

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

- Complete phase diagram and topological properties of interacting bosons in one-dimensional superlattices (*6 pages*) 134101
Tianhe Li, Huaiming Guo, Shu Chen, and Shun-Qing Shen
- Relaxed dispersion constraints and metamaterial effective parameters with physical meaning for all frequencies (*7 pages*) 134102
Christopher A. Dirdal, Tarjei Bondevik, and Johannes Skaar
- Structural, vibrational, and dielectric properties of Ruddlesden-Popper Ba_2ZrO_4 from first principles (*11 pages*) 134103
Lydie Louis and Serge M. Nakhmanson
- Noncentrosymmetric structural transitions in ultrashort ferroelectric $\text{AGaO}_3/\text{A}'\text{GaO}_3$ superlattices (*7 pages*) 134104
Nayoung Song, James M. Rondinelli, and Bog G. Kim
- Reconfigurable anisotropy and functional transformations with VO_2 -based metamaterial electric circuits (*10 pages*) 134105
Salvatore Savo, You Zhou, Giuseppe Castaldi, Massimo Moccia, Vincenzo Galdi, Shriram Ramanathan, and Yuki Sato
- Origin of the crossover between a freezing and a structural transition at low concentration in the relaxor ferroelectric $\text{K}_{1-x}\text{Li}_x\text{TaO}_3$ (*8 pages*) 134106
Ling Cai, Jean Toulouse, Leland Harriger, R. Gregory Downing, and L. A. Boatner
- A-site-driven ferroelectricity in strained ferromagnetic $\text{La}_2\text{NiMnO}_6$ thin films (*9 pages*) 134107
R. Takahashi, I. Ohkubo, K. Yamauchi, M. Kitamura, Y. Sakurai, M. Oshima, T. Oguchi, Y. Cho, and M. Lippmaa
- High pressure-temperature phase diagram and equation of state of titanium (*10 pages*) 134108
Agnès Dewaele, Vincent Stutzmann, Johann Bouchet, François Bottin, Florent Occelli, and Mohamed Mezouar
- Ethane-xenon mixtures under shock conditions (*9 pages*) 134109
Rudolph J. Magyar, Seth Root, Kyle Cochrane, Thomas R. Mattsson, and Dawn G. Flicker
- Interstitial silicon ions in rutile TiO_2 crystals (*7 pages*) 134110
E. M. Golden, N. C. Giles, Shan Yang (杨山), and L. E. Halliburton



CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 91, NUMBER 13

APRIL 2015-1(I)

Structure and energy of point defects in TiC: An <i>ab initio</i> study (11 pages)	134111
Weiwei Sun, Hossein Ehteshami, and Pavel A. Korzhavyi	
Finite-temperature properties of antiferroelectric PbZrO ₃ from atomistic simulations (6 pages)	134112
B. K. Mani, S. Lisenkov, and I. Ponomareva	
Domain pinning near a single-grain boundary in tetragonal and rhombohedral lead zirconate titanate films (12 pages)	134113
D. M. Marincel, H. R. Zhang, J. Britson, A. Belianinov, S. Jesse, S. V. Kalinin, L. Q. Chen, W. M. Rainforth, I. M. Reaney, C. A. Randall, and S. Trolier-McKinstry	
Wavelength dependence of nanosecond infrared laser-induced breakdown in water: Evidence for multiphoton initiation via an intermediate state (10 pages)	134114
Norbert Linz, Sebastian Freidank, Xiao-Xuan Liang, Hannes Vogelmann, Thomas Trickl, and Alfred Vogel	
Hysteretic phase transition sequence in 0.67Pb(Mg _{1/3} Nb _{2/3})O ₃ –0.33PbTiO ₃ single crystal driven by electric field and temperature (11 pages)	134115
Limei Zheng, Xiaoyan Lu, Hengshan Shang, Zengzhe Xi, Ruixue Wang, Junjun Wang, Peng Zheng, and Wenwu Cao	
General method to predict voltage-dependent ionic conduction in a solid electrolyte coating on electrodes (9 pages)	134116
Jie Pan, Yang-Tse Cheng, and Yue Qi	
Inhomogeneous, disordered, and partially ordered systems	
First-principles study of a sodium borosilicate glass-former. I. The liquid state (14 pages)	134201
Laurent Pedesseau, Simona Ispas, and Walter Kob	
First-principles study of a sodium borosilicate glass-former. II. The glass state (18 pages)	134202
Laurent Pedesseau, Simona Ispas, and Walter Kob	
Inherent structures in <i>m</i> -component spin glasses (10 pages)	134203
M. Baity-Jesi and G. Parisi	
Atomic-scale dynamics of a model glass-forming metallic liquid: Dynamical crossover, dynamical decoupling, and dynamical clustering (14 pages)	134204
Abhishek Jaiswal, Takeshi Egami, and Yang Zhang	
Dynamics, dynamical systems, lattice effects:	
 Heat-flux control and solid-state cooling by regulating chemical potential of photons in near-field electromagnetic heat transfer (8 pages)	134301
Kaifeng Chen, Parthiban Santhanam, Sunil Sandhu, Linxiao Zhu, and Shanhui Fan	
Theory of anharmonic phonons in two-dimensional crystals (20 pages)	134302
K. H. Michel, S. Costamagna, and F. M. Peeters	
Adiabatic many-body state preparation and information transfer in quantum dot arrays (7 pages)	134303
Umer Farooq, Abolfazl Bayat, Stefano Mancini, and Sougato Bose	
Dynamics of heat and mass transport in a quantum insulator (15 pages)	134304
Mateusz Łacki, Dominique Delande, and Jakub Zakrzewski	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 91, NUMBER 13

