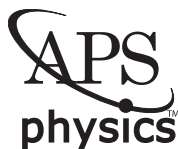


ARTICLES

Structure, structural phase transitions, mechanical properties, defects

- Reversible phase transition induced large piezoelectric response in Sm-doped BiFeO₃ with a composition near the morphotropic phase boundary (*7 pages*) 214101
Zhenyu Liao, Fei Xue, Wei Sun, Dongsheng Song, Qiqi Zhang, Jing-Feng Li, Long-Qing Chen, and Jing Zhu
- Formation enthalpies for transition metal alloys using machine learning (*12 pages*) 214102
Shashanka Ubaru, Agnieszka Międlar, Yousef Saad, and James R. Chelikowsky
-  Current-voltage characteristics of Weyl semimetal semiconducting devices, Veselago lenses, and hyperbolic Dirac phase (*13 pages*) 214103
R. D. Y. Hills, A. Kusmartseva, and F. V. Kusmartsev
- Elasticity and Poisson's ratio of hexagonal close-packed hydrogen at high pressures (*10 pages*) 214104
Alexander F. Goncharov, Michel Gauthier, Daniele Antonangeli, Simon Ayrinhac, Frédéric Decremps, Marc Morand, Alexei Grechnev, S. M. Tretyak, and Yu. A. Freiman
- Molecular detection on a defective MoS₂ monolayer by simultaneous conductance and force simulations (*9 pages*) 214105
C. González and Y. J. Dappe
- First-principles investigation of local structure deformation induced by x-ray irradiation in κ -(BEDT-TTF)₂Cu[N(CN)₂]Br (*7 pages*) 214106
Lijing Kang, Kazuto Akagi, Kouichi Hayashi, and Takahiko Sasaki
- First-principles investigation of phase stability in the Mg-Sc binary alloy (*10 pages*) 214107
Anirudh Raju Natarajan and Anton Van der Ven
- Migration mechanism for oversized solutes in cubic lattices: The case of yttrium in iron (*11 pages*) 214108
Jean-Louis Bocquet, Caroline Barouh, and Chu-Chun Fu
- Palladium-based ferroelectrics and multiferroics: Theory and experiment (*9 pages*) 214109
Shalini Kumari, Dhiren K. Pradhan, Nora Ortega, Kallol Pradhan, Christopher DeVreugd, Gopalan Srinivasan, Ashok Kumar, Tula R. Paudel, Evgeny Y. Tsymbal, Alice M. Bumstead, J. F. Scott, and Ram S. Katiyar
- Temperature-dependent far-infrared reflectance of an epitaxial (BaTiO₃)₈/(SrTiO₃)₄ superlattice (*10 pages*) 214110
V. Železný, O. Caha, A. Soukiassian, D. G. Schlom, and X. X. Xi



CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 95, NUMBER 21

JUNE 2017-1(I)

