

# PHYSICAL REVIEW B<sup>TM</sup>

## CONDENSED MATTER AND MATERIALS PHYSICS

Articles Published in FEBRUARY 2014

1(II)

*Published by*  
AMERICAN PHYSICAL SOCIETY<sup>TM</sup>

Volume 89

Third Series

Number 6

## RAPID COMMUNICATIONS

### Structure, structural phase transitions, mechanical properties, defects

Closed-circuit domain quadruplets in BaTiO<sub>3</sub> nanorods embedded in a SrTiO<sub>3</sub> 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. Lapyteva, and S. Flach

### Magnetism

Critical scaling in the cubic helimagnet Cu<sub>2</sub>OSeO<sub>3</sub> (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<sub>1-2x</sub>K<sub>2x</sub>Mn<sub>2</sub>As<sub>2</sub> (5 pages) ..... 060403(R)  
J. K. Glasbrenner and I. I. Mazin

Multiferroicity with coexisting isotropic and anisotropic spins in Ca<sub>3</sub>Co<sub>2-x</sub>Mn<sub>x</sub>O<sub>6</sub> (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



Tunneling, remanence, and frustration in dysprosium-based endohedral single-molecule magnets ( <i>4 pages</i> ) . . . . .	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 <sub>81</sub> Fe <sub>19</sub> /normal-metal bilayers ( <i>5 pages</i> ) . . . . .	060407(R)
M. Obstbaum, M. Härtinger, H. G. Bauer, T. Meier, F. Swientek, C. H. Back, and G. Woltersdorf	
<b>Superfluidity and superconductivity</b>	
Hysteretic behavior in the optical response of the underdoped Fe-arsenide Ba(Fe <sub>1-x</sub> Co <sub>x</sub> ) <sub>2</sub> As <sub>2</sub> in the electronic nematic phase ( <i>5 pages</i> ) . . . . .	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 ( <i>5 pages</i> ) . . . . .	060502(R)
D. Neilson, A. Perali, and A. R. Hamilton	
Amplitude Higgs mode in the 2H-NbSe <sub>2</sub> superconductor ( <i>5 pages</i> ) . . . . .	060503(R)
M.-A. Méasson, Y. Gallais, M. Cazayous, B. Clair, P. Rodière, L. Cario, and A. Sacuto	
Superconducting specific-heat jump $\Delta C_{el} \propto T_c^\beta$ ( $\beta \approx 2$ ) for K <sub>1-x</sub> Na <sub>x</sub> Fe <sub>2</sub> As <sub>2</sub> ( <i>5 pages</i> ) . . . . .	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 <sub>2</sub> Cu <sub>3</sub> O <sub>y</sub> ( <i>4 pages</i> ) . . . . .	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 <sub>3</sub> substrates ( <i>6 pages</i> ) . . . . .	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 ( <i>5 pages</i> ) . . . . .	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 ( <i>10 pages</i> ) . . . . .	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 ( <i>10 pages</i> ) . . . . .	064102
Tongjai Chookajorn and Christopher A. Schuh	
First-principles study of atomic ordering in fcc Ni-Cr alloys ( <i>12 pages</i> ) . . . . .	064103
Moshiour Rahaman, B. Johansson, and A. V. Ruban	
Molecular dynamics simulations of shock-compressed single-crystal silicon ( <i>10 pages</i> ) . . . . .	064104
Gabriele Mogni, Andrew Higginbotham, Katalin Gaál-Nagy, Nigel Park, and Justin S. Wark	
Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub> : A minimal induced-moment soft pseudospin glass perspective ( <i>5 pages</i> ) . . . . .	064105
David Sherrington	

