

PHYSICAL REVIEW B

For editorial and subscription correspondence,
please see inside front cover
(ISSN: 1098-0121)

PERIODICALS
Postmaster send address changes to:
American Institute of Physics
Suite 1NO1
2 Huntington Quadrangle
Melville, NY 11747-4502

THIRD SERIES, VOLUME 71, NUMBER 5

CONTENTS

FEBRUARY 2005-1(I)

BRIEF REPORTS

Structure, structural phase transitions, mechanical properties, defects

- Capillary sublimation of Ar in mesoporous glass (2 pages) 052101
Dirk Wallacher, Viktor P. Soprunyuk, Andriy V. Kityk, Patrick Huber, and Klaus Knorr
- Two-length-scale behavior near the ferroelectric phase transition of $\text{Sn}_2\text{P}_2\text{S}_6$ (4 pages) 052102
J. Hlinka, R. Currat, M. de Boissieu, F. Livet, and Yu. M. Vysochanskii
- Origin of hardness in nitride spinel materials (4 pages) 052103
Faming Gao, Rui Xu, and Kuan Liu
- Alternating covalent-ionic and metallic bonding in perovskite borides studied using *ab initio* methods (3 pages) 052104
Denis Music, Zhimei Sun, and Jochen M. Schneider

Inhomogeneous, disordered, and partially ordered systems

- Microscopic structure of tunneling systems in glasses (4 pages) 052201
P. Nalbach

Magnetism

- Structure and magnetic properties of the $\text{Fe}_3\text{O}_4(001)$ surface: *Ab initio* studies (4 pages) 052401
C. Cheng
- Impurity and boundary effects in one- and two-dimensional inhomogeneous Heisenberg antiferromagnets (4 pages) 052402
P. E. G. Assis, Valter L. Líbero, and K. Capelle
- Transition from the macrospin to chaotic behavior by a spin-torque driven magnetization precession of a square nanoelement (4 pages) 052403
D. Berkov and N. Gorn
- Magnetic response of the *CE* structure in the doping-free system $\text{NaMn}_7\text{O}_{12}$ (4 pages) 052404
F. Bolzoni, A. Prodi, A. Gauzzi, E. Gilioli, F. Licci, and M. Marezio
- Electronic structures and magnetic properties of LaAVMoO_6 ($A=\text{Ca}, \text{Sr}, \text{Ba}$): Investigation of possible half-metallic antiferromagnets (4 pages) 052405
Min Sik Park and B. I. Min
- Spontaneous-symmetry-breaking mechanism of adiabatic pumping (4 pages) 052406
Yaroslav Tserkovnyak and Arne Brataas



Copyright 2005 by The American Physical Society

(Continued)



1098-0121(20050201)71:5;1-T

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 71, NUMBER 5

FEBRUARY 2005-1(I)

Electronic structure of CrO_2 studied by magnetic circular dichroism in resonant photoemission (4 pages)	052407
C. F. Chang, D. J. Huang, A. Tanaka, G. Y. Guo, S. C. Chung, S.-T. Kao, S. G. Shyu, and C. T. Chen	
Exact results for Ising models on the triangular Kagomé lattice (3 pages)	052408
Junjuan Zheng and Gang Sun	
Unconventional magnetic transitions in the mineral clinoatacamite $\text{Cu}_2\text{Cl}(\text{OH})_3$ (4 pages)	052409
X. G. Zheng, T. Kawae, Y. Kashitani, C. S. Li, N. Tateiwa, K. Takeda, H. Yamada, C. N. Xu, and Y. Ren	
<i>Ab initio</i> investigation of magnetism in two-dimensional uranium systems (4 pages)	052410
Matej Komelj and Nataša Stojić	
Doping effect on the charge ordering in AlV_2O_4 (4 pages)	052411
Y. Horibe, K. Kurushima, S. Mori, T. Asada, Y. Koyama, M. Shingu, and T. Katsufuji	
Superfluidity and superconductivity	
Superconductivity competing with the incommensurate antiferromagnetic insulating state in the organic conductor $(\text{MDT-TS})(\text{AuI}_2)_{0.441}$ (4 pages)	052501
Tadashi Kawamoto, Yoshimasa Bando, Takehiko Mori, Kazuo Takimiya, and Tetsuo Otsubo	
Deviations from plastic barriers in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ thin films (4 pages)	052502
Y. Z. Zhang, Z. Wang, X. F. Lu, H. H. Wen, J. F. de Marneffe, R. Deltour, A. G. M. Jansen, and P. Wyder	
Paraconductivity of a mesoscopic superconducting tube in the nonohmic regime (4 pages)	052503
Carlos Carballeira and Victor V. Moshchalkov	
T linearity of in-plane resistivity in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ thin films (3 pages)	052504
Seongshik Oh, Tiziana Di Luccio, and J. N. Eckstein	
Loss of Andreev backscattering in superconducting quantum point contacts (4 pages)	052505
N. B. Kopnin, A. S. Mel'nikov, and V. M. Vinokur	
Supercurrent-phase relationship of a $\text{Nb}/\text{InAs}(2\text{DES})/\text{Nb}$ Josephson junction in overlapping geometry (4 pages)	052506
Mark Ebel, Christian Busch, Ulrich Merkt, Miroslav Grajcar, Tomáš Plecenik, and Evgeni Il'ichev	
Anomaly in $\text{YBa}_2\text{Cu}_4\text{O}_8$ charge distribution below T_c : A zero-field muon spin relaxation study (4 pages)	052507
P. Carretta, A. Keren, J. S. Lord, I. Zucca, S. M. Kazakov, and J. Karpinski	
Directing transport by polarized radiation in the presence of chaos and dissipation (4 pages)	052508
A. D. Chepelianskii and D. L. Shepelyansky	

