PHYSICAL REVIEW B™

For editorial and subscription correspondence, please see inside front cover
(ISSN: 1098-0121)

PERIODICALS
Postmaster send address changes to:

APS Subscription Services
P.O. Box 41
Annapolis Junction, MD 20701

THIRD SERIES, VOLUME 89, NUMBER 6 *CONTENTS* **FEBRUARY 2014-1(II)**

RAPID COMMUNICATIONS

Structure, structural phase transitions, mechanical properties, defects

Closed-circuit domain quadruplets in $BaTiO_3$ nanorods embedded in a $SrTiO_3$ film *(5 pages)* . . . . . 060101(R)
V. Stepkova, P. Marton, N. Setter, and J. Hlinka

Local fivefold symmetry in liquid and undercooled Ni probed by x-ray absorption spectroscopy and computer simulations *(4 pages)* . . . . . 060102(R)
A. Di Cicco, F. Iesari, S. De Panfilis, M. Celino, S. Giusepponi, and A. Filipponi

Inhomogeneous, disordered, and partially ordered systems

Interplay of force constants in the lattice dynamics of disordered alloys: An *ab initio* study *(5 pages)* . . . . . 060201(R)
Rajiv K. Chouhan, Aftab Alam, Subhradip Ghosh, and Abhijit Mookerjee

Probing the electronic structure of liquid water with many-body perturbation theory *(5 pages)* . . . . . 060202(R)
T. Anh Pham, Cui Zhang, Eric Schwegler, and Giulia Galli

Dynamics, dynamical systems, lattice effects:

Quantum chaotic subdiffusion in random potentials *(4 pages)* . . . . . 060301(R)
M. V. Ivanchenko, T. V. Laptyeva, and S. Flach

Magnetism

Critical scaling in the cubic helimagnet Cu_2OSeO_3 *(5 pages)* . . . . . 060401(R)
I. Živković, J. S. White, H. M. Rønnow, K. Prša, and H. Berger

Laser-induced spin dynamics in ferromagnetic (In,Mn)As at magnetic fields up to 7 T *(5 pages)* . . . . . 060402(R)
R. R. Subkhangulov, H. Munekata, Th. Rasing, and A. V. Kimel

First-principles evidence of Mn moment canting in hole-doped $Ba_{1-2x}K_{2x}Mn_2As_2$ *(5 pages)* . . . . . 060403(R)
J. K. Glasbrenner and I. I. Mazin

Multiferroicity with coexisting isotropic and anisotropic spins in $Ca_3Co_{2-x}Mn_xO_6$ *(5 pages)* . . . . . 060404(R)
Jae Wook Kim, Y. Kamiya, Eun Deok Mun, M. Jaime, N. Harrison, J. D. Thompson, V. Kiryukhin, H. T. Yi, Y. S. Oh, S.-W. Cheong, C. D. Batista, and V. S. Zapf

Controlling coherent and incoherent spin dynamics by steering the photoinduced energy flow *(5 pages)* . . . . . 060405(R)
D. Bossini, A. M. Kalashnikova, R. V. Pisarev, Th. Rasing, and A. V. Kimel

Copyright 2014 by American Physical Society

(Continued)

1098-0121(20140201)89:6;1-J

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).

PHYSICAL REVIEW B THIRD SERIES, VOLUME 89, NUMBER 6 FEBRUARY 2014-1(II)

Tunneling, remanence, and frustration in dysprosium-based endohedral single-molecule magnets *(4 pages)* . . . . . 060406(R)
Rasmus Westerström, Jan Dreiser, Cinthia Piamonteze, Matthias Muntwiler, Stephen Weyeneth, Karl Krämer, Shi-Xia Liu, Silvio Decurtins, Alexey Popov, Shangfeng Yang, Lothar Dunsch, and Thomas Greber

Inverse spin Hall effect in $Ni_{81}Fe_{19}$/normal-metal bilayers *(5 pages)* . . . . . 060407(R)
M. Obstbaum, M. Härtinger, H. G. Bauer, T. Meier, F. Swientek, C. H. Back, and G. Woltersdorf

Superfluidity and superconductivity

Hysteretic behavior in the optical response of the underdoped Fe-arsenide $Ba(Fe_{1-x}Co_x)_2As_2$ in the electronic nematic phase *(5 pages)* . . . . . 060501(R)
C. Mirri, A. Dusza, S. Bastelberger, J.-H. Chu, H.-H. Kuo, I. R. Fisher, and L. Degiorgi

Excitonic superfluidity and screening in electron-hole bilayer systems *(5 pages)* . . . . . 060502(R)
D. Neilson, A. Perali, and A. R. Hamilton