*(Continued)*

Crystal structure transformation in CeRuSn seen via the atomic pair distribution function ( <i>6 pages</i> ) . . . . .	064106
K. Prokeš, S. A. J. Kimber, J. A. Mydosh, and R. Pöttgen	
<i>Ab initio</i> study of the structural phase transitions of the double perovskites $Sr_2MWO_6$ ( $M=Zn, Ca, Mg$ ) ( <i>8 pages</i> ) . . . . .	064107
U. Petralanda and I. Etxebarria	
Peierls distortion, magnetism, and high hardness of manganese tetraboride ( <i>9 pages</i> ) . . . . .	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 Dubrovinskaja	
<i>Ab initio</i> study of AlN: Anisotropic thermal expansion, phase diagram, and high-temperature rocksalt to wurtzite phase transition ( <i>9 pages</i> ) . . . . .	064109
Steve Schmerler and Jens Kortus	
<b>Inhomogeneous, disordered, and partially ordered systems</b>	
Renormalization flow of the hierarchical Anderson model at weak disorder ( <i>8 pages</i> ) . . . . .	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 ( <i>9 pages</i> ) . . . . .	064202
J. Akola, P. Jóvári, I. Kaban, I. Voleská, J. Kolář, T. Wágner, and R. O. Jones	
<b>Dynamics, dynamical systems, lattice effects:</b>	
 Dynamical magnetic charges and linear magnetoelectricity ( <i>7 pages</i> ) . . . . .	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 ( <i>16 pages</i> ) . . . . .	064302
Ion Errea, Matteo Calandra, and Francesco Mauri	
Terahertz dynamics of ferroelectric vortices from first principles ( <i>6 pages</i> ) . . . . .	064303
Zhigang Gui and L. Bellaïche	
Numerical pump-probe experiments of laser-excited silicon in nonequilibrium phase ( <i>8 pages</i> ) . . . . .	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 ( <i>15 pages</i> ) . . . . .	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 ( <i>9 pages</i> ) . . . . .	064306
I. Rzdolski, V. L. Krutynskiy, 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 ( <i>7 pages</i> ) . . . . .	064307
Gyung-Min Choi, R. B. Wilson, and David G. Cahill	
Strong spin-phonon coupling in infrared and Raman spectra of $SrMnO_3$ ( <i>7 pages</i> ) . . . . .	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)*



Homogenization scheme for acoustic metamaterials ( <i>12 pages</i> ) . . . . .	064309
Min Yang, Guancong Ma, Ying Wu, Zhiyu Yang, and Ping Sheng	
Phonon spectrum of SrFe <sub>2</sub> As <sub>2</sub> determined using multizone phonon refinement ( <i>7 pages</i> ) . . . . .	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 ( <i>18 pages</i> ) . . . . .	064311
Amit Dey and Sudhakar Yarlagadda	
<b>Magnetism</b>	
Chemical pressure effects on magnetism in the quantum spin liquid candidates Yb <sub>2</sub> X <sub>2</sub> O <sub>7</sub> ( <i>X = Sn, Ti, Ge</i> ) ( <i>7 pages</i> ) . . . . .	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 ( <i>7 pages</i> ) . . . . .	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 <sub>2</sub> CoGe <sub>2</sub> O <sub>7</sub> ( <i>9 pages</i> ) . . . . .	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 ( <i>8 pages</i> ) . . . . .	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 ( <i>9 pages</i> ) . . . . .	064405
I. Turek, J. Kudrnovský, and V. Drchal	
Exploration of the helimagnetic and skyrmion lattice phase diagram in Cu <sub>2</sub> OSeO <sub>3</sub> using magnetoelectric susceptibility ( <i>5 pages</i> ) . . . . .	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 <sub>2</sub> Mo <sub>3</sub> O <sub>8</sub> ( <i>7 pages</i> ) . . . . .	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 ( <i>11 pages</i> ) . . . . .	064408
B. Lacoste, L. D. Buda-Prejbeanu, U. Ebels, and B. Dieny	
Long-range antiferromagnetic order in the frustrated XY pyrochlore antiferromagnet Er <sub>2</sub> Ge <sub>2</sub> O <sub>7</sub> ( <i>7 pages</i> ) . . . . .	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 <sub>2</sub> IrO <sub>4</sub> : A localized spin picture ( <i>9 pages</i> ) . . . . .	064410
Jun-ichi Igarashi and Tatsuya Nagao	
Magneto-optical analysis of stripe elements embedded in a synthetic antiferromagnet ( <i>10 pages</i> ) . . . . .	064411
M. Langer, A. Neudert, J. I. Mönch, R. Mattheis, K. Lenz, J. Fassbender, and J. McCord	