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

First-principles determination of the dynamical properties of $\text{Pb}_2\text{MgTeO}_6$ (9 pages)	054101
Razvan Caracas and Xavier Gonze	
Vacancies in ordered and disordered binary alloys treated with the cluster expansion (7 pages)	054102
A. Van der Ven and G. Ceder	
Density functional calculations of Ti-enhanced NaAlH_4 (10 pages)	054103
O. M. Løvvik and S. M. Opalka	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 71, NUMBER 5

FEBRUARY 2005-1(I)

Development of a bond-valence molecular-dynamics model for complex oxides (4 pages)	054104
Young-Han Shin, Valentino R. Cooper, Ilya Grinberg, and Andrew M. Rappe	
Formalism for obtaining nuclear momentum distributions by the deep inelastic neutron scattering technique (12 pages)	054105
J. J. Blostein, J. Dawidowski, and J. R. Granada	
Breakdown of the Born-Oppenheimer description explains neutron Compton-scattering anomaly (5 pages) . . .	054106
Nikitas I. Gidopoulos	
Origin of the intensity deficit in neutron Compton scattering (6 pages)	054107
G. F. Reiter and P. M. Platzman	
Structural phase transition of Fe grown on Au(111) (7 pages)	054108
D. T. Dekadjevi, B. J. Hickey, S. Brown, T. P. A. Hase, B. D. Fulthorpe, and B. K. Tanner	
Spatial ordering of primary defects at elevated temperatures (14 pages)	054109
A. A. Semenov and C. H. Woo	
Mean-field potential calculations of shock-compressed porous carbon (6 pages)	054110
Y. Wang, Z.-K. Liu, L.-Q. Chen, L. Burakovsky, D. L. Preston, W. Luo, B. Johansson, and R. Ahuja	
Molecular dynamics study of dislocation nucleation from a crack tip (10 pages)	054111
Berk Hess, Barend J. Thijsse, and Erik Van der Giessen	
Structural phase transition of germanium under uniaxial stress: An <i>ab initio</i> study (5 pages)	054112
Murat Durandurdu	

Inhomogeneous, disordered, and partially ordered systems

Intensity distribution of scalar waves propagating in random media (7 pages)	054201
P. Markoš and C. M. Soukoulis	
Structure, stability, and electronic properties of the <i>i</i> -AlPdMn quasicrystalline surface (14 pages)	054202
M. Krajčí and J. Hafner	
Universal fluctuations of the random lasing threshold in a sample of a finite area (8 pages)	054203
V. M. Apalkov and M. E. Raikh	
Experimentally constrained molecular relaxation: The case of glassy GeSe ₂ (5 pages)	054204
Parthapratim Biswas, De Nyago Tafen, and D. A. Drabold	
Dynamics of the quasiordered structure in the regioregulated π -conjugated polymer poly(4-methylthiazole-2,5-diyl) (11 pages)	054205
Seiichiro Mori, Yoshio Inoue, Takakazu Yamamoto, and Naoki Asakawa	
Models and modeling schemes for binary IV-VI glasses (15 pages)	054206
De Nyago Tafen and D. A. Drabold	

