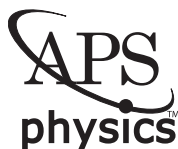


ARTICLES

Structure, structural phase transitions, mechanical properties, defects

- Interpretation of unexpected behavior of infrared absorption spectra of ScF_3 beyond the quasiharmonic approximation (9 pages) 214101
Sergei Piskunov, Pjotr A. Žgurs, Dmitry Bocharov, Alexei Kuzmin, Juris Purans, Aleksandr Kalinko, Robert A. Evarestov, Shehab E. Ali, and Francesco Rocca
- Quantum model for entropic springs (7 pages) 214102
Chiao-Hsuan Wang and Jacob M. Taylor
- Critical thickness for interface misfit dislocation formation in two-dimensional materials (8 pages) 214103
Brian C. McGuigan, Pascal Pochet, and Harley T. Johnson
- Potentially superhard hcp CrN_2 compound studied at high pressure (7 pages) 214104
Zhonglong Zhao, Kuo Bao, Fubo Tian, Defang Duan, Bingbing Liu, and Tian Cui
- Nonlinear elastic effects in phase field crystal and amplitude equations: Comparison to *ab initio* simulations of bcc metals and graphene (14 pages) 214105
Claas Hüter, Martin Friák, Marc Weikamp, Jörg Neugebauer, Nigel Goldenfeld, Bob Svendsen, and Robert Spatschek
- Ab initio* approach to structural, electronic, and ferroelectric properties of antimony sulphoiodide (9 pages) 214106
Danila Amoroso and Silvia Picozzi
- Bond-order potential for magnetic body-centered-cubic iron and its transferability (11 pages) 214107
Yi-Shen Lin, M. Mrovec, and V. Vitek
- Kinetics of the iron α - ϵ phase transition at high-strain rates: Experiment and model (6 pages) 214108
N. Amadou, T. de Resseguier, E. Brambrink, T. Vinci, A. Benuzzi-Mounaix, G. Huser, G. Morard, F. Guyot, K. Miyanishi, N. Ozaki, R. Kodama, and M. Koenig
- Zone-center phonons of bulk, few-layer, and monolayer $1T$ - TaS_2 : Detection of commensurate charge density wave phase through Raman scattering (7 pages) 214109
Oliver R. Albertini, Rui Zhao, Rebecca L. McCann, Simin Feng, Mauricio Terrones, James K. Freericks, Joshua A. Robinson, and Amy Y. Liu
- Dislocation patterning in a two-dimensional continuum theory of dislocations (10 pages) 214110
István Groma, Michael Zaiser, and Péter Dusán Ispánovity
- Density-based crystal plasticity: From the discrete to the continuum (12 pages) 214111
Pierre-Louis Valdenaire, Yann Le Bouar, Benoît Appolaire, and Alphonse Finel



CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 93, NUMBER 21

JUNE 2016-1(I)