Amplitude Higgs mode in the 2*H*-$NbSe_2$ superconductor *(5 pages)* . . . . . 060503(R)
M.-A. Méasson, Y. Gallais, M. Cazayous, B. Clair, P. Rodière, L. Cario, and A. Sacuto

Superconducting specific-heat jump $\Delta C_{\rm el} \propto T_c^{\beta}(\beta \approx 2)$ for $K_{1-x}Na_xFe_2As_2$ *(5 pages)* . . . . . 060504(R)
V. Grinenko, D. V. Efremov, S.-L. Drechsler, S. Aswartham, D. Gruner, M. Roslova, I. Morozov, K. Nenkov, S. Wurmehl, A. U. B. Wolter, B. Holzapfel, and B. Büchner

Absence of the $\frac{1}{8}$ anomaly in the oxygen isotope effect of $YBa_2Cu_3O_y$ *(4 pages)* . . . . . 060505(R)
K. Kamiya, T. Masui, S. Tajima, H. Bando, and Y. Aiura

Interface charge doping effects on superconductivity of single-unit-cell FeSe films on $SrTiO_3$ substrates *(6 pages)* 060506(R)
Wenhao Zhang, Zhi Li, Fangsen Li, Huimin Zhang, Junping Peng, Chenjia Tang, Qingyan Wang, Ke He, Xi Chen, Lili Wang, Xucun Ma, and Qi-Kun Xue

Anisotropic superconductivity in noncentrosymmetric BiPd *(5 pages)* . . . . . 060507(R)
L. Jiao, J. L. Zhang, Y. Chen, Z. F. Weng, Y. M. Shao, J. Y. Feng, X. Lu, B. Joshi, A. Thamizhavel, S. Ramakrishnan, and H. Q. Yuan

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

Deterministic electron ptychography at atomic resolution *(10 pages)* 064101
A. J. D'Alfonso, A. J. Morgan, A. W. C. Yan, P. Wang, H. Sawada, A. I. Kirkland, and L. J. Allen

Thermodynamics of stable nanocrystalline alloys: A Monte Carlo analysis *(10 pages)* 064102
Tongjai Chookajorn and Christopher A. Schuh

First-principles study of atomic ordering in fcc Ni-Cr alloys *(12 pages)* 064103
Moshiour Rahaman, B. Johansson, and A. V. Ruban

Molecular dynamics simulations of shock-compressed single-crystal silicon *(10 pages)* 064104
Gabriele Mogni, Andrew Higginbotham, Katalin Gaál-Nagy, Nigel Park, and Justin S. Wark

$Pb(Mg_{1/3}Nb_{2/3})O_3$: A minimal induced-moment soft pseudospin glass perspective *(5 pages)* 064105
David Sherrington

(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).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 89, NUMBER 6** **FEBRUARY 2014-1(II)**

Crystal structure transformation in CeRuSn seen via the atomic pair distribution function *(6 pages)* 064106
K. Prokeš, S. A. J. Kimber, J. A. Mydosh, and R. Pöttgen

Ab initio study of the structural phase transitions of the double perovskites Sr_2MWO_6 (M=Zn, Ca, Mg) *(8 pages)* 064107
U. Petralanda and I. Etxebarria

Peierls distortion, magnetism, and high hardness of manganese tetraboride *(9 pages)* 064108
Huiyang Gou, Alexander A. Tsirlin, Elena Bykova, Artem M. Abakumov, Gustaaf Van Tendeloo, Asta Richter, Sergey V. Ovsyannikov, Alexander V. Kurnosov, Dmytro M. Trots, Zuzana Konôpková, Hans-Peter Liermann, Leonid Dubrovinsky, and Natalia Dubrovinskaia

Ab initio study of AlN: Anisotropic thermal expansion, phase diagram, and high-temperature rocksalt to wurtzite phase transition *(9 pages)* 064109
Steve Schmerler and Jens Kortus

Inhomogeneous, disordered, and partially ordered systems

Renormalization flow of the hierarchical Anderson model at weak disorder *(8 pages)* 064201
F. L. Metz, L. Leuzzi, and G. Parisi

Structure, electronic, and vibrational properties of amorphous AsS_2 and $AgAsS_2$: Experimentally constrained density functional study *(9 pages)* 064202
J. Akola, P. Jóvári, I. Kaban, I. Voleská, J. Kolář, T. Wágner, and R. O. Jones

Dynamics, dynamical systems, lattice effects:

Dynamical magnetic charges and linear magnetoelectricity *(7 pages)* 064301
Meng Ye and David Vanderbilt

