

RAPID COMMUNICATIONS

Electronic structure and strongly correlated systems

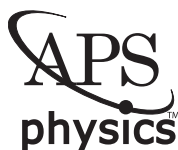
- Approximate method for controlling solid elastic waves by transformation media (*4 pages*) 201101(R)
Jin Hu, Zheng Chang, and Gengkai Hu
- Emergent electronic and magnetic state in $\text{Ca}_3\text{Ru}_2\text{O}_7$ induced by Ti doping (*4 pages*) 201102(R)
X. Ke, J. Peng, D. J. Singh, Tao Hong, Wei Tian, C. R. Dela Cruz, and Z. Q. Mao
- Topological insulators from complex orbital order in transition-metal oxides heterostructures (*5 pages*) 201103(R)
Andreas Rüegg and Gregory A. Fiete
- Possible interaction-driven topological phases in (111) bilayers of LaNiO_3 (*4 pages*) 201104(R)
Kai-Yu Yang, Wenguang Zhu, Di Xiao, Satoshi Okamoto, Ziqiang Wang, and Ying Ran
- Majorana fermions in a topological-insulator nanowire proximity-coupled to an *s*-wave superconductor (*4 pages*) 201105(R)
A. Cook and M. Franz
- Strong valence fluctuation effects in $\text{SmTr}_2\text{Al}_{20}$ ($\text{Tr} = \text{Ti, V, Cr}$) (*5 pages*) 201106(R)
Akito Sakai and Satoru Nakatsuji

Semiconductors I: bulk

- Spin-orbit coupling effect in (Ga,Mn)As films: Anisotropic exchange interactions and magnetocrystalline anisotropy (*5 pages*) 201201(R)
S. Mankovsky, S. Polesya, S. Bornemann, J. Minár, F. Hoffmann, C. H. Back, and H. Ebert

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

- Stress tuning of strong and weak couplings between quantum dots and cavity modes in microdisk microcavities (*4 pages*) 201301(R)
Hsuan Lin, Chia-Hsien Lin, Wei-Chen Lai, Yi-Shan Lee, Sheng-Di Lin, and Wen-Hao Chang
- Geometric blockade in a quantum dot coupled to two-dimensional and three-dimensional electron gases (*4 pages*) 201303(R)
K. Yamada, M. Stopa, T. Hatano, T. Yamaguchi, T. Ota, Y. Tokura, and S. Tarucha
- Strain effects on the electronic structure of SrTiO_3 : Toward high electron mobilities (*4 pages*) 201304(R)
A. Janotti, D. Steiauf, and C. G. Van de Walle
- Anomalous mass enhancement in strongly correlated quantum wells (*5 pages*) 201305(R)
Satoshi Okamoto



CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Thermopower with broken time-reversal symmetry (<i>4 pages</i>)	201306(R)
Keiji Saito, Giuliano Benenti, Giulio Casati, and Tomaž Prosen	
Thermoelectric transport of mesoscopic conductors coupled to voltage and thermal probes (<i>4 pages</i>)	201307(R)
David Sánchez and Llorenç Serra	
Detecting a Majorana-fermion zero mode using a quantum dot (<i>4 pages</i>)	201308(R)
Dong E. Liu and Harold U. Baranger	

Surface physics, nanoscale physics, low-dimensional systems

Graphene on Ni(111): Strong interaction and weak adsorption (<i>4 pages</i>)	201401(R)
F. Mittendorfer, A. Garhofer, J. Redinger, J. Klimeš, J. Harl, and G. Kresse	
Electronic energy level alignment at metal-molecule interfaces with a <i>GW</i> approach (<i>4 pages</i>)	201402(R)
Isaac Tamblyn, Pierre Darancet, Su Ying Quek, Stanimir A. Bonev, and Jeffrey B. Neaton	