High-temperature- and high-pressure-induced formation of the Laves-phase compound XeS_2 (6 pages)	214112
Xiaozhen Yan, Yangmei Chen, Shikai Xiang, Xiaoyu Kuang, Yan Bi, and Haiyan Chen	
Collective mode splitting in hybrid heterostructures (5 pages)	214113
Juan Gabriel Ramírez, J. de la Venta, Siming Wang, Thomas Saerbeck, Ali C. Basaran, X. Batlle, and Ivan K. Schuller	
Pressure effects on model ferroelectric $\text{BiFeO}_3\text{-PbTiO}_3$: Multiple phase transitions (6 pages)	214114
Abhisek Basu, Rajesh Jana, Rajeev Ranjan, and Goutam Dev Mukherjee	
Impact of local magnetism on stacking fault energies: A first-principles investigation for fcc iron (10 pages)	214115
I. Bleskov, T. Hickel, J. Neugebauer, and A. Ruban	
Inhomogeneous, disordered, and partially ordered systems	
Dramatically growing shear rigidity length scale in the supercooled glass former NiZr_2 (9 pages)	214201
Nicholas B. Weingartner, Ryan Soklaski, K. F. Kelton, and Zohar Nussinov	
Unveiling atomic-scale features of inherent heterogeneity in metallic glass by molecular dynamics simulations (7 pages)	214202
Y. C. Hu, P. F. Guan, M. Z. Li, C. T. Liu, Y. Yang, H. Y. Bai, and W. H. Wang	
Temperature and density dependence of the shear viscosity of liquid sodium (10 pages)	214203
N. Meyer, H. Xu, and J.-F. Wax	
Pressure-driven transformation of the ordering in amorphous network-forming materials (5 pages)	214204
Anita Zeidler and Philip S. Salmon	
Structural evolution mechanisms of amorphous and liquid As_2Se_3 at high pressures (8 pages)	214205
L. Properzi, M. Santoro, M. Minicucci, F. Iesari, M. Ciambezi, L. Nataf, Y. Le Godec, T. Irifune, F. Baudelet, and A. Di Cicco	
Topological Anderson insulators in systems without time-reversal symmetry (5 pages)	214206
Ying Su, Y. Avishai, and X. R. Wang	
Dynamics, dynamical systems, lattice effects:	
Phononic heat transport in the transient regime: An analytic solution (17 pages)	214301
Riku Tuovinen, Niko Säkkinen, Daniel Karlsson, Gianluca Stefanucci, and Robert van Leeuwen	
Different effects of electronic excitation on metals and semiconductors (9 pages)	214302
Gai-Qin Yan, Xin-Lu Cheng, Hong Zhang, Zhi-Yang Zhu, and Da-Hua Ren	
Phonon anharmonicity and components of the entropy in palladium and platinum (9 pages)	214303
Yang Shen, Chen W. Li, Xiaoli Tang, Hillary L. Smith, and B. Fultz	
Classical model of negative thermal expansion in solids with expanding bonds (7 pages)	214304
Joseph T. Schick and Andrew M. Rappe	
Phonon-glass dynamics in thermoelectric clathrates (7 pages)	214305
Yaping Liu, Qing Xi, Jun Zhou, Tsuneyoshi Nakayama, and Baowen Li	
Spin-phonon coupling and high-pressure phase transitions of RMnO_3 ($R = \text{Ca}$ and Pr): An inelastic neutron scattering and first-principles study (17 pages)	214306
S. K. Mishra, M. K. Gupta, R. Mittal, A. I. Kolesnikov, and S. L. Chaplot	

(Continued)