Glassy nature and glass-to-crystal transition in the binary metallic glass CuZr (11 pages)	214111
Zi-Yang Wei, Cheng Shang, Xiao-Jie Zhang, and Zhi-Pan Liu	
Frequency-dependent mechanical damping in alloys (8 pages)	214112
Raghavan Ranganathan, Yunfeng Shi, and Pawel Keblinski	
Tunable low-temperature dissipation scenarios in palladium nanomechanical resonators (9 pages)	214113
S. Rebari, Shelender Kumar, S. Indrajeet, Abhishek Kumar, Satyendra P. Pal, D. Weiss, and A. Venkatesan	
Simultaneous time-space resolved reflectivity and interferometric measurements of dielectrics excited with femtosecond laser pulses (13 pages)	214114
M. Garcia-Lechuga, L. Haahr-Lillevang, J. Siegel, P. Balling, S. Guizard, and J. Solis	
Phosphorus allotropes: Stability of black versus red phosphorus re-examined by means of the van der Waals inclusive density functional method (7 pages)	214115
Muratahan Aykol, Jeff W. Doak, and C. Wolverton	
Relativistic coupled-cluster and density-functional studies of argon at high pressure (10 pages)	214116
Peter Schwerdtfeger, Krista G. Steenbergen, and Elke Pahl	
Improved atomistic Monte Carlo models based on <i>ab-initio</i> -trained neural networks: Application to FeCu and FeCr alloys (11 pages)	214117
N. Castin, L. Messina, C. Domain, R. C. Pasianot, and P. Olsson	
Role of the A-site cation in determining the properties of the hybrid perovskite CH ₃ NH ₃ PbBr ₃ (7 pages)	214118
Sagar Sarkar and Priya Mahadevan	
Mott-to-Goodenough insulator-insulator transition in LiVO ₂ (7 pages)	214119
Alaska Subedi	
Synthesis of a polar ordered oxynitride perovskite (5 pages)	214120
Rajasekarakumar Vadapoo, Muhtar Ahart, Maddury Somayazulu, Nicholas Holtgrewe, Yue Meng, Zuzana Konopkova, Russell J. Hemley, and R. E. Cohen	
First-principles study on Ni ₃ Al (111) antiphase boundary with Ti and Hf impurities (9 pages)	214121
Ruoshi Sun, Christopher Woodward, and Axel van de Walle	
Inhomogeneous, disordered, and partially ordered systems	
Delocalized carriers in the <i>t</i> - <i>J</i> model with strong charge disorder (8 pages)	214201
Janez Bonča and Marcin Mierzejewski	
Polaron spin echo envelope modulations in an organic semiconducting polymer (14 pages)	214202
V. V. Mkhitarian and V. V. Dobrovitski	
Transport and optics at the node in a nodal loop semimetal (11 pages)	214203
S. P. Mukherjee and J. P. Carbotte	
Quantum dynamics of nuclear spins and spin relaxation in organic semiconductors (6 pages)	214204
V. V. Mkhitarian and V. V. Dobrovitski	
Cotunneling and polaronic effect in granular systems (18 pages)	214205
A. S. Ioselevich and V. V. Sivak	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 95, NUMBER 21

JUNE 2017-1(I)

Scaling of the Hall effects beyond the quantum resistance threshold in oxidized CoFeB (5 pages)	214206
A. Gerber and G. Kopnov	
Memory versus irreversibility in the thermal densification of amorphous glasses (10 pages)	214207
Z. Ovadyahu	
Dynamics, dynamical systems, lattice effects:	
Absorption spectrum of a two-level system subjected to a periodic pulse sequence (12 pages)	214301
H. F. Fotso and V. V. Dobrovitski	
Accurate interatomic force fields via machine learning with covariant kernels (10 pages)	214302
Aldo Glielmo, Peter Sollich, and Alessandro De Vita	
Unified quantum theory of elastic and inelastic atomic scattering from a physisorbed monolayer solid (12 pages)	214303
L. W. Bruch, F. Y. Hansen, and B. Dammann	
Dynamic strain-induced giant electroresistance and erasing effect in ultrathin ferroelectric tunnel-junction memory (7 pages)	214304
Hei-Man Yau, Zhongnan Xi, Xinxin Chen, Zheng Wen, Ge Wu, and Ji-Yan Dai	
Diffusely scattered and transmitted elastic waves by random rough solid-solid interfaces using an elastodynamic Kirchhoff approximation (13 pages)	214305
Fan Shi, Mike Lowe, and Richard Craster	
Acoustic properties of double-porosity granular polymers (10 pages)	214306
A. Alevizaki, R. Sainidou, P. Rembert, B. Morvan, and N. Stefanou	
Floquet time crystal in the Lipkin-Meshkov-Glick model (12 pages)	214307
Angelo Russomanno, Fernando Iemini, Marcello Dalmonte, and Rosario Fazio	
Zero-temperature localization in a sub-Ohmic spin-boson model investigated by an extended hierarchy equation of motion (8 pages)	214308
Chenru Duan, Zhoufei Tang, Jianshu Cao, and Jianlan Wu	
Rabi-like vibrational coherence transfer in a hydrogen-bonded charge transfer material (8 pages)	214309
Aaron S. Rury and Jahan M. Dawlaty	
Distinguishing between spatial coherence and temporal coherence of phonons (8 pages)	214310
Benoit Latour and Yann Chalopin	
Magnetism	
Spin dynamics of antiferromagnets in the presence of a homogeneous magnetization (16 pages)	214401
T. R. Kirkpatrick and D. Belitz	
First-order reversal curve of the magnetostructural phase transition in FeTe (8 pages)	214402
M. K. Frampton, J. Crocker, D. A. Gilbert, N. Curro, Kai Liu, J. A. Schneeloch, G. D. Gu, and R. J. Zieve	
Pressure effects in the itinerant antiferromagnetic metal TiAu (10 pages)	214403
C. T. Wolowiec, Y. Fang, C. A. McElroy, J. R. Jeffries, R. L. Stillwell, E. Svanidze, J. M. Santiago, E. Morosan, S. T. Weir, Y. K. Vohra, and M. B. Maple	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 95, NUMBER 21