ARTICLES

Electronic structure and strongly correlated systems

Method to include explicit correlations into density-functional calculations based on density-matrix functional theory (<i>11 pages</i>)	205101
Peter E. Blöchl and Christian F. J. Walther	
Density functional theory study on the electronic structure of <i>n</i> - and <i>p</i> -type doped SrTiO ₃ at anodic solid oxide fuel cell conditions (<i>9 pages</i>)	205102
Suwit Suthirakun, Salai Cheettu Ammal, Guoliang Xiao, Fanglin Chen, Hans-Conrad zur Loye, and Andreas Heyden	
Nonlinear transformation optics and engineering of the Kerr effect (<i>8 pages</i>)	205103
L. Bergamin, P. Alitalo, and S. A. Tretyakov	
Kinks in the electronic dispersion of the Hubbard model away from half filling (<i>13 pages</i>)	205104
Patrick Grete, Sebastian Schmitt, Carsten Raas, Frithjof B. Anders, and Götz S. Uhrig	
Core and shallow-core <i>d</i> - to <i>f</i> -shell excitations in rare-earth metals (<i>8 pages</i>)	205105
J. A. Bradley, K. T. Moore, G. van der Laan, J. P. Bradley, and R. A. Gordon	
Accurate and fast numerical solution of Poisson's equation for arbitrary, space-filling Voronoi polyhedra: Near-field corrections revisited (<i>8 pages</i>)	205106
Aftab Alam, Brian G. Wilson, and D. D. Johnson	
Hole spectral functions in lightly doped quantum antiferromagnets (<i>12 pages</i>)	205107
Satyaki Kar and Efstratios Manousakis	
Capturing long range correlations in two-dimensional quantum lattice systems using correlator product states (<i>13 pages</i>)	205108
S. Al-Assam, S. R. Clark, C. J. Foot, and D. Jaksch	
 Decay rates for topological memories encoded with Majorana fermions (<i>23 pages</i>)	205109
G. Goldstein and C. Chamon	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Mantle cloaking using thin patterned metasurfaces (<i>13 pages</i>)	205110
Pai-Yen Chen and Andrea Alù	
Common Fermi-liquid origin of T^2 resistivity and superconductivity in n -type SrTiO_3 (<i>11 pages</i>)	205111
D. van der Marel, J. L. M. van Mechelen, and I. I. Mazin	
Hall coefficient anomaly in the low-temperature high-field phase of $\text{Sr}_3\text{Ru}_2\text{O}_7$ (<i>5 pages</i>)	205112
R. A. Borzi, A. McCollam, J. A. N. Bruin, R. S. Perry, A. P. Mackenzie, and S. A. Grigera	
Nematic order in the vicinity of a vortex in superconducting FeSe (<i>9 pages</i>)	205113
Debanjan Chowdhury, Erez Berg, and Subir Sachdev	
Structural, electronic, magnetic, and thermal properties of single-crystalline $\text{UNi}_{0.5}\text{Sb}_2$ (<i>7 pages</i>)	205114
M. S. Torikachvili, B. K. Davis, K. Kothapalli, H. Nakotte, A. J. Schultz, E. D. Mun, and S. L. Bud'ko	
Real-time energy dynamics in spin- $\frac{1}{2}$ Heisenberg chains (<i>14 pages</i>)	205115
Stephan Langer, Markus Heyl, Ian P. McCulloch, and Fabian Heidrich-Meisner	
Frequency domain winding number and interaction effect on topological insulators (<i>4 pages</i>)	205116
Lei Wang, Xi Dai, and X. C. Xie	
Fluctuation-exchange approximation theory of the nonequilibrium singlet-triplet transition (<i>10 pages</i>)	205117
B. Horváth, B. Lazarovits, and G. Zaránd	
Multiband conduction in the type-I clathrate $\text{Ba}_8\text{Ge}_{43}\square_3$ (<i>8 pages</i>)	205118
C. Candolfi, A. Ormeci, U. Aydemir, M. Baitinger, N. Oeschler, Yu. Grin, and F. Steglich	
Calculated x-ray linear dichroism spectra for Gd-doped GaN (<i>4 pages</i>)	205119
Tawinan Cheiwchanchamnangij and Walter R. L. Lambrecht	
Phase separation and charge-ordered phases of the $d = 3$ Falicov-Kimball model at nonzero temperature: Temperature-density-chemical potential global phase diagram from renormalization-group theory (<i>13 pages</i>)	205120
Ozan S. Sariyer, Michael Hinczewski, and A. Nihat Berker	
