hiroshi Takatsu, Shingo Yonezawa, and Yoshiteru Maeno                                                                                                                   |        |
| Electronic structure and charge transfer processes in a Bi-Ca misfit cobaltate (11 pages) . . . . .                                                                                      | 035114 |
| E. Carleschi, M. Malvestuto, M. Zacchigna, A. Nicolaou, V. Brouet, S. Hébert, H. Muguerra, D. Grebille, and F. Parmigiani                                                                |        |
| Effects of contact and efficient charge transport in G4-DNA molecules (5 pages) . . . . .                                                                                                | 035115 |
| Ai-Min Guo and Shi-Jie Xiong                                                                                                                                                             |        |
| Fermi surface and surface electronic structure of delafossite PdCoO <sub>2</sub> (4 pages) . . . . .                                                                                     | 035116 |
| Kyoo Kim, Hong Chul Choi, and B. I. Min                                                                                                                                                  |        |
| Competition between spin density wave order and superconductivity in the underdoped cuprates (12 pages) . . . . .                                                                        | 035117 |
| Eun Gook Moon and Subir Sachdev                                                                                                                                                          |        |
| Excitation-energy dependence of transient grating spectroscopy in $\beta$ -carotene (10 pages) . . . . .                                                                                 | 035118 |
| Mitsuru Sugisaki, Masazumi Fujiwara, Selvakumar V. Nair, Harry E. Ruda, Richard J. Cogdell, and Hideki Hashimoto                                                                         |        |
| Kondo regime in triangular arrangements of quantum dots: Molecular orbitals, interference, and contact effects (13 pages) . . . . .                                                      | 035119 |
| E. Vernek, C. A. Büsser, G. B. Martins, E. V. Anda, N. Sandler, and S. E. Ulloa                                                                                                          |        |
| Temperature dependence of the Yb valence in YbCu <sub>5</sub> and YbCu <sub>5-x</sub> Al <sub>x</sub> Kondo compounds studied by x-ray spectroscopy (8 pages) . . . . .                  | 035120 |
| H. Yamaoka, I. Jarrige, N. Tsujii, N. Hiraoka, H. Ishii, and K-D. Tsuei                                                                                                                  |        |
| Multipole decomposition of LDA+ <i>U</i> energy and its application to actinide compounds (11 pages) . . . . .                                                                           | 035121 |
| Fredrik Bultmark, Francesco Cricchio, Oscar Grånäs, and Lars Nordström                                                                                                                   |        |

(Continued)

# CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 80, NUMBER 3

JULY 2009-15(I)

|                                                                                                                                              |        |
|----------------------------------------------------------------------------------------------------------------------------------------------|--------|
| Reversal of current blockade in nanotube-based field effect transistors through multiple trap correlations<br>(4 pages) .....                | 033402 |
| Jack Chan, Brian Burke, Kenneth Evans, Keith A. Williams, Smitha Vasudevan, Mingguo Liu,<br>Joe Campbell, and Avik W. Ghosh                  |        |
| Metallic behavior in the potassium-doped fullerene-cubane copolymer (4 pages) .....                                                          | 033403 |
| D. Quintavalle, F. Simon, G. Klupp, L. F. Kiss, G. Bortel, S. Pekker, and A. Jánossy                                                         |        |
| Tunable band gap and magnetic ordering by adsorption of molecules on graphene (4 pages) .....                                                | 033404 |
| Julia Berashevich and Tapash Chakraborty                                                                                                     |        |
| Single-component surface in binary self-assembled NaK nanoalloy clusters (4 pages) .....                                                     | 033405 |
| M. Tchapyguine, S. Legendre, A. Rosso, I. Bradeanu, G. Öhrwall, S. E. Canton, T. Andersson,<br>N. Mårtensson, S. Svensson, and O. Björneholm |        |
| First-principles analysis of lattice thermal conductivity in monolayer and bilayer graphene (4 pages) .....                                  | 033406 |
| B. D. Kong, S. Paul, M. Buongiorno Nardelli, and K. W. Kim                                                                                   |        |
| Stone-Wales defects in graphene and other planar $sp^2$ -bonded materials (4 pages) .....                                                    | 033407 |
| Jie Ma, Dario Alfè, Angelos Michaelides, and Enge Wang                                                                                       |        |
| Inelastic cotunneling mediated singlet-triplet transition in carbon nanotubes (4 pages) .....                                                | 033408 |
| S. Moriyama, J. Martinek, G. Ilnicki, T. Fuse, and K. Ishibashi                                                                              |        |
| Dispersion of metal-insulator-metal plasmon polaritons probed by cathodoluminescence imaging spectroscopy<br>(4 pages) .....                 | 033409 |
| Martin Kuttge, Wei Cai, F. Javier García de Abajo, and Albert Polman                                                                         |        |
| Dipole polarizability of isovalent carbon and boron cages and fullerenes (4 pages) .....                                                     | 033410 |
| Rajendra R. Zope and Tunna Baruah                                                                                                            |        |
| Coupled force-balance and scattering equations for nonlinear transport in quantum wires (4 pages) .....                                      | 033411 |
| Danhong Huang and Godfrey Gumbs                                                                                                              |        |
| Evidence of metallic nature of the surface bands of Au/Si(557) (4 pages) .....                                                               | 033412 |
| H. S. Kim, S. Y. Shin, S. H. Uhm, C. C. Hwang, D. Y. Noh, and J. W. Chung                                                                    |        |
| Induced current and Aharonov-Bohm effect in graphene (3 pages) .....                                                                         | 033413 |
| R. Jackiw, A. I. Milstein, S.-Y. Pi, and I. S. Terekhov                                                                                      |        |

## ARTICLES

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

|                                                                                                                                |        |
|--------------------------------------------------------------------------------------------------------------------------------|--------|
| Exact step-coupling theory for mode-coupling behavior in geometrical variation photonic crystal waveguides<br>(13 pages) ..... | 035101 |
| E. H. Khoo, A. Q. Liu, X. M. Zhang, E. P. Li, J. Li, D. Pinjala, and B. S. Luk'yanchuk                                         |        |
| Perturbation study of nonequilibrium quasiparticle spectra in an infinite-dimensional Hubbard lattice<br>(5 pages) .....       | 035102 |
| R. J. Heary and J. E. Han                                                                                                      |        |
| Correlation energy and spin susceptibility of a two-valley two-dimensional electron gas (7 pages) .....                        | 035103 |
| M. Marchi, S. De Palo, S. Moroni, and Gaetano Senatore                                                                         |        |
| Electromagnetically induced transparency and slow light in an array of metallic nanoparticles (6 pages) .....                  | 035104 |
| Vassilios Yannopapas, Emmanuel Paspalakis, and Nikolay V. Vitanov                                                              |        |

(Continued)