APRIL 2015-1(I)

Voltage noise, multiple phase-slips, and switching rates in moderately damped Josephson junctions (12 pages) . . .	134305
Martin Žonda, Wolfgang Belzig, and Tomáš Novotný	
Boundary scattering of phonons: Specularity of a randomly rough surface in the small-perturbation limit (9 pages)	134306
A. A. Maznev	
Magnetism	
Transport theory of metallic $B20$ helimagnets (9 pages)	134401
Jian Kang and Jiadong Zang	
Intraband and interband spin-orbit torques in noncentrosymmetric ferromagnets (9 pages)	134402
Hang Li, H. Gao, Liviu P. Zârbo, K. Výborný, Xuhui Wang, Ion Garate, Fatih Doğan, A. Čejchan, Jairo Sinova, T. Jungwirth, and Aurélien Manchon	
Magnetic single-domain state of the monochiral helimagnet MnSi in the zero-field limit: Magnetic properties study (6 pages)	134403
V. N. Narozhnyi and V. N. Krasnorussky	
 Classification and description of bosonic symmetry protected topological phases with semiclassical nonlinear sigma models (14 pages)	134404
Zhen Bi, Alex Rasmussen, Kevin Slagle, and Cenke Xu	
Strain dependence of antiferromagnetic interface coupling in $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrRuO}_3$ superlattices (7 pages) . . .	134405
Sujit Das, Andreas Herklotz, Eckhard Pippel, Er Jia Guo, Diana Rata, and Kathrin Dörr	
Magnetocaloric effects, quantum critical points, and the Berezinsky-Kosterlitz-Thouless transition in two-dimensional coupled spin-dimer systems (8 pages)	134406
Dominik Straßel, Peter Kopietz, and Sebastian Eggert	
Thickness and power dependence of the spin-pumping effect in $\text{Y}_3\text{Fe}_5\text{O}_{12}/\text{Pt}$ heterostructures measured by the inverse spin Hall effect (10 pages)	134407
M. B. Jungfleisch, A. V. Chumak, A. Kehlberger, V. Lauer, D. H. Kim, M. C. Onbasli, C. A. Ross, M. Kläui, and B. Hillebrands	
Temperature and field dependence of magnetic domains in $\text{La}_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$ (5 pages)	134408
Benjamin Bryant, Y. Moritomo, Y. Tokura, and G. Aeppli	
Anomalous Hall effect and current spin polarization in Co_2FeX Heusler compounds ($X = \text{Al, Ga, In, Si, Ge, and Sn}$): A systematic <i>ab initio</i> study (9 pages)	134409
Hung-Lung Huang, Jen-Chuan Tung, and Guang-Yu Guo	
Quantifying the deleterious role of strong correlations in $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ at the magnetocaloric transition (8 pages)	134410
J. A. Turcaud, A. M. Pereira, and L. F. Cohen	
Realization of the thermal equilibrium in inhomogeneous magnetic systems by the Landau-Lifshitz-Gilbert equation with stochastic noise, and its dynamical aspects (13 pages)	134411
Masamichi Nishino and Seiji Miyashita	
Effect of Bloch wave electron propagation and momentum-resolved signal detection on the quantitative and site-specific electron magnetic chiral dichroism of magnetic spinel oxide thin films (10 pages)	134412
B. Loukya, D. S. Negi, K. Dileep, N. Pachauri, A. Gupta, and R. Datta	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 91, NUMBER 13

APRIL 2015-1(I)