Particle-hole symmetry and interaction effects in the Kane-Mele-Hubbard model (<i>9 pages</i>)	205121
Dong Zheng, Guang-Ming Zhang, and Congjun Wu	
Instabilities of quadratic band crossing points (<i>8 pages</i>)	205122
Stefan Uebelacker and Carsten Honerkamp	
General spin-order theory via gauge Landau-Lifshitz equation (<i>6 pages</i>)	205123
You-Quan Li, Ye-Hua Liu, and Yi Zhou	
Intermediate-pressure phases of cerium studied by an LDA + Gutzwiller method (<i>6 pages</i>)	205124
Ming-Feng Tian, Xiaoyu Deng, Zhong Fang, and Xi Dai	
Variational Monte Carlo study of Anderson localization in the Hubbard model (<i>7 pages</i>)	205125
A. Farhoodfar, R. J. Gooding, and W. A. Atkinson	
Titanium forms a resonant level in the conduction band of PbTe (<i>5 pages</i>)	205126
Jan D. König, Michele D. Nielsen, Yi-Bin Gao, Markus Winkler, Alexandre Jacquot, Harald Böttner, and Joseph P. Heremans	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Role of hyperfine interaction for cavity-mediated coupling between spin qubits (7 pages)	205127
Julia Hildmann and Guido Burkard	
Edge states and topological phases in non-Hermitian systems (19 pages)	205128
Kenta Esaki, Masatoshi Sato, Kazuki Hasebe, and Mahito Kohmoto	
Time-dependent theory of nonlinear response and current fluctuations (8 pages)	205129
Ines Safi and Philippe Joyez	
Optical study of phonons and electronic excitations in tetragonal Sr_2VO_4 (6 pages)	205130
J. Teyssier, R. Vienne, E. Giannini, R. M. Eremina, A. Günther, J. Deisenhofer, M. V. Eremin, and D. van der Marel	
Low-energy excitations and singular contributions in the thermodynamics of clean Fermi liquids (25 pages)	205131
Hendrik Meier, Catherine Pépin, and Konstantin B. Efetov	
Nonstochastic algorithms for Jastrow-Slater and correlator product state wave functions (9 pages)	205132
Eric Neuscamman, Hitesh Changlani, Jesse Kinder, and Garnet Kin-Lic Chan	
Spin cluster operator theory for the kagome lattice antiferromagnet (21 pages)	205133
Kyunghwan Hwang, Yong Baek Kim, Jaehun Yu, and Kwon Park	
Structure of spinful quantum Hall states: A squeezing perspective (17 pages)	205134
E. Ardonne and N. Regnault	
Lattice dynamics and elastic properties of the 4f electron system: CeN (7 pages)	205135
V. Kanchana, G. Vaitheeswaran, Xinxin Zhang, Yanming Ma, A. Svane, and O. Eriksson	
 Bulk-edge correspondence in entanglement spectra (21 pages)	205136
Anushya Chandran, M. Hermanns, N. Regnault, and B. Andrei Bernevig	
Unified formalism for calculating polarization, magnetization, and more in a periodic insulator (14 pages)	205137
Kuang-Ting Chen and Patrick A. Lee	
Chemical pressure effects on structural, magnetic, and transport properties of $\text{Mn}_{1-x}\text{Co}_x\text{V}_2\text{O}_4$ (7 pages)	205138
A. Kiswandhi, J. S. Brooks, J. Lu, J. Whalen, T. Siegrist, and H. D. Zhou	
Semiconductors I: bulk	
Characterization of vibrational and mechanical properties of quaternary compounds $\text{Cu}_2\text{ZnSnS}_4$ and $\text{Cu}_2\text{ZnSnSe}_4$ in kesterite and stannite structures (7 pages)	205201
Tanju Gürel, Cem Sevik, and Tahir Çağın	
Defect evolution and impurity migration in Na-implanted ZnO (7 pages)	205202
Pekka T. Neuvonen, Lasse Vines, Vishnukanth Venkatachalapathy, Asier Zubiaga, Filip Tuomisto, Anders Hallén, Bengt G. Svensson, and Andrej Yu. Kuznetsov	
Self-diffusion in crystalline silicon: A Car-Parrinello molecular dynamics study (10 pages)	205203
Kenichi Koizumi, Mauro Boero, Yasuteru Shigeta, and Atsushi Oshiyama	
Carrier-mediated nonlocal ferromagnetic coupling between local magnetic polarons in Fe-doped In_2O_3 and Co-doped ZnO (6 pages)	205204
