

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 78, NUMBER 8

AUGUST 2008-15(II)

Angle-resolved electron energy-loss spectroscopy investigation of crystal-field transitions on MnO and NiO surfaces: Exchange scattering versus direct scattering (<i>7 pages</i>)	085438
F. Müller and S. Hüfner	
Phase diagram of the dissipative quantum particle in a box (<i>8 pages</i>)	085439
J. Sabio, L. Borda, F. Guinea, and F. Sols	

ERRATA

Erratum: Symmetry fingerprints of a benzene single-electron transistor: Interplay between Coulomb interaction and orbital symmetry [Phys. Rev. B 77 , 201406 (2008)] (<i>1 page</i>)	089901(E)
Georg Begemann, Dana Darau, Andrea Donarini, and Milena Grifoni	
Publisher's Note: Maximally localized Wannier functions within the FLAPW formalism [Phys. Rev. B 78 , 035120 (2008)] (<i>1 page</i>)	089902(E)
F. Freimuth, Y. Mokrousov, D. Wortmann, S. Heinze, and S. Blügel	
Publisher's Note: Conductivity of suspended and non-suspended graphene at finite gate voltage [Phys. Rev. B 78 , 085418 (2008)] (<i>1 page</i>)	089903(E)
T. Stauber, N. M. R. Peres, and A. H. Castro Neto	

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 78, NUMBER 8

AUGUST 2008-15(II)

Interaction of a CO molecule with a Pt monatomic wire: Electronic structure and ballistic conductance (11 pages)	085421
Gabriele Sciauzero, Andrea Dal Corso, Alexander Smogunov, and Erio Tosatti	
Exchange-split interface state at h-BN/Ni(111) (7 pages)	085422
Karen Zumbärgel, Kathrin Wulff, Christian Eibl, Markus Donath, and Matthias Hengsberger	
Scaling law of the giant Stark effect in boron nitride nanoribbons and nanotubes (5 pages)	085423
Fawei Zheng, Zhirong Liu, Jian Wu, Wenhui Duan, and Bing-Lin Gu	
Theory of the evolution of phonon spectra and elastic constants from graphene to graphite (17 pages)	085424
K. H. Michel and B. Verberck	
Electric charge enhancements in carbon nanotubes: Theory and experiments (5 pages)	085425
Zhao Wang, Mariusz Zdrojek, Thierry Mélin, and Michel Devel	
Charging of atoms, clusters, and molecules on metal-supported oxides: A general and long-ranged phenomenon (7 pages)	085426
Pentti Frondelius, Anders Hellman, Karoliina Honkala, Hannu Häkkinen, and Henrik Grönbeck	
Electronic properties of boron nitride nanocones under the influence of parallel and perpendicular external electric fields (6 pages)	085427
D. Pedreira, S. Azevedo, and M. Machado	
Positronium cooling into nanopores and nanochannels by phonon scattering (8 pages)	085428
S. Mariazzi, A. Salemi, and R. S. Brusa	
Density functional study of hydrogen adsorption on beryllium (0001) (7 pages)	085429
A. Allouche	
Line junction in a quantum Hall system with two filling fractions (9 pages)	085430
Diptiman Sen and Amit Agarwal	
Percolation scaling of $1/f$ noise in single-walled carbon nanotube films (9 pages)	085431
Ashkan Behnam, Gijs Bosman, and Ant Ural	
Optical conductivity of graphene in the visible region of the spectrum (8 pages)	085432
T. Stauber, N. M. R. Peres, and A. K. Geim	
Influence of elastic deformation of porous materials in adsorption-desorption process: A thermodynamic approach (12 pages)	085433
Annie Grosman and Camille Ortega	
Electronic and excitonic processes in light-emitting devices based on organic materials and colloidal quantum dots (8 pages)	085434
P. O. Anikeeva, C. F. Madigan, J. E. Halpert, M. G. Bawendi, and V. Bulović	
Estimates of effective Hubbard model parameters for C_{20} isomers (6 pages)	085435
Fei Lin and Erik S. Sørensen	
Superlubricity and tribochemistry of polyhydric alcohols (8 pages)	085436
C. Matta, L. Joly-Pottuz, M. I. De Barros Bouchet, J. M. Martin, M. Kano, Qing Zhang, and W. A. Goddard, III	
Dynamics in the quantum Hall effect and the phase diagram of graphene (31 pages)	085437
E. V. Gorbar, V. P. Gusynin, V. A. Miransky, and I. A. Shovkovy	