Resonant interactions between discrete phonons in quinhedron driven by nonlinear electron-phonon coupling (15 pages)	214307
Aaron S. Rury	
First-principles calculation and experimental investigation of lattice dynamics in the rare-earth pyrochlores $R_2\text{Ti}_2\text{O}_7$ ($R = \text{Tb, Dy, Ho}$) (13 pages)	214308
M. Ruminy, M. Núñez Valdez, B. Wehinger, A. Bosak, D. T. Adroja, U. Stühr, K. Iida, K. Kamazawa, E. Pomjakushina, D. Prabakaran, M. K. Haas, L. Bovo, D. Sheptyakov, A. Cervellino, R. J. Cava, M. Kenzelmann, N. A. Spaldin, and T. Fennell	
Magnetism	
 Magnetolectric and structural properties of Y_2CoMnO_6 : The role of antisite defects (12 pages)	214401
J. Blasco, J. García, G. Subías, J. Stankiewicz, J. A. Rodríguez-Velamazán, C. Ritter, J. L. García-Muñoz, and F. Fauth	
One-dimensional frustrated plaquette compass model: Nematic phase and spontaneous multimerization (16 pages)	214402
Wojciech Brzezicki and Andrzej M. Oleś	
Magnetic transitions in the topological magnon insulator $\text{Cu}(1,3\text{-bdc})$ (9 pages)	214403
R. Chisnell, J. S. Helton, D. E. Freedman, D. K. Singh, F. Demmel, C. Stock, D. G. Nocera, and Y. S. Lee	
Magnetovolume effect, macroscopic hysteresis, and moment collapse in the paramagnetic state of cubic MnGe under pressure (5 pages)	214404
N. Martin, M. Deutsch, J.-P. Itié, J.-P. Rueff, U. K. Rössler, K. Koepernik, L. N. Fomicheva, A. V. Tsvyashchenko, and I. Mirebeau	
Cycloidal versus skyrmionic states in mesoscopic chiral magnets (8 pages)	214405
Jeroen Mulkers, Milorad V. Milošević, and Bartel Van Waeyenberge	
Observation of large spin accumulation voltages in nondegenerate Si spin devices due to spin drift effect: Experiments and theory (9 pages)	214406
Takayuki Tahara, Yuichiro Ando, Makoto Kameno, Hayato Koike, Kazuhito Tanaka, Shinji Miwa, Yoshishige Suzuki, Tomoyuki Sasaki, Tohru Oikawa, and Masashi Shiraishi	
Structural and magnetic properties of the $5d^2$ double perovskites Sr_2BReO_6 ($B=\text{Y, In}$) (10 pages)	214407
A. A. Aczel, Z. Zhao, S. Calder, D. T. Adroja, P. J. Baker, and J.-Q. Yan	
Influence of the sputtering flow regime on the structural properties and magnetic behavior of Fe-Ga thin films ($\text{Ga} \sim 30 \text{ at.}\%$) (8 pages)	214408
A. Muñoz-Noval, A. Ordóñez-Fontes, and R. Ranchal	
Electronic and transport properties of the Mn-doped topological insulator Bi_2Te_3 : A first-principles study (8 pages)	214409
K. Carva, J. Kudrnovský, F. Mácá, V. Drchal, I. Turek, P. Baláž, V. Tkáč, V. Holý, V. Sechovský, and J. Honolka	
Ground-state candidate for the classical dipolar kagome Ising antiferromagnet (7 pages)	214410
I. A. Chioar, N. Rougemaille, and B. Canals	
Tunable Fano resonance and magneto-optical response in magnetoplasmonic structure fabricated by pure ferromagnetic metals (9 pages)	214411
Leyi Chen, Jinlong Gao, Wenbin Xia, Shaoyin Zhang, Shaolong Tang, Weiyi Zhang, Daoyong Li, Xiaoshan Wu, and Youwei Du	

(Continued)

Path to collapse for an isolated Néel skyrmion (6 pages)	214412
S. Rohart, J. Miltat, and A. Thiaville	
Observation of resistivity minimum at low temperature in $\text{Co}_x\text{Cu}_{1-x}$ ($x \sim 0.17\text{--}0.76$) nanostructured granular alloys (6 pages)	214413
S. Dhara, R. Roy Chowdhury, and B. Bandyopadhyay	
Exploring metamagnetism of single crystalline EuNiGe_3 by neutron scattering (7 pages)	214414
X. Fabrèges, A. Gukasov, P. Bonville, A. Maurya, A. Thamizhavel, and S. K. Dhar	
Absence of magnetic proximity effects in magnetoresistive $\text{Pt/CoFe}_2\text{O}_4$ hybrid interfaces (8 pages)	214415
M. Valvidares, N. Dix, M. Isasa, K. Ollefs, F. Wilhelm, A. Rogalev, F. Sánchez, E. Pellegrin, A. Bedoya-Pinto, P. Gargiani, L. E. Hueso, F. Casanova, and J. Fontcuberta	
Anisotropy: Spin order and magnetization of single-crystalline $\text{Cu}_4(\text{OH})_6\text{FBr}$ barlowite (6 pages)	214416
Tian-Heng Han, Eric D. Isaacs, John A. Schlueter, and John Singleton	
Quantum phase transitions in a generalized compass chain with three-site interactions (9 pages)	214417
Wen-Long You, Yu-Cheng Qiu, and Andrzej M. Oleś	
Anomalous Hall effect in localization regime (5 pages)	214418
Lin Wu, Kai Zhu, Di Yue, Yuan Tian, and Xiaofeng Jin	
Helical bunching and symmetry lowering inducing multiferroicity in Fe langasites (5 pages)	214419
L. Chaix, R. Ballou, A. Cano, S. Petit, S. de Brion, J. Ollivier, L.-P. Regnault, E. Ressouche, E. Constable, C. V. Colin, A. Zorko, V. Scagnoli, J. Balay, P. Lejay, and V. Simonet	
Resonant elastic x-ray scattering from the skyrmion lattice in Cu_2OSeO_3 (6 pages)	214420
S. L. Zhang, A. Bauer, H. Berger, C. Pfleiderer, G. van der Laan, and T. Hesjedal	
Quantum criticality and inhomogeneous magnetic order in Fe-doped $\alpha\text{-YbAlB}_4$ (8 pages)	214421
D. E. MacLaughlin, K. Kuga, Lei Shu, O. O. Bernal, P.-C. Ho, S. Nakatsuji, K. Huang, Z. F. Ding, C. Tan, and Jian Zhang	
Ultrafast changes of magnetic anisotropy driven by laser-generated coherent and noncoherent phonons in metallic films (10 pages)	214422
V. N. Kats, T. L. Linnik, A. S. Salasyuk, A. W. Rushforth, M. Wang, P. Wadley, A. V. Akimov, S. A. Cavill, V. Holy, A. M. Kalashnikova, and A. V. Scherbakov	
Enhanced Faraday rotation by crystals of core-shell magnetoplasmonic nanoparticles (7 pages)	214423
P. Varytis, P. A. Pantazopoulos, and N. Stefanou	
Influence of the critical Fe atomic volume on the magnetism of Fe-rich metallic glasses evidenced by pressure-dependent measurements (14 pages)	214424
L. F. Kiss, T. Kemény, J. Bednarčík, J. Gamcová, and H.-P. Liermann	
Energy dynamics in the Heisenberg-Kitaev spin chain (6 pages)	214425
Robin Steinigeweg and Wolfram Brenig	
 Highly anisotropic exchange interactions of $j_{\text{eff}} = \frac{1}{2}$ iridium moments on the fcc lattice in La_2BIrO_6 ($\text{B} = \text{Mg, Zn}$) (11 pages)	214426
A. A. Aczel, A. M. Cook, T. J. Williams, S. Calder, A. D. Christianson, G.-X. Cao, D. Mandrus, Yong-Baek Kim, and A. Paramakanti	