Shifei Qi, Fengxian Jiang, Jiuping Fan, H. Wu, S. B. Zhang, Gillian A. Gehring, Zhenyu Zhang, and Xiaohong Xu	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Quasiparticle band structures of β -HgS, HgSe, and HgTe (6 pages)	205205
A. Svane, N. E. Christensen, M. Cardona, A. N. Chantis, M. van Schilfgaarde, and T. Kotani	
Visible to vacuum-UV range optical absorption of oxygen dangling bonds in amorphous SiO ₂ (9 pages)	205206
Linards Skuja, Koichi Kajihara, Masahiro Hirano, and Hideo Hosono	
Inverse design approach to hole doping in ternary oxides: Enhancing <i>p</i> -type conductivity in cobalt oxide spinels (8 pages)	205207
J. D. Perkins, T. R. Paudel, A. Zakutayev, P. F. Ndione, P. A. Parilla, D. L. Young, S. Lany, D. S. Ginley, A. Zunger, N. H. Perry, Y. Tang, M. Grayson, T. O. Mason, J. S. Bettinger, Y. Shi, and M. F. Toney	
High-pressure optical studies of donor-acceptor polymer heterojunctions (5 pages)	205208
K. Paudel, M. Chandrasekhar, U. Scherf, E. Preis, and S. Guha	
Study of the ferroelectric phase transition in germanium telluride using time-domain terahertz spectroscopy (8 pages)	205209
Filip Kadlec, Christelle Kadlec, Petr Kužel, and Jan Petzelt	
<i>Ab initio</i> study on band-gap narrowing in SrTiO ₃ with Nb-C-Nb codoping (8 pages)	205210
Wu-Jun Shi and Shi-Jie Xiong	
Fluorescence and polarization spectroscopy of single silicon vacancy centers in heteroepitaxial nanodiamonds on iridium (8 pages)	205211
Elke Neu, Martin Fischer, Stefan Gsell, Matthias Schreck, and Christoph Becher	
Synthesis, structure, and magnetic properties of the layered iron oxychalcogenide Na ₂ Fe ₂ Se ₂ O (4 pages)	205212
J. B. He, D. M. Wang, H. L. Shi, H. X. Yang, J. Q. Li, and G. F. Chen	
Correlation of photocurrent and electroabsorption spectra and their temperature dependence for conjugated light emitting polymers: The origin of the corresponding density of states (12 pages)	205213
Awnish K. Tripathi and Y. N. Mohapatra	
Temperature dependence of the upper-branch polariton population in an organic semiconductor microcavity (8 pages)	205214
David M. Coles, Paolo Michetti, Caspar Clark, Ali M. Adawi, and David G. Lidzey	
Low-temperature magnetotransport of the narrow-gap semiconductor FeSb ₂ (5 pages)	205215
H. Takahashi, R. Okazaki, Y. Yasui, and I. Terasaki	
Excitonic transition dynamics on front and back surfaces of ZnO thin films (5 pages)	205216
Sun-Kyun Lee, Bong-Joon Kwon, Yong-Hoon Cho, Hang-Ju Ko, and Takafumi Yao	
Chemical stability of the magnetic oxide EuO directly on silicon observed by hard x-ray photoemission spectroscopy (7 pages)	205217
C. Caspers, M. Müller, A. X. Gray, A. M. Kaiser, A. Gloskovskii, C. S. Fadley, W. Drube, and C. M. Schneider	
Semiconductors II: surfaces, interfaces, microstructures, and related topics	
Mechanism of Fermi level pinning at metal/germanium interfaces (5 pages)	205301
K. Kasahara, S. Yamada, K. Sawano, M. Miyao, and K. Hamaya	
Magnetoresistance effects and phase coherent transport phenomena in a magnetic nonplanar two-dimensional hole system (8 pages)	205302
Stefan Knott, Thomas Ch. Hirschmann, Ursula Wurstbauer, Wolfgang Hansen, and Werner Wegscheider	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Carrier confinement in GaN/Al _x Ga _{1-x} N nanowire heterostructures ($0 < x \leq 1$) (14 pages)	205303
Florian Furtmayr, Jörg Teubert, Pascal Becker, Sonia Conesa-Boj, Joan Ramon Morante, Alexey Chernikov, Sören Schäfer, Sangam Chatterjee, Jordi Arbiol, and Martin Eickhoff	
Electronic properties of polar and nonpolar InN surfaces: A quasiparticle picture (8 pages)	205304
A. Belabbes, J. Furthmüller, and F. Bechstedt	
Spin-phonon coupling in single Mn-doped CdTe quantum dot (15 pages)	205305
C. L. Cao, L. Besombes, and J. Fernández-Rossier	
Room-temperature <i>p</i> -induced surface ferromagnetism: First-principles study (5 pages)	205306