Anharmonic free energies and phonon dispersions from the stochastic self-consistent harmonic approximation: Application to platinum and palladium hydrides *(16 pages)* 064302
Ion Errea, Matteo Calandra, and Francesco Mauri

Terahertz dynamics of ferroelectric vortices from first principles *(6 pages)* 064303
Zhigang Gui and L. Bellaiche

Numerical pump-probe experiments of laser-excited silicon in nonequilibrium phase *(8 pages)* 064304
S. A. Sato, K. Yabana, Y. Shinohara, T. Otobe, and G. F. Bertsch

Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations *(15 pages)* 064305
Lianhua He, Fang Liu, Geoffroy Hautier, Micael J. T. Oliveira, Miguel A. L. Marques, Fernando D. Vila, J. J. Rehr, G.-M. Rignanese, and Aihui Zhou

Femtosecond laser-induced optical anisotropy in a two-dimensional lattice of magnetic dots *(9 pages)* 064306
I. Razdolski, V. L. Krutyanskiy, T. V. Murzina, Th. Rasing, and A. V. Kimel

Indirect heating of Pt by short-pulse laser irradiation of Au in a nanoscale Pt/Au bilayer *(7 pages)* 064307
Gyung-Min Choi, R. B. Wilson, and David G. Cahill

Strong spin-phonon coupling in infrared and Raman spectra of $SrMnO_3$ *(7 pages)* 064308
S. Kamba, V. Goian, V. Skoromets, J. Hejtmánek, V. Bovtun, M. Kempa, F. Borodavka, P. Vaněk, A. A. Belik, J. H. Lee, O. Pacherová, and K. M. Rabe

(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).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 89, NUMBER 6** **FEBRUARY 2014-1(II)**

Homogenization scheme for acoustic metamaterials *(12 pages)* 064309
Min Yang, Guancong Ma, Ying Wu, Zhiyu Yang, and Ping Sheng

Phonon spectrum of $SrFe_2As_2$ determined using multizone phonon refinement *(7 pages)* 064310
D. Parshall, R. Heid, J. L. Niedziela, Th. Wolf, M. B. Stone, D. L. Abernathy, and D. Reznik

Polaron dynamics and decoherence in an interacting two-spin system coupled to an optical-phonon environment *(18 pages)* 064311
Amit Dey and Sudhakar Yarlagadda

Magnetism

Chemical pressure effects on magnetism in the quantum spin liquid candidates $Yb_2X_2O_7$ (X = Sn, Ti, Ge) *(7 pages)* 064401
Z. L. Dun, M. Lee, E. S. Choi, A. M. Hallas, C. R. Wiebe, J. S. Gardner, E. Arrighi, R. S. Freitas, A. M. Arevalo-Lopez, J. P. Attfield, H. D. Zhou, and J. G. Cheng

Spin excitations in cubic maghemite nanoparticles studied by time-of-flight neutron spectroscopy *(7 pages)* 064402
S. Disch, R. P. Hermann, E. Wetterskog, A. A. Podlesnyak, K. An, T. Hyeon, G. Salazar-Alvarez, L. Bergström, and Th. Brückel

Evolution of two-dimensional antiferromagnetism with temperature and magnetic field in multiferroic $Ba_2CoGe_2O_7$ *(9 pages)* 064403
V. Hutanu, A. P. Sazonov, M. Meven, G. Roth, A. Gukasov, H. Murakawa, Y. Tokura, D. Szaller, S. Bordács, I. Kézsmárki, V. K. Guduru, L. C. J. M. Peters, U. Zeitler, J. Romhányi, and B. Náfrádi

Spin-dependent optical response of multiferroic EuO: First-principles DFT calculations *(8 pages)* 064404
Wen-Yi Tong, Hang-Chen Ding, Yong-Chao Gao, Shi-Jing Gong, Xiangang Wan, and Chun-Gang Duan

Fermi sea term in the relativistic linear muffin-tin-orbital transport theory for random alloys *(9 pages)* 064405
I. Turek, J. Kudrnovský, and V. Drchal

Exploration of the helimagnetic and skyrmion lattice phase diagram in Cu_2OSeO_3 using magnetoelectric susceptibility *(5 pages)* 064406
A. A. Omrani, J. S. White, K. Prša, I. Živković, H. Berger, A. Magrez, Ye-Hua Liu, J. H. Han, and H. M. Rønnow