(Continued)

Dynamic modulation of the transport properties of the $\text{LaAlO}_3/\text{SrTiO}_3$ interface using uniaxial strain (7 pages)	214427
Fan Zhang, Yue-Wen Fang, Ngai Yui Chan, Wing Chong Lo, Dan Feng Li, Chun-Gang Duan, Feng Ding, and Ji Yan Dai	
Spin-wave and electromagnon dispersions in multiferroic MnWO_4 as observed by neutron spectroscopy: Isotropic Heisenberg exchange versus anisotropic Dzyaloshinskii-Moriya interaction (8 pages)	214428
Y. Xiao (肖荫果), C. M. N. Kumar, S. Nandi, Y. Su (苏夷希), W. T. Jin (金文涛), Z. Fu (付振东), E. Faulhaber, A. Schneidewind, and Th. Brückel	
Phenomenology of chiral damping in noncentrosymmetric magnets (5 pages)	214429
Collins Ashu Akosa, Ioan Mihai Miron, Gilles Gaudin, and Aurélien Manchon	
Magnetic ordering in the ultrapure site-diluted spin chain materials $\text{SrCu}_{1-x}\text{Ni}_x\text{O}_2$ (6 pages)	214430
G. Simutis, M. Thede, R. Saint-Martin, A. Mohan, C. Baines, Z. Guguchia, R. Khasanov, C. Hess, A. Revcolevschi, B. Büchner, and A. Zheludev	
⚡ Challenges in design of Kitaev materials: Magnetic interactions from competing energy scales (21 pages)	214431
Stephen M. Winter, Ying Li, Harald O. Jeschke, and Roser Valentí	
Gapless quantum spin liquid ground state in the spin-1 antiferromagnet $6\text{HB-Ba}_3\text{NiSb}_2\text{O}_9$ (6 pages)	214432
J. A. Quilliam, F. Bert, A. Manseau, C. Darie, C. Guillot-Deudon, C. Payen, C. Baines, A. Amato, and P. Mendels	
Lieb-Mattis ferrimagnetism in magnetic semiconductors (6 pages)	214433
R. O. Kuzian, J. Richter, M. D. Kuz'min, and R. Hayn	
Crossed responses of spin and orbital magnetism in topological insulators (8 pages)	214434
Ryota Nakai and Kentaro Nomura	
Spin-rotational-invariant theory of transition-metal magnetism at finite temperatures: Systematic study of a single-site model (11 pages)	214435
G. M. Pastor and J. Dorantes-Dávila	
Spin-wave localization in tangentially magnetized films (8 pages)	214436
Elena V. Tartakovskaya, Martha Pardavi-Horvath, and Robert D. McMichael	
⚡ Spin-wave excitation modes in thick vortex-state circular ferromagnetic nanodots (10 pages)	214437
R. V. Verba, A. Hierro-Rodriguez, D. Navas, J. Ding, X. M. Liu, A. O. Adeyeye, K. Y. Guslienko, and G. N. Kakazei	
Ground-state phases of the spin-1 J_1 - J_2 Heisenberg antiferromagnet on the honeycomb lattice (17 pages)	214438
P. H. Y. Li and R. F. Bishop	
First-principles studies of the Gilbert damping and exchange interactions for half-metallic Heuslers alloys (14 pages)	214439
Jonathan Chico, Samara Keshavarz, Yaroslav Kvashnin, Manuel Pereiro, Igor Di Marco, Corina Etz, Olle Eriksson, Anders Bergman, and Lars Bergqvist	
Static magnetic proximity effect in $\text{Pt/Ni}_{1-x}\text{Fe}_x$ bilayers investigated by x-ray resonant magnetic reflectivity (9 pages)	214440
C. Klewe, T. Kuschel, J.-M. Schmalhorst, F. Bertram, O. Kuschel, J. Wollschläger, J. Strempfer, M. Meinert, and G. Reiss	