Effect of CoO/Ni orthogonal exchange coupling on perpendicular anisotropy of Ni films on Pd(001) (5 pages) . . .	134413
P. Kuświk, P. L. Gastelois, M. M. Soares, H. C. N. Tolentino, M. De Santis, A. Y. Ramos, A. D. Lamirand, M. Przybylski, and J. Kirschner	
Competing chiral orders in the topological Haldane-Hubbard model of spin- $\frac{1}{2}$ fermions and bosons (7 pages) . . .	134414
C. Hickey, P. Rath, and A. Paramakanti	
Local magnetism and structural properties of Heusler Ni ₂ MnGa alloys (10 pages)	134415
M. Belesi, L. Giebeler, C. G. F. Blum, U. K. Rößler, B. Büchner, and S. Wurmehl	
Inclined magnetic structure of iron borate Pr _x Y _{1-x} Fe ₃ (BO ₃) ₄ : A neutron diffraction study and crystal-field calculations (11 pages)	134416
C. Ritter, A. I. Pankrats, A. A. Demidov, D. A. Velikanov, V. L. Temerov, and I. A. Gudim	
Spectroscopic evidence of band Jahn-Teller distortion upon martensitic phase transition in Heusler-type Ni-Fe(Co)-Ga ferromagnetic shape-memory alloy films (6 pages)	134417
K. Sumida, K. Shirai, S. Zhu, M. Taniguchi, M. Ye, S. Ueda, Y. Takeda, Y. Saitoh, I. R. Aseguinolaza, J. M. Barandiarán, V. A. Chernenko, and A. Kimura	
Bridging the gap between discrete and continuous magnetic models in the scaling approach (7 pages)	134418
E. A. Velásquez, J. Mazo-Zuluaga, P. Vargas, and J. Mejía-López	
Phases and phase transitions of a perturbed Kekulé-Kitaev model (14 pages)	134419
Eoin Quinn, Subhro Bhattacharjee, and Roderich Moessner	
Thermal conductivity of IPA-CuCl ₃ : Evidence for ballistic magnon transport and the limited applicability of the Bose-Einstein condensation model (8 pages)	134420
Z. Y. Zhao, B. Tong, X. Zhao, L. M. Chen, J. Shi, F. B. Zhang, J. D. Song, S. J. Li, J. C. Wu, H. S. Xu, X. G. Liu, and X. F. Sun	
Universal distribution of magnetic anisotropy of impurities in ordered and disordered nanograins (10 pages)	134421
A. Szilva, P. Balla, O. Eriksson, G. Zaránd, and L. Szunyogh	
Two-stage Kondo effect in T-shaped double quantum dots with ferromagnetic leads (14 pages)	134422
Krzysztof P. Wójcik and Ireneusz Weymann	
Magnons and excitation continuum in XXZ triangular antiferromagnetic model: Application to Ba ₃ CoSb ₂ O ₉ (8 pages)	134423
E. A. Ghioldi, A. Mezio, L. O. Manuel, R. R. P. Singh, J. Oitmaa, and A. E. Trumper	
Ferromagnetic resonance in a topographically modulated permalloy film (6 pages)	134424
J. Sklenar, P. Tucciarone, R. J. Lee, D. Tice, R. P. H. Chang, S. J. Lee, I. P. Nevirkovets, O. Heinonen, and J. B. Ketterson	
Muon spin rotation and neutron scattering study of the noncentrosymmetric tetragonal compound CeAuAl ₃ (12 pages)	134425
D. T. Adroja, C. de la Fuente, A. Fraile, A. D. Hillier, A. Daoud-Aladine, W. Kockelmann, J. W. Taylor, M. M. Koza, E. Burzurí, F. Luis, J. I. Arnaud, and A. del Moral	
Close correlation between magnetic properties and the soft phonon mode of the structural transition in BaFe ₂ As ₂ and SrFe ₂ As ₂ (6 pages)	134426
D. Parshall, L. Pintschovius, J. L. Niedziela, J.-P. Castellan, D. Lamago, R. Mittal, Th. Wolf, and D. Reznik	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 91, NUMBER 13

APRIL 2015-1(I)