Guntram Fischer, Nadiezhda Sanchez, Waheed Adeagbo, Martin Lüders, Zdzisława Szotek, Walter M. Temmerman, Arthur Ernst, Wolfram Hergert, and M. Carmen Muñoz	
Direct versus indirect optical recombination in Ge films grown on Si substrates (6 pages)	205307
G. Grzybowski, R. Roucka, J. Mathews, L. Jiang, R. T. Beeler, J. Kouvetakis, and J. Menéndez	
Extracting the density profile of an electronic wave function in a quantum dot (6 pages)	205308
Erin E. Boyd and Robert M. Westervelt	
Electronic structure of realistically extended atomistically resolved disordered Si:P δ -doped layers (9 pages)	205309
Sunhee Lee, Hoon Ryu, Huw Campbell, Lloyd C. L. Hollenberg, Michelle Y. Simmons, and Gerhard Klimeck	
Tuning interchain and intrachain interactions in polyfluorene copolymers (7 pages)	205311
Ya-Shih Huang, Johannes Gierschner, Johanna P. Schmidtke, Richard H. Friend, and David Beljonne	
Dynamics of excitons and free carriers in hybrid organic-inorganic quantum well structures (7 pages)	205312
Yu. Gladush, C. Piermarocchi, and V. Agronovich	
Coherent photocurrent control in a magnetic field through quantum interference (18 pages)	205313
Kiran M. Rao and J. E. Sipe	
<i>Ab initio</i> study of the early stages of gas-phase water oxidation of the Si(100) (2 × 1):H surface (8 pages)	205314
R. Lelis-Sousa and M. J. Caldas	
Femtosecond optical excitation of coherent acoustic phonons in a piezoelectric <i>p-n</i> junction (12 pages)	205315
Yu-Chieh Wen, Gia-Wei Chern, Kung-Hsuan Lin, Jeffrey Jarren Yeh, and Chi-Kuang Sun	
Mechanically probing coherent tunneling in a double quantum dot (6 pages)	205316
J. Gardner, S. D. Bennett, and A. A. Clerk	
Reconstruction dependent growth of lead phthalocyanine layers on GaAs(001) surfaces (5 pages)	205317
Linda Riele, Thomas Bruhn, Vanessa Rackwitz, Regina Passmann, Bjørn-Ove Fimland, Norbert Esser, and Patrick Vogt	
Effect of doping on performance of organic solar cells (14 pages)	205318
V. A. Trukhanov, V. V. Bruevich, and D. Yu. Paraschuk	
Unraveling of free-carrier absorption for terahertz radiation in heterostructures (6 pages)	205319
Andreas Wacker, Gerald Bastard, Francesca Carosella, Robson Ferreira, and Emmanuel Dupont	
Capacitively coupled double quantum dot system in the Kondo regime (10 pages)	205320
Irisnei L. Ferreira, P. A. Orellana, G. B. Martins, F. M. Souza, and E. Vernek	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Spin density waves in a semiconductor superlattice in a tilted magnetic field (<i>10 pages</i>)	205321
Liqu Zheng, D. C. Marinescu, and G. F. Giuliani	
Optimal quantum control for conditional rotation of exciton qubits in semiconductor quantum dots (<i>11 pages</i>) . . .	205322
Reuble Mathew, Craig E. Pryor, Michael E. Flatté, and Kimberley C. Hall	
Electron and hole gas in modulation-doped GaAs/Al _{1-x} Ga _x As radial heterojunctions (<i>9 pages</i>)	205323
Andrea Bertoni, Miquel Royo, Farah Mahawish, and Guido Goldoni	
Connectivity of edge and surface states in topological insulators (<i>5 pages</i>)	205324
Yongjin Jiang, Feng Lu, Feng Zhai, Tony Low, and Jiangping Hu	
Tunable band gaps in bilayer transition-metal dichalcogenides (<i>10 pages</i>)	205325
Ashwin Ramasubramaniam, Doron Naveh, and Elias Towe	
Multidimensional nanoscale materials from fused quantum dots (<i>5 pages</i>)	205326
Luis Tortajada, Lucas V. Besteiro, Murilo L. Tiago, L. J. Gallego, James R. Chelikowsky, and M. M. G. Alemany	
Magneto-optical Faraday and Kerr effects in topological insulator films and in other layered quantized Hall systems (<i>13 pages</i>)	205327
Wang-Kong Tse and A. H. MacDonald	
 Measurement of statistical nuclear spin polarization in a nanoscale GaAs sample (<i>8 pages</i>)	205328
