

711
p59/r6

PHYSICAL REVIEW BTM

CONDENSED MATTER AND MATERIALS PHYSICS

Articles Published in DECEMBER 2013

1(I)

Published by
AMERICAN PHYSICAL SOCIETYTM

Volume 88

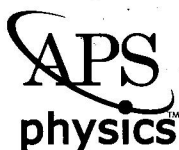
Third Series

Number 21

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

- Modified embedded-atom method used to derive interatomic potentials for defects and phase formation in the W-C system (9 pages) 214101
P. H. Chen and K. Nordlund
- Role of screened exact exchange in accurately describing properties of transition metal oxides: Modeling defects in LaAlO₃ (5 pages) 214102
Fedwa El-Mellouhi, Edward N. Brothers, Melissa J. Lucero, and Gustavo E. Scuseria
- Theory of local electric polarization and its relation to internal strain: Impact on polarization potential and electronic properties of group-III nitrides (22 pages) 214103
Miguel A. Caro, Stefan Schulz, and Eoin P. O'Reilly
- Charge ordering transition in GdBaCo₂O₅: Evidence of reentrant behavior (10 pages) 214104
M. Allieta, M. Scavini, L. Lo Presti, M. Coduri, L. Loconte, S. Cappelli, C. Oliva, P. Ghigna, P. Pattison, and V. Scagnoli
- Formation of monoclinic nanodomains at the morphotropic phase boundary of ferroelectric systems (6 pages) ... 214105
X. Q. Ke, D. Wang, X. Ren, and Y. Wang
- Dynamical symmetry breaking with optimal control: Reducing the number of pieces (6 pages) 214106
Matthew J. M. Power and Gabriele De Chiara
- Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure (6 pages) 214107
Qingfeng Zeng, Junhui Peng, Artem R. Oganov, Qiang Zhu, Congwei Xie, Xiaodong Zhang, Dong Dong, Litong Zhang, and Laifei Cheng
- Pressure-induced phase-transition sequence in CoF₂: An experimental and first-principles study on the crystal, vibrational, and electronic properties (15 pages) 214108
J. A. Barreda-Argüeso, S. López-Moreno, M. N. Sanz-Ortiz, F. Aguado, R. Valiente, J. González, F. Rodríguez, A. H. Romero, A. Muñoz, L. Nataf, and F. Baudelet
- Mott transition in CaFe₂O₄ at around 50 GPa (5 pages) 214109
Eran Greenberg, Gregory H. Rozenberg, Weiming Xu, Moshe P. Pasternak, Catherine McCammon, Konstantin Glazyrin, and Leonid S. Dubrovinsky