Local magnetism and spin correlations in the geometrically frustrated cluster magnet $LiZn_2Mo_3O_8$ *(7 pages)* 064407
J. P. Sheckelton, F. R. Foronda, LiDong Pan, C. Moir, R. D. McDonald, T. Lancaster, P. J. Baker, N. P. Armitage, T. Imai, S. J. Blundell, and T. M. McQueen

Magnetization dynamics of an in-plane magnetized synthetic ferrimagnetic free layer submitted to spin-transfer torques and applied field *(11 pages)* 064408
B. Lacoste, L. D. Buda-Prejbeanu, U. Ebels, and B. Dieny

Long-range antiferromagnetic order in the frustrated *XY* pyrochlore antiferromagnet $Er_2Ge_2O_7$ *(7 pages)* 064409
X. Li, W. M. Li, K. Matsubayashi, Y. Sato, C. Q. Jin, Y. Uwatoko, T. Kawae, A. M. Hallas, C. R. Wiebe, A. M. Arevalo-Lopez, J. P. Attfield, J. S. Gardner, R. S. Freitas, H. D. Zhou, and J.-G. Cheng

Magnetic excitation in resonant inelastic x-ray scattering of Sr_2IrO_4: A localized spin picture *(9 pages)* 064410
Jun-ichi Igarashi and Tatsuya Nagao

Magneto-optical analysis of stripe elements embedded in a synthetic antiferromagnet *(10 pages)* 064411
M. Langer, A. Neudert, J. I. Mönch, R. Mattheis, K. Lenz, J. Fassbender, and J. McCord

(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).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 89, NUMBER 6** **FEBRUARY 2014-1(II)**

Theory of magnon-skyrmion scattering in chiral magnets *(7 pages)* 064412
Junichi Iwasaki, Aron J. Beekman, and Naoto Nagaosa

Control of skyrmion magnetic bubble gyration *(5 pages)* 064413
Kyoung-Woong Moon, Byong Sun Chun, Wondong Kim, Z. Q. Qiu, and Chanyong Hwang

Proposal for direct measurement of random fields in the $LiHo_xY_{1-x}F_4$ crystal *(9 pages)* 064414
Yoav G. Pollack and Moshe Schechter

Intrinsic insulating ferromagnetism in manganese oxide thin films *(7 pages)* 064415
Y. S. Hou, H. J. Xiang, and X. G. Gong

Stability of two-dimensional skyrmions in thin films of $Mn_{1-x}Fe_xSi$ investigated by the topological Hall effect *(6 pages)* 064416
T. Yokouchi, N. Kanazawa, A. Tsukazaki, Y. Kozuka, M. Kawasaki, M. Ichikawa, F. Kagawa, and Y. Tokura

Magnetic structure and spin excitations in $BaMn_2Bi_2$ *(6 pages)* 064417
S. Calder, B. Saparov, H. B. Cao, J. L. Niedziela, M. D. Lumsden, A. S. Sefat, and A. D. Christianson

Magnetism of $Pd_{1-x}Ni_x$ alloys near the critical concentration for ferromagnetism *(13 pages)* 064418
G. M. Kalvius, O. Hartmann, R. Wäppling, A. Günther, A. Krimmel, A. Loidl, D. E. MacLaughlin, O. O. Bernal, G. J. Nieuwenhuys, M. C. Aronson, R. P. Dickey, M. B. Maple, A. Amato, and C. Baines

Influence of material defects on current-driven vortex domain wall mobility *(5 pages)* 064419
Jonathan Leliaert, Ben Van de Wiele, Arne Vansteenkiste, Lasse Laurson, Gianfranco Durin, Luc Dupré, and Bartel Van Waeyenberge

Unconventional critical scaling of magnetization in ferromagnetic uranium superconductors UGe_2 and URhGe *(8 pages)* 064420
Naoyuki Tateiwa, Yoshinori Haga, Tatsuma D. Matsuda, Etsuji Yamamoto, and Zachary Fisk

Corner contribution to cluster numbers in the Potts model *(8 pages)* 064421
István A. Kovács, Eren Metin Elçi, Martin Weigel, and Ferenc Iglói

Magnetic ordering with reduced cerium moments in hole-doped $CeOs_2Al_{10}$ *(5 pages)* 064422
D. D. Khalyavin, D. T. Adroja, A. Bhattacharyya, A. D. Hillier, P. Manuel, A. M. Strydom, J. Kawabata, and T. Takabatake

Observation of a giant Kerr rotation in a ferromagnetic transition metal by M-edge resonant magneto-optic Kerr effect *(6 pages)* 064423
Sh. Yamamoto, M. Taguchi, M. Fujisawa, R. Hobara, S. Yamamoto, K. Yaji, T. Nakamura, K. Fujikawa, R. Yukawa, T. Togashi, M. Yabashi, M. Tsunoda, S. Shin, and I. Matsuda