Fei Xue (薛飞), D. P. Weber, P. Peddibhotla, and M. Poggio	
Effect of photoinduced charge displacement on organic optoelectronic conversion (<i>5 pages</i>)	205329
Laigui Hu, Akito Iwasaki, Rie Suizu, Yukiko Noda, Bo Li, Hirofumi Yoshikawa, Michio M. Matsushita, Kunio Awaga, and Hiroshi Ito	
Phonons in Bi ₂ S ₃ nanostructures: Raman scattering and first-principles studies (<i>8 pages</i>)	205330
Yanyuan Zhao, Kun Ting Eddie Chua, Chee Kwan Gan, Jun Zhang, Bo Peng, Zeping Peng, and Qihua Xiong	
Efficient simulation of multidimensional phonon transport using energy-based variance-reduced Monte Carlo formulations (<i>15 pages</i>)	205331
Jean-Philippe M. Péraud and Nicolas G. Hadjiconstantinou	
Zeeman splitting and spin dynamics tuning by exciton charging in two-dimensional systems (<i>7 pages</i>)	205332
Leonardo K. Castelano, Daniel Ferreira Cesar, Victor Lopez-Richard, Gilmar E. Marques, Odilon D. D. Couto Jr., Fernando Iikawa, Rudolf Hey, and Paulo V. Santos	
Surface physics, nanoscale physics, low-dimensional systems	
Consonant diminution of lattice and electronic coupling between a film and a substrate: Pb on Ge(100) (<i>5 pages</i>)	205401
Pei-Wen Chen, Yu-Hsuan Lu, Tay-Rong Chang, Chi-Bin Wang, Li-Yen Liang, Chung-Huang Lin, Cheng-Maw Cheng, Ku-Ding Tsuei, H.-T. Jeng, and S.-J. Tang	
Plasmons in Pb nanowire arrays on Si(557): Between one and two dimensions (<i>8 pages</i>)	205402
T. Block, C. Tegenkamp, J. Baringhaus, H. Pfnür, and T. Inaoka	
Ferroelectricity and ferromagnetism in EuTiO ₃ nanowires (<i>11 pages</i>)	205403
Anna N. Morozovska, Maya D. Glinchuk, Rakesh K. Behera, Basil Zaulychny, Chaitanya S. Deo, and Eugene A. Eliseev	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Substantial reduction of Stone-Wales activation barrier in fullerene (7 pages)	205404
Mukul Kabir, Swarnakamal Mukherjee, and Tanusri Saha-Dasgupta	
Microscopic theory of absorption and ultrafast many-particle kinetics in graphene (14 pages)	205406
Ermin Malic, Torben Winzer, Evgeny Bobkin, and Andreas Knorr	
Raman spectroscopy of the internal strain of a graphene layer grown on copper tuned by chemical vapor deposition (5 pages)	205407
V. Yu, E. Whiteway, J. Maassen, and M. Hilke	
Direct electrode-electrode tunneling in break-junction measurements of molecular conductance (12 pages)	205408
B. Gotsmann, H. Riel, and E. Lörtscher	
RKKY coupling between impurity spins in graphene nanoflakes (10 pages)	205409
Karol Szałowski	
Universal scaling relations for the thermoelectric power factor of semiconducting nanostructures (10 pages)	205410
Jane E. Cornett and Oded Rabin	
 Spectroscopic signatures of many-body interactions and delocalized states in self-assembled lateral quantum dot molecules (8 pages)	205411
X. Zhou, S. Sanwlani, W. Liu, J. H. Lee, Zh. M. Wang, G. Salamo, and M. F. Doty	
Tuning the band gap and magnetic properties of BN sheets impregnated with graphene flakes (5 pages)	205412
M. Kan, J. Zhou, Q. Wang, Q. Sun, and P. Jena	
Interplay of epitaxial strain and rotations in PbTiO ₃ /PbZrO ₃ superlattices from first principles (7 pages)	205413
Jeroen L. Blok, Dave H. A. Blank, Guus Rijnders, Karin M. Rabe, and David Vanderbilt	
Disorder-induced metallicity in amorphous graphene (5 pages)	205414
Erik Holmström, Jonas Fransson, Olle Eriksson, Raquel Lizárraga, Biplab Sanyal, Sumanta Bhandary, and Mikhail I. Katsnelson	
All-electron <i>GW</i> methods implemented in molecular orbital space: Ionization energy and electron affinity of conjugated molecules (6 pages)	205415
San-Huang Ke	
Theory of nonequilibrium single-electron dynamics in STM imaging of dangling bonds on a hydrogenated silicon surface (14 pages)	205416
Lucian Livadaru, Jason Pitters, Marco Taucer, and Robert A. Wolkow	