(Continued)

Theoretical formalism for collective spin-wave edge excitations in arrays of dipolarly interacting magnetic nanodots (20 pages)	214441
Ivan Lisenkov, Vasyl Tyberkevych, Sergey Nikitov, and Andrei Slavin	
Superfluidity and superconductivity	
Ultrastrong coupling in two-resonator circuit QED (8 pages)	214501
A. Baust, E. Hoffmann, M. Haeberlein, M. J. Schwarz, P. Eder, J. Goetz, F. Wulschner, E. Xie, L. Zhong, F. Quijandría, D. Zueco, J.-J. García Ripoll, L. García-Álvarez, G. Romero, E. Solano, K. G. Fedorov, E. P. Menzel, F. Deppe, A. Marx, and R. Gross	
Josephson junction through a disordered topological insulator with helical magnetization (9 pages)	214502
Alexander Zyuzin, Mohammad Alidoust, and Daniel Loss	
Superconductivity and ferromagnetism in hole-doped RbEuFe ₄ As ₄ (9 pages)	214503
Yi Liu, Ya-Bin Liu, Zhang-Tu Tang, Hao Jiang, Zhi-Cheng Wang, Abduweli Ablimit, Wen-He Jiao, Qian Tao, Chun-Mu Feng, Zhu-An Xu, and Guang-Han Cao	
Topological superconductivity in quantum Hall–superconductor hybrid systems (7 pages)	214504
Björn Zocher and Bernd Rosenow	
Flat-band superconductivity in strained Dirac materials (5 pages)	214505
V. J. Kauppila, F. Aikebaier, and T. T. Heikkilä	
Electron doping evolution of the magnetic excitations in NaFe _{1-x} Co _x As (13 pages)	214506
Scott V. Carr, Chenglin Zhang, Yu Song, Guotai Tan, Yu Li, D. L. Abernathy, M. B. Stone, G. E. Granroth, T. G. Perring, and Pengcheng Dai	
Effects of order parameter self-consistency in a $s_{\pm}$ - s junction (12 pages)	214507
Rosa Rodríguez-Mota, Erez Berg, and T. Pereg-Barnea	
Superconducting electron and hole lenses (8 pages)	214508
H. Cheraghchi, H. Esmailzadeh, and A. G. Moghaddam	
Magnetic behavior of dirty multiband superconductors near the upper critical field (7 pages)	214509
Mikhail Silaev	
Effects of electron correlation, electron-phonon coupling, and spin-orbit coupling on the isovalent Pd-substituted superconductor SrPt ₃ P (6 pages)	214510
Kangkang Hu, Bo Gao, Qiucheng Ji, Yonghui Ma, Wei Li, Xuguang Xu, Hui Zhang, Gang Mu, Fuqiang Huang, Chuanbing Cai, Xiaoming Xie, and Mianheng Jiang	
Probing unconventional superconductivity in inversion-symmetric doped Weyl semimetal (7 pages)	214511
Youngseok Kim, Moon Jip Park, and Matthew J. Gilbert	
Simultaneous investigation of shear modulus and torsional resonance of solid ⁴ He (5 pages)	214512
Jaeho Shin, Jaewon Choi, Keiya Shirahama, and Eunseong Kim	
Extracting paramagnon excitations from resonant inelastic x-ray scattering experiments (4 pages)	214513
Jagat Lamsal and Wouter Montfrooij	
Characterizing p -wave superconductivity using the spin structure of Shiba states (10 pages)	214514
V. Kaladzhyan, C. Bena, and P. Simon	