*(Continued)*

Theory of magnon-skyrmion scattering in chiral magnets ( <i>7 pages</i> ) . . . . .	064412
Junichi Iwasaki, Aron J. Beekman, and Naoto Nagaosa	
Control of skyrmion magnetic bubble gyration ( <i>5 pages</i> ) . . . . .	064413
Kyoung-Woong Moon, Byong Sun Chun, Wondong Kim, Z. Q. Qiu, and Chanyong Hwang	
Proposal for direct measurement of random fields in the $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ crystal ( <i>9 pages</i> ) . . . . .	064414
Yoav G. Pollack and Moshe Schechter	
Intrinsic insulating ferromagnetism in manganese oxide thin films ( <i>7 pages</i> ) . . . . .	064415
Y. S. Hou, H. J. Xiang, and X. G. Gong	
Stability of two-dimensional skyrmions in thin films of $\text{Mn}_{1-x}\text{Fe}_x\text{Si}$ investigated by the topological Hall effect ( <i>6 pages</i> ) . . . . .	064416
T. Yokouchi, N. Kanazawa, A. Tsukazaki, Y. Kozuka, M. Kawasaki, M. Ichikawa, F. Kagawa, and Y. Tokura	
Magnetic structure and spin excitations in $\text{BaMn}_2\text{Bi}_2$ ( <i>6 pages</i> ) . . . . .	064417
S. Calder, B. Saporov, H. B. Cao, J. L. Niedziela, M. D. Lumsden, A. S. Sefat, and A. D. Christianson	
☞ Magnetism of $\text{Pd}_{1-x}\text{Ni}_x$ alloys near the critical concentration for ferromagnetism ( <i>13 pages</i> ) . . . . .	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 ( <i>5 pages</i> ) . . . . .	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 $\text{UGe}_2$ and $\text{URhGe}$ ( <i>8 pages</i> ) . . . . .	064420
Naoyuki Tateiwa, Yoshinori Haga, Tatsuma D. Matsuda, Etsuji Yamamoto, and Zachary Fisk	
Corner contribution to cluster numbers in the Potts model ( <i>8 pages</i> ) . . . . .	064421
István A. Kovács, Eren Metin Elçi, Martin Weigel, and Ferenc Igloi	
Magnetic ordering with reduced cerium moments in hole-doped $\text{CeOs}_2\text{Al}_{10}$ ( <i>5 pages</i> ) . . . . .	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 ( <i>6 pages</i> ) . . . . .	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: $\text{DyN}$ , $\text{ErN}$ , and $\text{HoN}$ ( <i>7 pages</i> ) . . . . .	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 ( <i>7 pages</i> ) . . . . .	064425
M. E. Knoester, Jairo Sinova, and R. A. Duine	
☞ Spin-orbit torques and anisotropic magnetization damping in skyrmion crystals ( <i>6 pages</i> ) . . . . .	064426
Kjetil M. D. Hals and Arne Brataas	

(Continued)

Dissipationless spin current between two coupled ferromagnets ( <i>9 pages</i> ) . . . . .	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 ( <i>11 pages</i> ) . . . . .	064428
S. A. Nikolaev and I. V. Solovyev	
<b>Superfluidity and superconductivity</b>	
Josephson $\pi$ state induced by valley polarization ( <i>5 pages</i> ) . . . . .	064501
Jun Wang, Y. H. Yang, and K. S. Chan	
Tunable critical supercurrent and spin-asymmetric Josephson effect in superlattices ( <i>11 pages</i> ) . . . . .	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 ( <i>9 pages</i> ) . . . . .	064503
Ryota Nakai and Kentaro Nomura	
Electron bubbles in liquid $^4\text{He}$ containing a small number of electrons ( <i>6 pages</i> ) . . . . .	064504
Wanchun Wei, Zhuolin Xie, and Humphrey J. Maris	
Multiband effects on Fulde-Ferrell-Larkin-Ovchinnikov states of Pauli-limited superconductors ( <i>16 pages</i> ) . . . . .	064505
Masahiro Takahashi, Takeshi Mizushima, and Kazushige Machida	
Bose-Hubbard model with occupation-parity couplings ( <i>9 pages</i> ) . . . . .	064506
Kuei Sun and C. J. Bolech	
Strong thermal fluctuations in cuprate superconductors in magnetic fields above $T_c$ ( <i>7 pages</i> ) . . . . .	064507
Xujiang Jiang, Dingping Li, and Baruch Rosenstein	
Size effects in superconducting thin films coupled to a substrate ( <i>10 pages</i> ) . . . . .	064508
Aurelio Romero-Bermúdez and Antonio M. García-García	
First-principles study of the minimal model of magnetic interactions in Fe-based superconductors ( <i>7 pages</i> ) . . . . .	064509
J. K. Glasbrenner, J. P. Velev, and I. I. Mazin	
Anomalous impurity effects in the iron-based superconductor $\text{KFe}_2\text{As}_2$ ( <i>5 pages</i> ) . . . . .	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 $\text{LaFe}(\text{As}_{1-x}\text{P}_x)(\text{O}_{1-y}\text{F}_y)$ : $^{31}\text{P}$ -NMR studies ( <i>6 pages</i> ) . . . . .	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 ( <i>5 pages</i> ) . . . . .	064512
Jie Ren and Jian-Xin Zhu	
Interplay of classical and quantum capacitance in a one-dimensional array of Josephson junctions ( <i>10 pages</i> ) . . . . .	064513
Pedro Ribeiro and Antonio M. García-García	

(Continued)

Strong electron pairing at the iron $3d_{xz,yz}$ orbitals in hole-doped $\text{BaFe}_2\text{As}_2$ superconductors revealed by angle-resolved photoemission spectroscopy ( <i>12 pages</i> ) . . . . .	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	