Charge trapping and scattering in epitaxial graphene (5 pages)	205417
Damon B. Farmer, Vasili Perebeinos, Yu-Ming Lin, Christos Dimitrakopoulos, and Phaedon Avouris	
Structural coupling across the LaAlO ₃ /SrTiO ₃ interface: High-resolution x-ray diffraction study (6 pages)	205418
J. E. Boschker, C. Folkman, C. W. Bark, Å. F. Monsen, E. Folven, J. K. Grepstad, E. Wahlström, C. B. Eom, and T. Tybell	
Electroluminescence of molecules in a scanning tunneling microscope: Role of tunneling electrons and surface plasmons (9 pages)	205419
Guangjun Tian and Yi Luo	
Electronic structure of PTCDA on Sn/Si(111)- $\sqrt{3} \times \sqrt{3}$ (8 pages)	205420
H. M. Zhang, J. B. Gustafsson, and L. S. O. Johansson	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Edge effects in graphene nanostructures: Semiclassical theory of spectral fluctuations and quantum transport (<i>19 pages</i>)	205421
Jürgen Wurm, Klaus Richter, and İnanç Adagideli	
Commensurate-incommensurate phase transition in chlorine monolayer chemisorbed on Ag(111): Direct observation of crowdfion condensation into a domain-wall fluid (<i>8 pages</i>)	205422
B. V. Andryushechkin, V. V. Cherkez, B. Kierren, Y. Fagot-Revurat, D. Malterre, and K. N. Eltsov	
Hydrogenated graphene on silicon dioxide surfaces (<i>7 pages</i>)	205423
P. Havu, M. Ijäs, and A. Harju	
Electron transmission through atomic steps of Bi ₂ Se ₃ and Bi ₂ Te ₃ surfaces (<i>14 pages</i>)	205424
Katsuyoshi Kobayashi	
Charge transmission through a single oligomer: Effects of photoinduced Frenkel-exciton formation (<i>14 pages</i>)	205425
Luxia Wang and Volkhard May	
☞ Ferroelectricity in a quasiamorphous ultrathin BaTiO ₃ film (<i>7 pages</i>)	205426
J. L. Wang, A. Pancotti, P. Jégou, G. Niu, B. Gautier, Y. Y. Mi, L. Torteche, S. Yin, B. Vilquin, and N. Barrett	
Modeling the constant-current distance-voltage mode of scanning tunneling spectroscopy (<i>8 pages</i>)	205427
Alex Pronschinske, Daniel J. Mardit, and Daniel B. Dougherty	
Manipulating light polarization with ultrathin plasmonic metasurfaces (<i>6 pages</i>)	205428
Yang Zhao and Andrea Alù	
Origin of conductivity crossover in entangled multiwalled carbon nanotube networks filled by iron (<i>10 pages</i>)	205429
George Chimowa, Ella C. Linganis, Dmitry Churochkin, Neil J. Coville, and Somnath Bhattacharyya	
Structural and electronic properties of Sc _n O _m ($n = 1 - 3$, $m = 1 - 2n$) clusters: Theoretical study using screened hybrid density functional theory (<i>7 pages</i>)	205430
Yu Yang, Haitao Liu, and Ping Zhang	
Multiscale magnetic study of Ni(111) and graphene on Ni(111) (<i>10 pages</i>)	205431
L. V. Dzemiantsova, M. Karolak, F. Lofink, A. Kubetzka, B. Sachs, K. von Bergmann, S. Hankemeier, T. O. Wehling, R. Frömter, H. P. Oepen, A. I. Lichtenstein, and R. Wiesendanger	
Electrostatic stability of insulating surfaces: Theory and applications (<i>16 pages</i>)	205432
Massimiliano Stengel	
One-dimensional physics in transition metal nanowires: Phases and elementary excitations (<i>11 pages</i>)	205433
Jun-ichi Okamoto and A. J. Millis	
Steps on rutile TiO ₂ (110): Active sites for water and methanol dissociation (<i>6 pages</i>)	205434
Umberto Martinez, Lasse B. Vilhelmsen, Henrik H. Kristoffersen, Jess Stausholm-Møller, and Bjørk Hammer	
Thickness and fluctuations of free and adsorbed liquid films (<i>11 pages</i>)	205435
Eva M. Fernández, Enrique Chacón, and Pedro Tarazona	
From fused aromatics to graphene-like nanoribbons: The effects of multiple terminal groups, length and symmetric pathways on charge transport (<i>9 pages</i>)	205436
Ante Bilić, Julian D. Gale, and Stefano Sanvito	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