JUNE 2017-1(I)

Phase diagram of weakly coupled Heisenberg spin chains subject to a uniform Dzyaloshinskii-Moriya interaction (25 pages)	214404
Wen Jin and Oleg A. Starykh	
Inverse spin Hall effect in the semiconductor (Ga,Mn)As at room temperature (7 pages)	214405
J. B. S. Mendes, S. L. A. Mello, O. Alves Santos, R. O. Cunha, R. L. Rodríguez-Suárez, A. Azevedo, and S. M. Rezende	
Superexchange theory of electronic polarization driven by relativistic spin-orbit interaction at half filling (13 pages)	214406
I. V. Solov'yev	
Dipolar ferromagnetism in three-dimensional superlattices of nanoparticles (8 pages)	214407
Bassel Alkadour, J. I. Mercer, J. P. Whitehead, B. W. Southern, and J. van Lierop	
Magnon dispersion in $\text{Ca}_2\text{Ru}_{1-x}\text{Ti}_x\text{O}_4$: Impact of spin-orbit coupling and oxygen moments (14 pages)	214408
S. Kunkemöller, E. Komleva, S. V. Streltsov, S. Hoffmann, D. I. Khomskii, P. Steffens, Y. Sidis, K. Schmalzl, and M. Braden	
Finite-temperature fidelity and von Neumann entropy in the honeycomb spin lattice with quantum Ising interaction (9 pages)	214409
Yan-Wei Dai, Qian-Qian Shi, Sam Young Cho, Murray T. Batchelor, and Huan-Qiang Zhou	
Entanglement scaling and spatial correlations of the transverse-field Ising model with perturbations (8 pages)	214410
Richard Cole, Frank Pollmann, and Joseph J. Betouras	
Topological properties of a coupled spin-photon system induced by damping (7 pages)	214411
Michael Harder, Lihui Bai, Paul Hyde, and Can-Ming Hu	
Critical behavior of $\text{Mg}_{1-x}\text{Fe}_x\text{O}$ at the pressure-induced iron spin-state crossover (8 pages)	214412
K. Glazyrin, R. Sinmyo, E. Bykova, M. Bykov, V. Cerantola, M. Longo, C. McCammon, Vitali B. Prakapenka, and Leonid Dubrovinsky	
Spin pumping, dissipation, and direct and alternating inverse spin Hall effects in magnetic-insulator/normal-metal bilayers (14 pages)	214413
André Kapelrud and Arne Brataas	
Anisotropy-governed competition of magnetic phases in the honeycomb quantum magnet $\text{Na}_3\text{Ni}_2\text{SbO}_6$ studied by dilatometry and high-frequency ESR (7 pages)	214414
J. Werner, W. Hergert, M. Gertig, J. Park, C. Koo, and R. Klingeler	
Phase diagram of multiferroic $\text{KCu}_3\text{As}_2\text{O}_7(\text{OD})_3$ (10 pages)	214415
Gørn J. Nilsen, Virginie Simonet, Claire V. Colin, Ryutaro Okuma, Yoshihiko Okamoto, Masashi Tokunaga, Thomas C. Hansen, Dmitry D. Khalyavin, and Zenji Hiroi	
Detection of induced paramagnetic moments in Pt on $\text{Y}_3\text{Fe}_5\text{O}_{12}$ via x-ray magnetic circular dichroism (7 pages)	214416
Takashi Kikkawa, Motohiro Suzuki, Jun Okabayashi, Ken-ichi Uchida, Daisuke Kikuchi, Zhiyong Qiu, and Eiji Saitoh	
Magnetism and ultrafast magnetization dynamics of Co and CoMn alloys at finite temperature (12 pages)	214417
R. Chimata, E. K. Delczeg-Czirjak, A. Szilva, R. Cardias, Y. O. Kvashnin, M. Pereiro, S. Mankovsky, H. Ebert, D. Thonig, B. Sanyal, A. B. Klautau, and O. Eriksson	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 95, NUMBER 21

JUNE 2017-1(I)