(Continued)

σ -bonding contribution of a strong π -acceptor molecule: Surface chemical bond of SO_2 on Ni(100) (5 pages)	085405
T. Tokushima, K. Sodeyama, Y. Harada, Y. Takata, M. Nagasono, Y. Kitajima, Y. Tamenori, H. Ohashi, S. Tsuneyuki, A. Hiraya, and S. Shin	
Periodized discrete elasticity models for defects in graphene (11 pages)	085406
A. Carpio and L. L. Bonilla	
Shuttle instability induced by an ac gate in a nanoelectromechanical single-electron transistor (9 pages)	085407
Norihiro Nishiguchi	
Optimization of metal dispersion in doped graphitic materials for hydrogen storage (5 pages)	085408
Gyubong Kim, Seung-Hoon Jhi, Noejung Park, Steven G. Louie, and Marvin L. Cohen	
Charge-memory polaron effect in molecular junctions (6 pages)	085409
Dmitry A. Ryndyk, Pino D'Amico, Gianaurelio Cuniberti, and Klaus Richter	
Zeeman-level lifetimes in $\text{Er}^{3+}:\text{Y}_2\text{SiO}_5$ (7 pages)	085410
S. R. Hastings-Simon, B. Lauritzen, M. U. Staudt, J. L. M. van Mechelen, C. Simon, H. de Riedmatten, M. Afzelius, and N. Gisin	
Experimental study of Coulomb corrections and single-particle energies for single-walled carbon nanotubes using cross-polarized photoluminescence (5 pages)	085411
K.-C. Chuang (莊凱捷), A. Nish, J.-Y. Hwang (黃炯源), G. W. Evans, and R. J. Nicholas	
Non-cubic distortions in quadratic $E \otimes e$ Jahn-Teller systems (8 pages)	085412
Elie A. Moujaes, Janette L. Dunn, and Colin A. Bates	
Tuning the gap in bilayer graphene using chemical functionalization: Density functional calculations (5 pages)	085413
D. W. Boukhvalov and M. I. Katsnelson	
Near-field radiative heat transfer for structured surfaces (9 pages)	085414
Svend-Age Biehs, Oliver Huth, and Felix Rütting	
Conductivity of defectless graphene (4 pages)	085415
Alexander B. Kashuba	
Quantum critical transport in clean graphene (12 pages)	085416
Lars Fritz, Jörg Schmalian, Markus Müller, and Subir Sachdev	
Stability and magnetism of hydrogen dimers on graphene (8 pages)	085417
Yves Ferro, D. Teillet-Billy, N. Rougeau, V. Sidis, S. Morisset, and Alain Allouche	
Conductivity of suspended and non-suspended graphene at finite gate voltage (13 pages)	085418
T. Stauber, N. M. R. Peres, and A. H. Castro Neto	
Electronic potential of a chemisorption interface (7 pages)	085419
Jin Zhao, Niko Pontius, Aimo Winkelmann, Vahit Sametoglu, Atsushi Kubo, Andrei G. Borisov, Daniel Sánchez-Portal, V. M. Silkin, Eugene V. Chulkov, Pedro M. Echenique, and Hrvoje Petek	
Molecular dynamics simulation study of nanoscale passive oxide growth on Ni-Al alloy surfaces at low temperatures (17 pages)	085420
Subramanian K. R. S. Sankaranarayanan and Shriram Ramanathan	

(Continued)