| | |
|---|--------|
| Pressure-induced stacking sequence variations in gold from first principles (<i>6 pages</i>) | 214110 |
| Takahiro Ishikawa, Kuniko Kato, Masaya Nomura, Naoshi Suzuki, Hitose Nagara, and Katsuya Shimizu | |
| Finite-temperature properties of strongly anharmonic and mechanically unstable crystal phases from first principles (<i>13 pages</i>) | 214111 |
| John C. Thomas and Anton Van der Ven | |
| Simulation of uranium dioxide polymorphs and their phase transitions (<i>12 pages</i>) | 214112 |
| Paul C. M. Fossati, Laurent Van Brutzel, Alain Chartier, and Jean-Paul Crocombette | |
| Isotopic differentiation and sublattice melting in dense dynamic ice (<i>8 pages</i>) | 214113 |
| Andreas Hermann, N. W. Ashcroft, and Roald Hoffmann | |
| Alignment of ferroelectric polarization and defect complexes in copper-doped potassium niobate (<i>13 pages</i>) | 214114 |
| Sabine Körbel and Christian Elsässer | |
| Control of oxygen octahedral rotations and physical properties in SrRuO ₃ films (<i>11 pages</i>) | 214115 |
| Wenlai Lu, Ping Yang, Wen Dong Song, Gan Moog Chow, and Jing Sheng Chen | |
| Defect ordering and defect–domain-wall interactions in PbTiO ₃ : A first-principles study (<i>7 pages</i>) | 214116 |
| Anand Chandrasekaran, Dragan Damjanovic, Nava Setter, and Nicola Marzari | |
| Native point defects in LaAlO ₃ : A hybrid functional study (<i>8 pages</i>) | 214117 |
| Minseok Choi, Anderson Janotti, and Chris G. Van de Walle | |
| Inhomogeneous, disordered, and partially ordered systems | |
| Long-time relaxation of ion-bombarded silicon studied with the kinetic activation-relaxation technique: Microscopic description of slow aging in a disordered system (<i>9 pages</i>) | 214201 |
| Laurent Karim Béland and Normand Mousseau | |
| Geometrically frustrated magnetism of spins on icosahedral clusters: The Gd ₃ Au ₁₃ Sn ₄ quasicrystalline approximant (<i>11 pages</i>) | 214202 |
| P. Koželj, S. Jazbec, S. Vrtnik, A. Jelen, J. Dolinšek, M. Jagodič, Z. Jagličić, P. Boulet, M. C. de Weerd, J. Ledieu, J. M. Dubois, and V. Fournée | |
| Dynamics, dynamical systems, lattice effects: | |
| Nonlinear dynamics of a microelectromechanical oscillator with delayed feedback (<i>5 pages</i>) | 214301 |
| R. van Leeuwen, D. M. Karabacak, H. S. J. van der Zant, and W. J. Venstra | |
| Picosecond Joule heating in photoconductive switch electrodes (<i>7 pages</i>) | 214302 |
| Bjorn Vermeersch, Gilles Pernot, Hong Lu, Je-Hyeong Bahk, Art Gossard, and Ali Shakouri | |
| <i>Ab initio</i> study of the unusual thermal transport properties of boron arsenide and related materials (<i>12 pages</i>) | 214303 |
| D. A. Broido, L. Lindsay, and T. L. Reinecke | |
| Transverse thermoelectric effects in platinum strips on permalloy films (<i>6 pages</i>) | 214304 |
| S. H. Wang, L. K. Zou, J. W. Cai, B. G. Shen, and J. R. Sun | |
| Magnetism | |
| Asymmetric magnetic domain-wall motion by the Dzyaloshinskii-Moriya interaction (<i>5 pages</i>) | 214401 |
| Soong-Geun Je, Duck-Ho Kim, Sang-Cheol Yoo, Byoung-Chul Min, Kyung-Jin Lee, and Sug-Bong Choe | |

(Continued)

| | |
|---|--------|
| Multishell contribution to the Dzyaloshinskii-Moriya spiraling in MnSi-type crystals (<i>13 pages</i>) | 214402 |
| Viacheslav A. Chizhikov and Vladimir E. Dmitrienko | |
| Separation of longitudinal spin Seebeck effect from anomalous Nernst effect: Determination of origin of transverse thermoelectric voltage in metal/insulator junctions (<i>11 pages</i>) | 214403 |
| T. Kikkawa, K. Uchida, S. Daimon, Y. Shiomi, H. Adachi, Z. Qiu, D. Hou, X.-F. Jin, S. Maekawa, and E. Saitoh | |
| Ultrafast demagnetization after laser irradiation in transition metals: <i>Ab initio</i> calculations of the spin-flip electron-phonon scattering with reduced exchange splitting (<i>11 pages</i>) | 214404 |
| Christian Illg, Michael Haag, and Manfred Fähnle | |
| Pure spin current-induced domain wall motion probed by localized spin signal detection (<i>7 pages</i>) | 214405 |
| Nils Motzko, Björn Burkhardt, Nils Richter, Robert Reeve, Piotr Laczkowski, Williams Savero Torres, Laurent Vila, Jean-Philippe Attané, and Mathias Kläui | |
| Large enhancement of emergent magnetic fields in MnSi with impurities and pressure (<i>5 pages</i>) | 214406 |
| Benjamin J. Chapman, Maxwell G. Grossnickle, Thomas Wolf, and Minhyea Lee | |
| Effect of hydrogen adsorption on the magnetic properties of a surface nanocluster of iron (<i>8 pages</i>) | 214407 |
| Pavel F. Bessarab, Valery M. Uzdin, and Hannes Jónsson | |
| Quantitative stray field imaging of a magnetic vortex core (<i>5 pages</i>) | 214408 |
| J.-P. Tetienne, T. Hingant, L. Rondin, S. Rohart, A. Thiaville, J.-F. Roch, and V. Jacques | |
| ☞ Phase-space Berry phases in chiral magnets: Dzyaloshinskii-Moriya interaction and the charge of skyrmions (<i>11 pages</i>) | 214409 |
| Frank Freimuth, Robert Bamler, Yuriy Mokrousov, and Achim Rosch | |
| Stabilization of spin-zero Ru ⁴⁺ through epitaxial strain in SrRuO ₃ thin films (<i>5 pages</i>) | 214410 |
| A. J. Grutter, F. J. Wong, C. A. Jenkins, E. Arenholz, A. Vailionis, and Y. Suzuki | |
| Quantum phase transitions out of a $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological phase (<i>8 pages</i>) | 214411 |
| Saeed S. Jahromi, S. Farhad Masoudi, Mehdi Kargarian, and Kai Phillip Schmidt | |
| Thermal drag in spin ladders coupled to phonons (<i>8 pages</i>) | 214412 |
| Christian Bartsch and Wolfram Brenig | |
| Magnetocrystalline anisotropy energy of Fe(001) and Fe(110) slabs and nanoclusters: A detailed local analysis within a tight-binding model (<i>9 pages</i>) | 214413 |
| Dongzhe Li, Alexander Smogunov, Cyrille Barreateau, François Ducastelle, and Daniel Spanjaard | |
| Thermally activated switching rate of a nanomagnet in the presence of spin torque (<i>6 pages</i>) | 214414 |
| Tomohiro Taniguchi, Yasuhiro Utsumi, and Hiroshi Imamura | |
| Circularly polarized x-ray scattering investigation of spin-lattice coupling in TbMnO ₃ in crossed electric and magnetic fields (<i>13 pages</i>) | 214415 |
| H. C. Walker, F. Fabrizi, L. Paolasini, F. de Bergevin, D. Prabhakaran, A. T. Boothroyd, and D. F. McMorrow | |
| Photoinduced dynamics of spinel MnV ₂ O ₄ (<i>7 pages</i>) | 214416 |
| K. Takubo, Y. Onishi, A. Furuhashi, A. Nogami, and T. Katsufuji | |
| Current-induced torques and interfacial spin-orbit coupling (<i>7 pages</i>) | 214417 |
| Paul M. Haney, Hyun-Woo Lee, Kyung-Jin Lee, Aurélien Manchon, and M. D. Stiles | |