Flows of Rényi entropies (<i>10 pages</i>)	205437
Yu. V. Nazarov	
Influence of intrinsic electronic properties on light transmission through subwavelength holes on gold and MgB ₂ thin films (<i>6 pages</i>)	205438
Xu Fang, Chenggang Zhuang, Zhenchao Wen, Xiufeng Han, Qingrong Feng, X. X. Xi, Franco Nori, Xincheng Xie, Qian Niu, and Xianggang Qiu	
Optical properties of periodic arrays of subwavelength slits in a perfect metal (<i>11 pages</i>)	205439
B. Sturman, E. Podivilov, and M. Gorkunov	
 Berry phase and pseudospin winding number in bilayer graphene (<i>5 pages</i>)	205440
Cheol-Hwan Park and Nicola Marzari	
Electronic and optical properties of a circular graphene quantum dot in a magnetic field: Influence of the boundary conditions (<i>12 pages</i>)	205441
M. Grujić, M. Zarenia, A. Chaves, M. Tadić, G. A. Farias, and F. M. Peeters	
Interaction of W(CO) ₆ with SiO ₂ surfaces: A density functional study (<i>7 pages</i>)	205442
Kaliappan Muthukumar, Ingo Opahle, Juan Shen, Harald O. Jeschke, and Roser Valentí	
Size-dependent persistent photocurrent and surface band bending in <i>m</i> -axial GaN nanowires (<i>7 pages</i>)	205443
Hsin-Yi Chen, Reui-San Chen, Nitin K. Rajan, Fu-Chieh Chang, Li-Chyong Chen, Kuei-Hsien Chen, Ying-Jay Yang, and Mark A. Reed	
Effects of domains in phonon conduction through hybrid boron nitride and graphene sheets (<i>5 pages</i>)	205444
H. Sevinçli, W. Li, N. Mingo, G. Cuniberti, and S. Roche	
Optical response and ground state of graphene (<i>13 pages</i>)	205445
T. Stroucken, J. H. Grönqvist, and S. W. Koch	
First-principles study of the oxygen evolution reaction of lithium peroxide in the lithium-air battery (<i>9 pages</i>)	205446
Yifei Mo, Shyue Ping Ong, and Gerbrand Ceder	
Adsorption of hydrogen on the interface of a graphene/boron nitride hybrid atomic membrane (<i>7 pages</i>)	205447
Ting Cao (曹霆), Ji Feng (冯济), and E. G. Wang (王恩哥)	
Landau levels in asymmetric graphene trilayers (<i>7 pages</i>)	205448
S. H. R. Sena, J. M. Pereira Jr., F. M. Peeters, and G. A. Farias	
Dephasing and hyperfine interaction in carbon nanotube double quantum dots: The clean limit (<i>20 pages</i>)	205449
Andres A. Reynoso and Karsten Flensberg	
Self-consistent full counting statistics of inelastic transport (<i>8 pages</i>)	205450
Tae-Ho Park and Michael Galperin	
Packing efficiency and accessible surface area of crumpled graphene (<i>7 pages</i>)	205451
Steven W. Cranford and Markus J. Buehler	
Quantum size effects on chemisorption properties: CO on ultrathin Cu films from first principles (<i>8 pages</i>)	205452
L. Mouketo, N. Bingeli, and B. M'Passi-Mabiala	
Density functional theory study of the γ -MnOOH (010) surface: Response to oxygen and water partial pressures and temperature (<i>15 pages</i>)	205453
Gloria A. E. Oxford and Anne M. Chaka	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 84, NUMBER 20

NOVEMBER 2011-15(II)

ERRATA

Publisher's Note: Site dilution in the Kitaev honeycomb model [Phys. Rev. B 84 , 115146 (2011)] (<i>1 page</i>)	209901(E)
A. J. Willans, J. T. Chalker, and R. Moessner	
Publisher's Note: Quasiparticle band structures of β -HgS, HgSe, and HgTe [Phys. Rev. B 84 , 205205 (2011)] (<i>1 page</i>)	209902(E)
A. Svane, N. E. Christensen, M. Cardona, A. N. Chantis, M. van Schilfgaarde, and T. Kotani	