Voltage control of magnetocrystalline anisotropy in ferromagnetic-semiconductor-piezoelectric hybrid structures (5 pages)	085314
A. W. Rushforth, E. De Ranieri, J. Zemen, J. Wunderlich, K. W. Edmonds, C. S. King, E. Ahmad, R. P. Campion, C. T. Foxon, B. L. Gallagher, K. Výborný, J. Kučera, and T. Jungwirth	
Quantum many-body theory of qubit decoherence in a finite-size spin bath (13 pages)	085315
Wen Yang and Ren-Bao Liu	
Impact of strain waves traveling across a quantum dot on the optical response of the dot: Distinction between strain waves of different origin (8 pages)	085316
J. Huneke, A. Krügel, T. Kuhn, A. Vagov, and V. M. Axt	
Atomic structure of chlorinated Si(113) surfaces (8 pages)	085317
J. I. Flege, Th. Schmidt, M. Siebert, G. Materlik, and J. Falta	
Reflection and diffraction at the end of a cylindrical dielectric nanowire: Exact analytical solution (11 pages)	085318
V. G. Bordo	
Electronic structure and chemical and magnetic interactions in ZnO doped with Co and Al: Experiments and <i>ab initio</i> density-functional calculations (9 pages)	085319
Diana Iuşan, Ronny Knut, Biplab Sanyal, Olof Karis, Olle Eriksson, Victoria A. Coleman, Gunnar Westin, J. Magnus Wikberg, and Peter Svedlindh	
Terahertz photoconductivity of mobile electrons in nanoporous InP honeycombs (4 pages)	085320
J. Lloyd-Hughes, S. K. E. Merchant, L. Sirbu, I. M. Tiginyanu, and M. B. Johnston	
Agglomeration and uniform growth of Si ₃ N ₄ on Si(100): Experiments and first-principles calculations (9 pages)	085321
Koichi Kato, Daisuke Matsushita, Koichi Muraoka, and Yasushi Nakasaki	
Optically detected magnetic resonance in (Zn,Mn)Se/(Zn,Be)Se quantum wells (8 pages)	085322
V. Yu. Ivanov, M. Godlewski, D. R. Yakovlev, M. K. Kneip, M. Bayer, S. M. Ryabchenko, and A. Waag	
Atomic and energy structure of InAs/AlAs quantum dots (10 pages)	085323
T. S. Shamirzaev, A. V. Nenashev, A. K. Gutakovskii, A. K. Kalagin, K. S. Zhuravlev, M. Larsson, and P. O. Holtz	
Surface physics, nanoscale physics, low-dimensional systems	
Magnetoplasmons in layered graphene structures (5 pages)	085401
Oleg L. Berman, Godfrey Gumbs, and Yurii E. Lozovik	
Thermal radiation spectra of individual subwavelength microheaters (5 pages)	085402
Yat-Yin Au, Helgi Skuli Skulason, Snorri Ingvarsson, Levente J. Klein, and Hendrik F. Hamann	
Experimental and theoretical study of the morphology of commensurate and incommensurate graphene layers on Ni single-crystal surfaces (8 pages)	085403
D. Usachov, A. M. Dobrotvorskii, A. Varykhalov, O. Rader, W. Gudat, A. M. Shikin, and V. K. Adamchuk	
Bayesian approach to the calculation of lateral interactions: NO/Rh(111) (9 pages)	085404
A. P. J. Jansen and C. Popa	

(Continued)

Role of diatomic hydrogen in the electronic structure of ZnO (5 pages)	085213
S. Zh. Karazhanov and A. G. Ulyashin	
First-principles study of native defects in CdGeAs ₂ (11 pages)	085214
Tula R. Paudel and Walter R. L. Lambrecht	
Role of oxygen defects in diluted Mn:Ge (7 pages)	085215
A. Continenza and G. Profeta	
Semiconductors II: surfaces, interfaces, microstructures, and related topics	
Multiterminal multimode spin-dependent scattering matrix formalism: Electron and hole quantum spin transport in multiterminal junctions (10 pages)	085301
P. Brusheim, D. Csontos, U. Zülicke, and H. Q. Xu	
Phonon-assisted tunneling between singlet states in two-electron quantum dot molecules (8 pages)	085302
A. Grodecka, P. Machnikowski, and J. Förstner	
Metastable anisotropy orientation of nematic quantum Hall fluids (9 pages)	085303
Daniel G. Barci and Zochil González Arenas	
Optical spectra of a quantum dot in a microcavity in the nonlinear regime (11 pages)	085304
E. del Valle, F. P. Laussy, F. M. Souza, and I. A. Shelykh	
Interaction matrix element fluctuations in ballistic quantum dots: Random wave model (13 pages)	085305
L. Kaplan and Y. Alhassid	
Warming in systems with a discrete spectrum: Spectral diffusion of two-dimensional electrons in a magnetic field (4 pages)	085306
N. Romero Kalmanovitz, A. A. Bykov, Sergey Vitkalov, and A. I. Toropov	
Giant optical Faraday rotation induced by a single-electron spin in a quantum dot: Applications to entangling remote spins via a single photon (5 pages)	085307
C. Y. Hu, A. Young, J. L. O'Brien, W. J. Munro, and J. G. Rarity	
Method to study highly correlated nanostructures: The logarithmic-discretization embedded-cluster approximation (16 pages)	085308
E. V. Anda, G. Chiappe, C. A. Büsler, M. A. Davidovich, G. B. Martins, F. Heidrich-Meisner, and E. Dagotto	
Skyrme and Wigner crystals in graphene (13 pages)	085309
R. Côté, J.-F. Jobidon, and H. A. Fertig	
von Neumann-Wigner theorem in quantum dot molecules (4 pages)	085310
L.-X. Zhang, D. V. Melnikov, and J.-P. Leburton	
Fourier analyses of commensurability oscillations in Fibonacci lateral superlattices (10 pages)	085311
Akira Endo and Yasuhiro Iye	
Spin precession due to a non-Abelian spin-orbit gauge field (7 pages)	085312
Jyh-Shinn Yang, Xiao-Gang He, Son-Hsien Chen, and Ching-Ray Chang	
Effective phonon bottleneck in the carrier thermalization of InAs/GaAs quantum dots (6 pages)	085313
S. Sanguinetti, M. Guzzi, E. Grilli, M. Gurioli, L. Seravalli, P. Frigeri, S. Franchi, M. Capizzi, S. Mazzuccato, and A. Polimeni	