Paths to collapse for isolated skyrmions in few-monolayer ferromagnetic films (<i>12 pages</i>)	214418
Dusan Stosic, Jeroen Mulkers, Bartel Van Waeyenberge, Teresa B. Ludermir, and Milorad V. Milošević	
Field-induced metamagnetic transitions and two-dimensional excitations in ludwigite $\text{Co}_{4.76}\text{Al}_{1.24}(\text{O}_2\text{BO}_3)_2$ (<i>6 pages</i>)	214419
C. P. C. Medrano, D. C. Freitas, E. C. Passamani, C. B. Pinheiro, E. Baggio-Saitovitch, M. A. Continentino, and D. R. Sanchez	
Cascades of phase transitions in spiral magnets caused by dipolar forces (<i>9 pages</i>)	214420
O. I. Utesov and A. V. Syromyatnikov	
Longitudinal spin Seebeck effect in permalloy separated from the anomalous Nernst effect: Theory and experiment (<i>8 pages</i>)	214421
J. Holanda, O. Alves Santos, R. O. Cunha, J. B. S. Mendes, R. L. Rodríguez-Suárez, A. Azevedo, and S. M. Rezende	
Anisotropic Dzyaloshinskii-Moriya interaction in ultrathin epitaxial Au/Co/W(110) (<i>6 pages</i>)	214422
Lorenzo Camosi, Stanislas Rohart, Olivier Fruchart, Stefania Pizzini, Mohamed Belmeguenai, Yves Roussigné, Andreï Stashkevich, Salim Mourad Cherif, Laurent Ranno, Maurizio de Santis, and Jan Vogel	
Temperature-dependent magnetic damping of yttrium iron garnet spheres (<i>8 pages</i>)	214423
H. Maier-Flaig, S. Klingler, C. Dubs, O. Surzhenko, R. Gross, M. Weiler, H. Huebl, and S. T. B. Goennenwein	
Spin-wave modes in ferromagnetic nanodisks, their excitation via alternating currents and fields, and auto-oscillations (<i>15 pages</i>)	214424
D. Mancilla-Almonacid and R. E. Arias	
Magnetic phase diagram of CeCu_2Ge_2 up to 15 T: On the route to understand field-induced phase transitions (<i>10 pages</i>)	214425
P. Geselbracht, A. Schneidewind, M. Doerr, S. Granovsky, M. Rotter, M. Loewenhaupt, G. W. Scheerer, Z. Ren, and K. Prokeš	
Magnetization process in a frustrated plaquette dimerized ladder (<i>13 pages</i>)	214426
F. Elias, M. Arlego, and C. A. Lamas	
Equilibrium magnetization and magnetization relaxation of multicore magnetic nanoparticles (<i>10 pages</i>)	214427
Patrick Ilg	
Superfluidity and superconductivity	
Collective mode contributions to the Meissner effect: Fulde-Ferrell and pair-density wave superfluids (<i>6 pages</i>)	214501
Rufus Boyack, Chien-Te Wu, Brandon M. Anderson, and K. Levin	
Higgs modes in the pair density wave superconducting state (<i>10 pages</i>)	214502
Rodrigo Soto-Garrido, Yuxuan Wang, Eduardo Fradkin, and S. Lance Cooper	
Stability of flat zero-energy states at the dirty surface of a nodal superconductor (<i>11 pages</i>)	214503
Satoshi Ikegaya and Yasuhiro Asano	
Giant ultrafast Kerr effect in superconductors (<i>5 pages</i>)	214504
Charles W. Robson, Kieran A. Fraser, and Fabio Biancalana	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 95, NUMBER 21

JUNE 2017-1(I)