Dynamics, dynamical systems, lattice effects, quantum solids

Effects of electron-phonon coupling range on the polaron formation (6 pages)	054301
C. A. Perroni, V. Cataudella, G. De Filippis, and V. Marigliano Ramaglia	
Far-field imaging of acoustic waves by a two-dimensional sonic crystal (6 pages)	054302
Chunying Qiu, Xiangdong Zhang, and Zhengyou Liu	

(Continued)

Vibrational and crystalline properties of polymorphic CuInC_2 ($C=\text{Se}, \text{S}$) chalcogenides (9 pages)	054303
J. Álvarez-García, B. Barcones, A. Pérez-Rodríguez, A. Romano-Rodríguez, J. R. Morante, A. Janotti, Su-Huai Wei, and R. Scheer	
Magnetism	
Memory in a magnetic nanoparticle system: Polydispersity and interaction effects (8 pages)	054401
S. Chakraverty, M. Bandyopadhyay, S. Chatterjee, S. Dattagupta, A. Frydman, S. Sengupta, and P. A. Sreeram	
Origin of magnetic frustrations in Fe-Ni Invar alloys (4 pages)	054402
A. V. Ruban, M. I. Katsnelson, W. Olovsson, S. I. Simak, and I. A. Abrikosov	
Hydrodynamic approach to coherent nuclear-spin transport (7 pages)	054403
D. Greenbaum, M. Kindermann, C. Ramanathan, and D. G. Cory	
Magnetoresistivity in the clustered state of $\text{La}_{0.7-x}\text{Y}_x\text{Ca}_{0.3}\text{MnO}_3$ manganites (7 pages)	054404
J. A. Souza and R. F. Jardim	
Perturbative approach to J mixing in f -electron systems: Application to actinide dioxides (7 pages)	054405
N. Magnani, P. Santini, G. Amoretti, and R. Caciuffo	
Quantum dynamics in single-spin measurement (6 pages)	054406
Stefano Mancini, David Vitali, and Héctor Moya-Cessa	
Self-consistent theory of current-induced switching of magnetization (16 pages)	054407
D. M. Edwards, F. Federici, J. Mathon, and A. Umerski	
Anisotropic Hall effect in single-crystal heavy-fermion YbAgGe (8 pages)	054408
Sergey L. Bud'ko, Emilia Morosan, and Paul C. Canfield	
Mössbauer characterization of ^{57}Fe dopant ions across the insulator-metal transition in $\text{ANi}_{0.98}\text{Fe}_{0.02}\text{O}_3$ ($A=\text{Nd}, \text{Lu}$) perovskites (7 pages)	054409
Igor Presniakov, Gérard Demazeau, Alexey Baranov, Alexey Sobolev, and Konstantin Pokholok	
Analytical model to understand the colossal magnetocaloric effect (6 pages)	054410
P. J. von Ranke, N. A. de Oliveira, C. Mello, A. Magnus G. Carvalho, and S. Gama	
Tailoring perpendicular exchange bias in $[\text{Pt}/\text{Co}]\text{-IrMn}$ multilayers (7 pages)	054411
J. Sort, V. Baltz, F. Garcia, B. Rodmacq, and B. Dieny	
Effect of spin fluctuations on thermal expansion characteristics in paramagnetic Laves-phase $\text{Lu}(\text{Co}_{1-x}\text{Ga}_x)_2$ compounds (6 pages)	054412
M. Ohta, A. Fujita, K. Fukamichi, H. Saito, E. Matsubara, and H. Takahashi	
Numerical evidence of a spin-1/2 chain approaching a spin-1 chain (5 pages)	054413
Hsiang-Hsuan Hung and Chang-De Gong	
Structural and magnetic properties of $\text{Fe}[\text{Fe}(\text{CN})_6]\cdot 4\text{H}_2\text{O}$ (7 pages)	054414
Amit Kumar, S. M. Yusuf, and L. Keller	
Group theory and octupolar order in URu_2Si_2 (10 pages)	054415
Annamária Kiss and Patrik Fazekas	
Correlation between tunneling magnetoresistance and magnetization in dipolar-coupled nanoparticle arrays (8 pages)	054416
D. Kechrakos and K. N. Trohidou	