(Continued)

| | |
|--|--------|
| Spin- $\frac{1}{2}$ J_1 - J_2 Heisenberg model on a cross-stripped square lattice (<i>15 pages</i>) | 214418 |
| R. F. Bishop, P. H. Y. Li, and C. E. Campbell | |
| Inelastic neutron scattering study of crystal field excitations of Nd^{3+} in NdFeAsO (<i>6 pages</i>) | 214419 |
| Y. Xiao, M. Zbiri, R. A. Downie, J.-W. G. Bos, Th. Brückel, and T. Chatterji | |
| Discrete helicoidal states in chiral magnetic thin films (<i>6 pages</i>) | 214420 |
| M. N. Wilson, E. A. Karhu, D. P. Lake, A. S. Quigley, S. Meynell, A. N. Bogdanov, H. Fritzsche, U. K. Röbler, and T. L. Monchesky | |
| Magnetic quantum diesel engine in Ni_2 (<i>11 pages</i>) | 214421 |
| C. D. Dong, G. Lefkidis, and W. Hübner | |
| Quantum Monte Carlo simulations for stacked spin-ladder systems containing low concentrations of nonmagnetic impurities: Application to the low-temperature broadening of NMR spectra in SrCu_2O_3 (<i>10 pages</i>) | 214422 |
| Robert Achleitner, Hans Gerd Evertz, Masatoshi Imada, Ralf Gamillscheg, and Peter Mohn | |
| Intrinsic magnetic order and inhomogeneous transport in Gd-implanted zinc oxide (<i>5 pages</i>) | 214423 |
| John Kennedy, Grant V. M. Williams, Peter P. Murmu, and Ben J. Ruck | |
| Extended reciprocal space observation of artificial spin ice with x-ray resonant magnetic scattering (<i>7 pages</i>) | 214424 |
| J. Perron, L. Anghinolfi, B. Tudu, N. Jaouen, J.-M. Tonnerre, M. Sacchi, F. Nolting, J. Lüning, and L. J. Heyderman | |
| Spin-polarized photoelectrons resonantly excited by circularly polarized light from a fractional Ag film on $\text{GaAs}(100)$ (<i>6 pages</i>) | 214425 |
| P. Klaer, F. Schertz, M. Lehr, G. Schönhense, and H. J. Elmers | |
| Surface critical exponents at a discontinuous bulk transition (<i>6 pages</i>) | 214426 |
| Linjun Li and Michel Pleimling | |
| Rotation sense of the magnetization in the Co/CoO exchange-bias system probed with anisotropic magnetoresistance measurements (<i>4 pages</i>) | 214427 |
| Steven Brems, Haoliang Liu, Kristiaan Temst, and Chris Van Haesendonck | |
| Magnon spectrum in the domain ferromagnetic state of antisite-disordered double perovskites (<i>7 pages</i>) | 214428 |
| Subrat Kumar Das, Viveka Nand Singh, and Pinaki Majumdar | |
| Effects of pressure on the magnetic-structural and Griffiths-like transitions in $\text{Dy}_5\text{Si}_3\text{Ge}$ (<i>9 pages</i>) | 214429 |
| N. Marcano, P. A. Algarabel, J. Rodríguez Fernández, C. Magén, L. Morellón, Niraj K. Singh, K. A. Gschneidner, Jr., V. K. Pecharsky, and M. R. Ibarra | |
| Insights into the phase diagram of bismuth ferrite from quasiharmonic free-energy calculations (<i>16 pages</i>) | 214430 |
| Claudio Cazorla and Jorge Íñiguez | |
| Testing dependence of anomalous Hall effect on resistivity in SrRuO_3 by its increase with electron irradiation (<i>4 pages</i>) | 214431 |
| Noam Haham, Marcin Konczykowski, Bouwe Kuiper, Gertjan Koster, and Lior Klein | |
| Spin Hall effect induced by Bi impurities in Cu: Skew scattering and side-jump (<i>8 pages</i>) | 214432 |
| Peter M. Levy, Hongxin Yang, Mairbek Chshiev, and Albert Fert | |
| Spiral magnetic structure in the iron diarsenate $\text{LiFeAs}_2\text{O}_7$: A neutron diffraction study (<i>9 pages</i>) | 214433 |
| Gwenaëlle Rousse, Juan Rodríguez-Carvajal, Calin Wurm, and Christian Masquelier | |