Nature of the effective interaction in electron-doped cuprate superconductors: A sign-problem-free quantum Monte Carlo study (7 pages)	214505
Zi-Xiang Li, Fa Wang, Hong Yao, and Dung-Hai Lee	
Superconductivity and charge-carrier localization in ultrathin $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4/\text{La}_2\text{CuO}_4$ bilayers (12 pages)	214506
K. Sen, P. Marsik, S. Das, E. Perret, R. de Andres Prada, A. Alberca, N. Biškup, M. Varela, and C. Bernhard	
Dynamic transition of vortices into phase slips and generation of vortex-antivortex pairs in thin film Josephson junctions under dc and ac currents (19 pages)	214507
Ahmad Sheikhzada and Alex Gurevich	
Damped spin excitations in a doped cuprate superconductor with orbital hybridization (8 pages)	214508
O. Ivashko, N. E. Shaik, X. Lu, C. G. Fatuzzo, M. Dantz, P. G. Freeman, D. E. McNally, D. Destraz, N. B. Christensen, T. Kurosawa, N. Momono, M. Oda, C. E. Matt, C. Monney, H. M. Rønnow, T. Schmitt, and J. Chang	
Finite-energy spin fluctuations as a pairing glue in systems with coexisting electron and hole bands (6 pages)	214509
Masahiro Nakata, Daisuke Ogura, Hidetomo Usui, and Kazuhiko Kuroki	
Ru doping in iron-based pnictides: The “unfolded” dominant role of structural effects for superconductivity (11 pages)	214510
M. Reticcioli, G. Profeta, C. Franchini, and A. Continenza	
Superconductivity with broken time-reversal symmetry in ion-irradiated $\text{Ba}_{0.27}\text{K}_{0.73}\text{Fe}_2\text{As}_2$ single crystals (5 pages)	214511
V. Grinenko, P. Materne, R. Sarkar, H. Luetkens, K. Kihou, C. H. Lee, S. Akhmadaliev, D. V. Efremov, S.-L. Drechsler, and H.-H. Klauss	
Optical investigation of $\text{BaFe}_2(\text{As}_{0.77}\text{P}_{0.23})_2$: Spin-fluctuation-mediated superconductivity under pressure (12 pages)	214512
E. Uykur, T. Kobayashi, W. Hirata, S. Miyasaka, S. Tajima, and C. A. Kuntscher	
Quantum paraelectricity probed by superconducting resonators (6 pages)	214513
D. Davidovikj, N. Manca, H. S. J. van der Zant, A. D. Caviglia, and G. A. Steele	
Electron-phonon superconductivity in the filled skutterudites $\text{LaRu}_4\text{P}_{12}$, $\text{LaRu}_4\text{As}_{12}$, and $\text{LaPt}_4\text{Ge}_{12}$ (13 pages)	214514
H. M. Tütüncü, Ertuğrul Karaca, and G. P. Srivastava	
Three superconducting phases with different categories of pairing in hole- and electron-doped $\text{LaFeAs}_{1-x}\text{P}_x\text{O}$ (8 pages)	214515
S. Miyasaka, M. Uekubo, H. Tsuji, M. Nakajima, S. Tajima, T. Shiotani, H. Mukuda, H. Sagayama, H. Nakao, R. Kumai, and Y. Murakami	

COMMENTS

Comment on “Cluster expansion and the configurational theory of alloys” (3 pages)	216201
Tim Mueller	
Reply to “Comment on ‘Cluster expansion and the configurational theory of alloys’” (4 pages)	216202
J. M. Sanchez	

(Continued)

ERRATA

Publisher's Note: Enhanced ferroelectric polarization in epitaxial $(\text{Pb}_{1-x}\text{La}_x)(\text{Zr}_{0.52}\text{Ti}_{0.48})\text{O}_3$ thin films due to low La doping [Phys. Rev. B 95 , 174304 (2017)] (<i>1 page</i>)	219901(E)
Devajyoti Mukherjee, Mahesh Hordagoda, David Pesquera, Dipankar Ghosh, Jacob L. Jones, Pritish Mukherjee, and Sarath Witanachchi	
Publisher's Note: Josephson effect in a multiorbital model for Sr_2RuO_4 [Phys. Rev. B 95 , 174518 (2017)] (<i>1 page</i>)	219902(E)
Kohei Kawai, Keiji Yada, Yukio Tanaka, Yasuhiro Asano, Alexander A. Golubov, and Satoshi Kashiwaya	
Publisher's Note: Achiral tilted domain walls in perpendicularly magnetized nanowires [Phys. Rev. B 95 , 180406(R) (2017)] (<i>1 page</i>)	219903(E)
B. Boehm, A. Bisig, A. Bischof, G. Stefanou, B. J. Hickey, and R. Allenspach	
Publisher's Note: Phase-field study of ripening and rearrangement of precipitates under chemomechanical coupling [Phys. Rev. B 95 , 174101 (2017)] (<i>1 page</i>)	219904(E)
C. Schwarze, A. Gupta, T. Hickel, and R. Darvishi Kamachali	
Erratum: Unraveling the composition dependence of the martensitic transformation temperature: A first-principles study of Ti-Ta alloys [Phys. Rev. B 94 , 224104 (2016)] (<i>1 page</i>)	219905(E)
Tanmoy Chakraborty, Jutta Rogal, and Ralf Drautz	