Intrinsic reduction of the ordered $4f$ magnetic moments in semiconducting rare-earth nitride thin films: DyN, ErN, and HoN *(7 pages)* 064424
D. L. Cortie, J. D. Brown, S. Brück, T. Saerbeck, J. P. Evans, H. Fritzsche, X. L. Wang, J. E. Downes, and F. Klose

Phenomenology of current-skyrmion interactions in thin films with perpendicular magnetic anisotropy *(7 pages)* 064425
M. E. Knoester, Jairo Sinova, and R. A. Duine

Spin-orbit torques and anisotropic magnetization damping in skyrmion crystals *(6 pages)* 064426
Kjetil M. D. Hals and Arne Brataas

(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).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 89, NUMBER 6** **FEBRUARY 2014-1(II)**

Dissipationless spin current between two coupled ferromagnets *(9 pages)* 064427
Wei Chen, Peter Horsch, and Dirk Manske

Orbital magnetization of insulating perovskite transition-metal oxides with a net ferromagnetic moment in the ground state *(11 pages)* 064428
S. A. Nikolaev and I. V. Solovyev

Superfluidity and superconductivity

Josephson π state induced by valley polarization *(5 pages)* 064501
Jun Wang, Y. H. Yang, and K. S. Chan

Tunable critical supercurrent and spin-asymmetric Josephson effect in superlattices *(11 pages)* 064502
Juha M. Kreula, Miikka O. J. Heikkinen, Francesco Massel, and Päivi Törmä

Disorder effects on thermal transport on the surface of topological superconductors by the self-consistent Born approximation *(9 pages)* 064503
Ryota Nakai and Kentaro Nomura

Electron bubbles in liquid ^{4}He containing a small number of electrons *(6 pages)* 064504
Wanchun Wei, Zhuolin Xie, and Humphrey J. Maris

Multiband effects on Fulde-Ferrell-Larkin-Ovchinnikov states of Pauli-limited superconductors *(16 pages)* 064505
Masahiro Takahashi, Takeshi Mizushima, and Kazushige Machida

Bose-Hubbard model with occupation-parity couplings *(9 pages)* 064506
Kuei Sun and C. J. Bolech

Strong thermal fluctuations in cuprate superconductors in magnetic fields above T_c *(7 pages)* 064507
Xujiang Jiang, Dingping Li, and Baruch Rosenstein

Size effects in superconducting thin films coupled to a substrate *(10 pages)* 064508
Aurelio Romero-Bermúdez and Antonio M. García-García

First-principles study of the minimal model of magnetic interactions in Fe-based superconductors *(7 pages)* 064509
J. K. Glasbrenner, J. P. Velev, and I. I. Mazin

Anomalous impurity effects in the iron-based superconductor KFe_2As_2 *(5 pages)* 064510
A. F. Wang, S. Y. Zhou, X. G. Luo, X. C. Hong, Y. J. Yan, J. J. Ying, P. Cheng, G. J. Ye, Z. J. Xiang, S. Y. Li, and X. H. Chen

Enhancement of superconducting transition temperature due to antiferromagnetic spin fluctuations in iron pnictides $LaFe(As_{1-x}P_x)(O_{1-y}F_y)$: ^{31}P-NMR studies *(6 pages)* 064511
H. Mukuda, F. Engetsu, K. Yamamoto, K. T. Lai, M. Yashima, Y. Kitaoka, A. Takemori, S. Miyasaka, and S. Tajima

Asymmetric Andreev reflection induced electrical and thermal Hall-like effects in metal/anisotropic superconductor junctions *(5 pages)* 064512
Jie Ren and Jian-Xin Zhu

Interplay of classical and quantum capacitance in a one-dimensional array of Josephson junctions *(10 pages)* 064513
Pedro Ribeiro and Antonio M. García-García

(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).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 89, NUMBER 6** **FEBRUARY 2014-1(II)**

Strong electron pairing at the iron $3d_{xz,yz}$ orbitals in hole-doped $BaFe_2As_2$ superconductors revealed by angle-resolved photoemission spectroscopy *(12 pages)* 064514

D. V. Evtushinsky, V. B. Zabolotnyy, T. K. Kim, A. A. Kordyuk, A. N. Yaresko, J. Maletz, S. Aswartham, S. Wurmehl, A. V. Boris, D. L. Sun, C. T. Lin, B. Shen, H. H. Wen, A. Varykhalov, R. Follath, B. Büchner, and S. V. Borisenko

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).