(Continued)

Superfluidity and superconductivity

- Sound velocities of hexagonal close-packed H_2 and He under pressure (*5 pages*) 214501
 Yu. A. Freiman, Alexei Grechnev, S. M. Tretyak, A. F. Goncharov, C. S. Zha, and Russell J. Hemley
- Superconducting current and proximity effect in ABA and ABC multilayer graphene Josephson junctions (*5 pages*) 214502
 W. A. Muñoz, L. Covaci, and F. M. Peeters
- Chiral phases of superfluid 3He in an anisotropic medium (*15 pages*) 214503
 J. A. Sauls
- Networks of Josephson junctions and their synchronization (*4 pages*) 214504
 Yurii N. Ovchinnikov and Vladimir Z. Kresin
- Quantum Monte Carlo study of the dynamic structure factor in the gas and crystal phase of hard-sphere bosons (*11 pages*) 214505
 R. Rota, F. Tramonto, D. E. Galli, and S. Giorgini
- Muon spin relaxation and electron/neutron diffraction studies of $BaTi_2(As_{1-x}Sb_x)_2O$: Absence of static magnetism and superlattice reflections (*5 pages*) 214506
 Y. Nozaki, K. Nakano, T. Yajima, H. Kageyama, B. Frandsen, L. Liu, S. Cheung, T. Goko, Y. J. Uemura, T. S. J. Munsie, T. Medina, G. M. Luke, J. Munevar, D. Nishio-Hamane, and C. M. Brown
- Classification of ground states and normal modes for phase-frustrated multicomponent superconductors (*17 pages*) 214507
 Daniel Weston and Egor Babaev
- Leggett modes in iron-based superconductors as a probe of time-reversal symmetry breaking (*20 pages*) 214508
 M. Marciiani, L. Fanfarillo, C. Castellani, and L. Benfatto
- Ⓔ Microwave conductivity and superfluid density in strongly overdoped $Tl_2Ba_2CuO_{6+\delta}$ (*12 pages*) 214509
 D. Deepwell, D. C. Peets, C. J. S. Truncik, N. C. Murphy, M. P. Kennett, W. A. Huttema, Ruixing Liang, D. A. Bonn, W. N. Hardy, and D. M. Broun
- Evolution of the Fermi surface topology in doped 122 iron pnictides (*7 pages*) 214510
 Lihua Pan, Jian Li, Yuan-Yen Tai, Matthias J. Graf, Jian-Xin Zhu, and C. S. Ting
- Superconductivity in $Fe_{1.05}Te:O_x$ single crystals (*5 pages*) 214511
 Z. T. Zhang, Z. R. Yang, W. J. Lu, X. L. Chen, L. Li, Y. P. Sun, C. Y. Xi, L. S. Ling, C. J. Zhang, L. Pi, M. L. Tian, and Y. H. Zhang
- Pressure-induced $0-\pi$ transitions and supercurrent crossover in antiferromagnetic weak links (*4 pages*) 214512
 Henrik Enoksen, Jacob Linder, and Asle Sudbø
- Transverse forces on a vortex in lattice models of superfluids (*7 pages*) 214513
 E. B. Sonin
- Time-reversal anomaly and Josephson effect in time-reversal-invariant topological superconductors (*7 pages*) 214514
 Suk Bum Chung, Joshua Horowitz, and Xiao-Liang Qi
- Devil's staircases and continued fractions in Josephson junctions (*6 pages*) 214515
 Yu. M. Shukrinov, S. Yu. Medvedeva, A. E. Botha, M. R. Kolahchi, and A. Irie