(Continued)

Phase diagram of the t - U - J_1 - J_2 chain at half filling (10 pages)	085128
X. Huang, E. Szirmai, F. Gebhard, J. Sólyom, and R. M. Noack	
Stability of the U(1) spin liquid with a spinon Fermi surface in 2+1 dimensions (13 pages)	085129
Sung-Sik Lee	
Charge pumping and noise in a one-dimensional wire with weak electron-electron interactions (11 pages)	085130
P. Devillard, V. Gasparian, and T. Martin	
Spectroscopy of $\text{Yb}^{3+}:\text{CaF}_2$: From isolated centers to clusters (12 pages)	085131
V. Petit, P. Camy, J.-L. Doualan, X. Portier, and R. Moncorgé	
Semiconductors I: bulk	
Validity of the Slater-Janak transition-state model within the LDA+ U approach (7 pages)	085201
Simone Sanna, Th. Frauenheim, and U. Gerstmann	
Evolution of vacancy-related defects upon annealing of ion-implanted germanium (5 pages)	085202
J. Slotte, M. Rummukainen, F. Tuomisto, V. P. Markevich, A. R. Peaker, C. Jaynes, and R. M. Gwilliam	
Energetics of endohedral atoms in type-I clathrates observed by soft x-ray spectroscopy (6 pages)	085203
Jun Tang, Takeshi Rachi, Ryotaro Kumashiro, Marcos A. Avila, Kouichirou Suekuni, Toshiro Takabatake, FangZhun Guo, Keisuke Kobayashi, Koji Akai, and Katsumi Tanigaki	
Motion-dependent magnetic properties of excitons in CdTe (13 pages)	085204
L. C. Smith, J. J. Davies, D. Wolverson, S. Crampin, R. T. Cox, J. Cibert, H. Mariette, V. P. Kochereshko, M. Wiater, G. Karczewski, and T. Wojtowicz	
Formation and origin of the dominating electron trap in irradiated p -type silicon (7 pages)	085205
Lasse Vines, E. V. Monakhov, A. Yu. Kuznetsov, R. Kozłowski, P. Kaminski, and B. G. Svensson	
Electronic structure of transition-metal impurities in semiconductors: Cu in GaP (11 pages)	085206
O. V. Farberovich, A. Yaresko, K. Kikoin, and V. Fleurov	
Effect of Gaussian disorder on the voltage dependence of the current density in sandwich-type devices based on organic semiconductors (16 pages)	085207
S. L. M. van Mensfoort and R. Coehoorn	
Hole transport in polyfluorene-based sandwich-type devices: Quantitative analysis of the role of energetic disorder (10 pages)	085208
S. L. M. van Mensfoort, S. I. E. Vulto, R. A. J. Janssen, and R. Coehoorn	
Compositional dependence of ferromagnetism in (Al,Ga,Mn)As magnetic semiconductors (6 pages)	085209
A. W. Rushforth, N. R. S. Farley, R. P. Campion, K. W. Edmonds, C. R. Staddon, C. T. Foxon, B. L. Gallagher, and K. M. Yu	
Exciton-phonon coupling in diindenoperylene thin films (10 pages)	085210
U. Heinemeyer, R. Scholz, L. Gisslén, M. I. Alonso, J. O. Ossó, M. Garriga, A. Hinderhofer, M. Kytka, S. Kowarik, A. Gerlach, and F. Schreiber	
Electronic and optical properties of ferromagnetic $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ in a multiband tight-binding approach (10 pages)	085211
Marko Turek, Jens Siewert, and Jaroslav Fabian	
Generalized valence-force-field model of (Ga,In)(N,P) ternary alloys (10 pages)	085212
Koushik Biswas, Alberto Franceschetti, and Stephan Lany	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 78, NUMBER 8