Separation of magnetic and superconducting behavior in $\text{YBa}_2\text{Cu}_3\text{O}_{6.33}$ ($T_c = 8.4$ K) (19 pages)	134427
Zahra Yamani, W. J. L. Buyers, F. Wang, Y.-J. Kim, J.-H. Chung, S. Chang, P. M. Gehring, G. Gasparovic, C. Stock, C. L. Broholm, J. C. Baglo, Ruixing Liang, D. A. Bonn, and W. N. Hardy	
Activation of antiferromagnetic domain switching in exchange-coupled Fe/CoO/MgO(001) systems (5 pages) . . .	134428
Q. Li, G. Chen, T. P. Ma, J. Zhu, A. T. N'Diaye, L. Sun, T. Gu, Y. Huo, J. H. Liang, R. W. Li, C. Won, H. F. Ding, Z. Q. Qiu, and Y. Z. Wu	
Superfluidity and superconductivity	
Tunneling spectroscopy and Majorana modes emergent from topological gapless phases in high- T_c cuprate superconductors (14 pages)	134501
Jun-Ting Kao, Shin-Ming Huang, Chung-Yu Mou, and C. C. Tsuei	
Reversed anisotropy of the in-plane resistivity in the antiferromagnetic phase of iron tellurides (7 pages)	134502
L. Liu, T. Mikami, M. Takahashi, S. Ishida, T. Kakeshita, K. Okazaki, A. Fujimori, and S. Uchida	
Continuous and discontinuous dark solitons in polariton condensates (5 pages)	134503
Stavros Komineas, Stephen P. Shipman, and Stephanos Venakides	
Modeling and simulations of quantum phase slips in ultrathin superconducting wires (12 pages)	134504
Andreas Andersson and Jack Lidmar	
Locally gauge-invariant spin response of $^3\text{He-B}$ films with Majorana surface states (7 pages)	134505
Edward Taylor, A. John Berlinsky, and Catherine Kallin	
Partially ordered vortex lattices in the high-field low-temperature mixed state of quasi-two-dimensional organic superconductors (5 pages)	134506
A. Maniv, V. Zhuravlev, T. Maniv, O. Ofer, R. Rommel, J. Müller, and J. E. Sonier	
Scattering length of Andreev reflection from quantized vortices in $^3\text{He-B}$ (7 pages)	134507
Y. A. Sergeev, C. F. Barenghi, S. N. Fisher, V. Tsepelin, and N. Suramlishvili	
Evidence of double-gap superconductivity in noncentrosymmetric $\text{Nb}_{0.18}\text{Re}_{0.82}$ single crystals (7 pages)	134508
C. Cirillo, R. Fittipaldi, M. Smidman, G. Carapella, C. Attanasio, A. Vecchione, R. P. Singh, M. R. Lees, G. Balakrishnan, and M. Cuoco	
Emergence of superconductivity in a doped single-valley quadratic band crossing system of spin- $\frac{1}{2}$ fermions (9 pages)	134509
Kelly Ann Pawlak, James M. Murray, and Oskar Vafek	
Quasiparticle interference patterns in a topological superconductor (11 pages)	134510
Aaron Farrell, Maxime Beaudry, M. Franz, and T. Pereg-Barnea	
Theoretical study of correlation between spin fluctuations and T_c in isovalent-doped 1111 iron-based superconductors (7 pages)	134511
Hayato Arai, Hidetomo Usui, Katsuhiko Suzuki, Yuki Fuseya, and Kazuhiko Kuroki	
Large Chern-number topological superfluids in a coupled-layer system (6 pages)	134512
Beibing Huang, Chun Fai Chan, and Ming Gong	
Effects of lasing in a one-dimensional quantum metamaterial (7 pages)	134513
Hidehiro Asai, Sergey Savel'ev, Shiro Kawabata, and Alexandre M. Zagoskin	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 91, NUMBER 13

APRIL 2015-1(I)

Time-reversal-invariant topological superconductivity in n -doped BiH (<i>11 pages</i>)	134514
Fan Yang, Cheng-Cheng Liu, Yu-Zhong Zhang, Yugui Yao, and Dung-Hai Lee	

ERRATA

Erratum: Electron energy loss and inelastic x-ray scattering cross sections from time-dependent density-functional perturbation theory [Phys. Rev. B 88 , 064301 (2013)] (<i>1 page</i>)	139901(E)
Iurii Timrov, Nathalie Vast, Ralph Gebauer, and Stefano Baroni	
Publisher's Note: Quantifying the deleterious role of strong correlations in $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ at the magnetocaloric transition [Phys. Rev. B 91 , 134410 (2015)] (<i>1 page</i>)	139902(E)
J. A. Turcaud, A. M. Pereira, and L. F. Cohen	
Erratum: Dynamics of entanglement entropy and entanglement spectrum crossing a quantum phase transition [Phys. Rev. B 89 , 104303 (2014)] (<i>1 page</i>)	139903(E)
Elena Canovi, Elisa Ercolessi, Piero Naldesi, Luca Taddia, and Davide Vodola	