(Continued)

| | |
|---|--------|
| Magnetic structure of superconducting $\text{Eu}(\text{Fe}_{0.82}\text{Co}_{0.18})_2\text{As}_2$ as revealed by single-crystal neutron diffraction (7 pages) | 214516 |
| W. T. Jin, S. Nandi, Y. Xiao, Y. Su, O. Zaharko, Z. Guguchia, Z. Bukowski, S. Price, W. H. Jiao, G. H. Cao, and Th. Brückel | |
| Lattice dynamical signature of charge density wave formation in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (11 pages) | 214517 |
| M. Bakr, S. M. Souliou, S. Blanco-Canosa, I. Zegkinoglou, H. Gretarsson, J. Stremper, T. Loew, C. T. Lin, R. Liang, D. A. Bonn, W. N. Hardy, B. Keimer, and M. Le Tacon | |
| Disorder effects on superconducting tendencies in the checkerboard Hubbard model (13 pages) | 214518 |
| Peter M. Smith and Malcolm P. Kennett | |

ERRATA

| | |
|--|-----------|
| Publisher's Note: Spin motive force induced by Rashba interaction in the strong sd coupling regime [Phys. Rev. B 87 , 054403 (2013)] (1 page) | 219901(E) |
| Gen Tatara, Noriyuki Nakabayashi, and Kyung-Jin Lee | |
| Publisher's Note: Topological rf SQUID with a frustrating π junction for probing the Majorana bound state [Phys. Rev. B 88 , 184512 (2013)] (1 page) | 219902(E) |
| P. Lucignano, F. Tafuri, and A. Tagliacozzo | |
| Erratum: High-dimensional fractionalization and spinon deconfinement in pyrochlore antiferromagnets [Phys. Rev. B 75 , 094411 (2007)] (1 page) | 219903(E) |
| Z. Nussinov, C. D. Batista, B. Normand, and S. A. Trugman | |
| Erratum: Parametric amplification in Josephson junction embedded transmission lines [Phys. Rev. B 87 , 144301 (2013)] (2 pages) | 219904(E) |
| Oded Yaakobi, Lazar Friedland, Chris Macklin, and Irfan Siddiqi | |
| Erratum: Generalized Gilbert equation including inertial damping: Derivation from an extended breathing Fermi surface model [Phys. Rev. B 84 , 172403 (2011)] (1 page) | 219905(E) |
| Manfred Fähnle, Daniel Steiauf, and Christian Illg | |
| Publisher's Note: First-order ferroelastic transition in a magnetoelectric multiferroic: CuCrO_2 [Phys. Rev. B 88 , 224104 (2013)] (1 page) | 219906(E) |
| O. Aktas, G. Quirion, T. Otani, and T. Kimura | |
| Erratum: Interface-induced d -wave pairing [Phys. Rev. B 84 , 100510(R) (2011)] (1 page) | 219907(E) |
| C. Stephanos, T. Kopp, J. Mannhart, and P. J. Hirschfeld | |
| Publisher's Note: Magnetocrystalline anisotropy energy of Fe(001) and Fe(110) slabs and nanoclusters: A detailed local analysis within a tight-binding model [Phys. Rev. B 88 , 214413 (2013)] (1 page) | 219908(E) |
| Dongzhe Li, Alexander Smogunov, Cyrille Barreateau, François Ducastelle, and Daniel Spanjaard | |