AUGUST 2008-15(II)

Physical origin of the resonant mode deep inside the stop band of a metallodielectric photonic crystal (4 pages)	085110
Minfeng Chen, Shawn-Yu Lin, Hung-Chun Chang, and Allan S. P. Chang	
Electronic structure of Ga-, In-, and Tl-doped PbTe: A supercell study of the impurity bands (8 pages)	085111
Khang Hoang and S. D. Mahanti	
Dynamical theory of artificial optical magnetism produced by rings of plasmonic nanoparticles (10 pages) ...	085112
Andrea Alù and Nader Engheta	
Theoretical study of quasiparticle inelastic lifetimes as applied to aluminum (13 pages)	085113
I. A. Nechaev, I. Yu. Sklyadneva, V. M. Silkin, P. M. Echenique, and E. V. Chulkov	
Band offsets of ultrathin high- κ oxide films with Si (10 pages)	085114
Eric Bersch, Sylvie Rangan, Robert Allen Bartynski, Eric Garfunkel, and Elio Vescovo	
Efficiency of energy transfer in a light-harvesting system under quantum coherence (7 pages)	085115
Alexandra Olaya-Castro, Chiu Fan Lee, Francesca Fassioli Olsen, and Neil F. Johnson	
Magnetic and surface plasmon resonances for periodic lattices of plasmonic split-ring resonators (8 pages)	085116
Ruey-Lin Chern	
Microscopic origin of the different colors displayed by $\text{MgAl}_2\text{O}_4\text{:Cr}^{3+}$ and emerald (7 pages)	085117
J. M. García-Lastra, M. T. Barriuso, J. A. Aramburu, and M. Moreno	
Ground-state phase diagrams of the generalized Falicov-Kimball model with Hund coupling (9 pages)	085118
Romuald Lemański and Jakub Wrzodak	
Gauge approach to the specific heat in the normal state of cuprates (5 pages)	085119
P. A. Marchetti and A. Ambrosetti	
Evidence for a band broadening across the ferromagnetic transition of $\text{Cr}_{1/3}\text{NbSe}_2$ (6 pages)	085120
W. Z. Hu, G. T. Wang, Rongwei Hu, C. Petrovic, E. Morosan, R. J. Cava, Z. Fang, and N. L. Wang	
Trap saturation in InP:Fe by optical interband excitation (7 pages)	085121
M. P. Petrov, V. V. Bryksin, B. Hilling, M. Lemmer, and M. Imlau	
Nature of the $\text{Fe}^{4/2}$ center in KTaO_3 : A density functional theory study (7 pages)	085122
A. Trueba, P. García-Fernández, J. M. García-Lastra, M. T. Barriuso, J. A. Aramburu, and M. Moreno	
Negative differential resistance in molecular junctions: Application to graphene ribbon junctions (8 pages)	085123
Hosein Cheraghchi and Keivan Esfarjani	
Fluctuating stripes in strongly correlated electron systems and the nematic-smectic quantum phase transition (30 pages)	085124
Kai Sun, Benjamin M. Fregoso, Michael J. Lawler, and Eduardo Fradkin	
Accurate GW self-energies in a plane-wave basis using only a few empty states: Towards large systems (9 pages)	085125
Fabien Bruneval and Xavier Gonze	
Exact-exchange Kohn-Sham potential, surface energy, and work function of jellium slabs (12 pages)	085126
C. M. Horowitz, C. R. Proetto, and J. M. Pitarke	
Self-consistent theory of molecular switching (12 pages)	085127
F. Pistolesi, Ya. M. Blanter, and Ivar Martin	

(Continued)

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).