(Continued)

Spin-orbit coupling and odd-parity superconductivity in the quasi-one-dimensional compound $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$ (6 pages)	214515
Christian Platt, Weeje Cho, Ross H. McKenzie, Ronny Thomale, and S. Raghu	
Rashba versus Kohn-Luttinger: Evolution of p -wave superconductivity in magnetized two-dimensional Fermi gases subject to spin-orbit interactions (9 pages)	214516
Ethan Lake, Caleb Webb, D. A. Pesin, and O. A. Starykh	
Large quantum superpositions of a nanoparticle immersed in superfluid helium (4 pages)	214517
O. Lychkovskiy	
Paramagnetic excited vortex states in superconductors (14 pages)	214518
Rodolpho Ribeiro Gomes, Mauro M. Doria, and Antonio R. de C. Romaguera	
Doping evolution of the superconducting gap structure in the underdoped iron arsenide $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ revealed by thermal conductivity (7 pages)	214519
J.-Ph. Reid, M. A. Tanatar, X. G. Luo, H. Shakeripour, S. René de Cotret, A. Juneau-Fecteau, J. Chang, B. Shen, H.-H. Wen, H. Kim, R. Prozorov, N. Doiron-Leyraud, and Louis Taillefer	

ERRATA

Publisher's Note: Crucial role of interlayer distance for antiferromagnet-induced perpendicular magnetic anisotropy [Phys. Rev. B 92 , 214435 (2015)] (1 page)	219901(E)
Bo-Yao Wang, Po-Han Lin, Ming-Shian Tsai, Chun-Wei Shih, Meng-Ju Lee, Chun-Wei Huang, Nae-Yeou Jih, Pei-Yu Cheng, and Der-Hsin Wei	
Publisher's Note: Evolution of damping in ferromagnetic/nonmagnetic thin film bilayers as a function of nonmagnetic layer thickness [Phys. Rev. B 93 , 054402 (2016)] (1 page)	219902(E)
S. Azzawi, A. Ganguly, M. Tokaç, R. M. Rowan-Robinson, J. Sinha, A. T. Hindmarch, A. Barman, and D. Atkinson	
Publisher's Note: Charge avalanches and depinning in the Coulomb glass: The role of long-range interactions [Phys. Rev. B 93 , 094429 (2016)] (1 page)	219903(E)
Juan Carlos Andresen, Yohanes Pramudya, Helmut G. Katzgraber, Creighton K. Thomas, Gergely T. Zimanyi, and V. Dobrosavljević	
Erratum: High-pressure x-ray-diffraction study of $\alpha\text{-AlPO}_4$ [Phys. Rev. B 62 , 8824 (2000)] (1 page)	219904(E)
Surinder M. Sharma, Nandini Garg, and S. K. Sikka	
Publisher's Note: Umbrella-coplanar transition in the triangular XXZ model with arbitrary spin [Phys. Rev. B 93 , 224402 (2016)] (1 page)	219905(E)
Giacomo Marmorini, Daisuke Yamamoto, and Ippei Danshita	
Erratum: Spin transfer torque in antiferromagnetic spin valves: From clean to disordered regimes [Phys. Rev. B 89 , 174430 (2014)] (1 page)	219906(E)
Hamed Ben Mohamed Saidaoui, Aurelien Manchon, and Xavier Waintal	