X-ray absorption studies of the local structure and f -level occupancy in $\text{CeIr}_{1-x}\text{Rh}_x\text{In}_5$ (8 pages)	054417
M. Daniel, S.-W. Han, C. H. Booth, A. L. Cornelius, P. G. Pagliuso, J. L. Sarrao, and J. D. Thompson	
Atomistic simulation of AlO_x magnetic tunnel junction growth (8 pages)	054418
Xiao Wang Zhou and Haydn N. G. Wadley	
Magnetic structure of $\beta\text{-ErD}_2$: Long-range and short-range order from powder neutron diffraction (6 pages) . .	054419
P. Vajda, G. André, T. J. Udovic, R. W. Erwin, and Q. Huang	
Spin state of LaCoO_3 : Dependence on CoO_6 octahedra geometry (6 pages)	054420
K. Knížek, P. Novák, and Z. Jirák	
Superfluidity and superconductivity	
Properties of the superconducting state in a two-band model (18 pages)	054501
E. J. Nicol and J. P. Carbotte	
Doping phase diagram of $\text{Y}_{1-x}\text{Ca}_x\text{Ba}_2(\text{Cu}_{1-y}\text{Zn}_y)_3\text{O}_{7-\delta}$ from transport measurements: Tracking the pseudogap below T_c (8 pages)	054502
S. H. Naqib, J. R. Cooper, J. L. Tallon, R. S. Islam, and R. A. Chakalov	
Josephson vortex state across the phase diagram of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$: A magneto-optics study (9 pages)	054503
S. V. Dordevic, Seiki Komiya, Yoichi Ando, Y. J. Wang, and D. N. Basov	
Magnetic interactions in a single-band model for the cuprates and ruthenates (19 pages)	054504
P. Monthoux and G. G. Lonzarich	
Spin-charge coupling in lightly doped $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (10 pages)	054505
Shiliang Li, Stephen D. Wilson, David Mandrus, Bairu Zhao, Y. Onose, Y. Tokura, and Pengcheng Dai	
Boson structures in the relation between optical conductivity and quasiparticle dynamics (10 pages)	054506
J. P. Carbotte, E. Schachinger, and J. Hwang	
Static charge-imbalance effects in intrinsic Josephson systems (14 pages)	054507
J. Keller and D. A. Ryndyk	
t - J model for a bilayer: Coexisting superconductivity and planar-flux phases (5 pages)	054508
Hongbo Zhao and Jan R. Engelbrecht	
Anisotropic nonmonotonic behavior of the superconducting critical current in thin $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ films on vicinal SrTiO_3 surfaces (9 pages)	054509
C. Cantoni, D. T. Verebelyi, E. D. Specht, J. Budai, and D. K. Christen	
Phase diffusion and fractional Shapiro steps in superconducting quantum point contacts (10 pages)	054510
Raphaël Duprat and Alfredo Levy Yeyati	
Anomalous paramagnetic effects in the mixed state of $\text{LuNi}_2\text{B}_2\text{C}$ (5 pages)	054511
Tuson Park, A. Malinowski, M. F. Hundley, J. D. Thompson, Y. Sun, M. B. Salamon, Eun Mi Choi, Heon Jung Kim, Sung-Ik Lee, P. C. Canfield, and V. G. Kogan	
Underbarrier nucleation kinetics in a metastable quantum liquid near the liquid-gas spinodal line (9 pages) . .	054512
S. N. Burmistrov, L. B. Dubovskii, and Y. Okuda	
Variational Monte Carlo study of local order in liquid and solid ^4He with shadow wave functions (7 pages) . .	054513
Li Hui and Francesco Pederiva	

Anomalous enhancement of electronic heat capacity in the organic conductors κ -(BEDT-TTF) ₄ Hg _{3-δ} X ₈ (X=Br,Cl) (4 pages)	054514
Akihito Naito, Yasuhiro Nakazawa, Kazuya Saito, Hiromi Taniguchi, Kazushi Kanoda, and Michio Sorai	
Binding of charge carriers in the extended t - J model (6 pages)	054515
J. M. Tipper, C. Genert, and K. J. E. Vos	
Fast partial decoherence of a superconducting flux qubit in a spin bath (7 pages)	054516
Jacek Dziarmaga	

ERRATA

Erratum: Evidence of two different Mn states in CaCu ₃ Mn ₄ O ₁₂ derivatives with colossal magnetoresistance [Phys. Rev. B 70 , 024419 (2004)] (1 page)	059901(E)
J. Sánchez-Benítez, C. Prieto, A. de Andrés, J. A. Alonso, M. J. Martínez-Lope, and M. T. Casais	
Erratum: Crystal structure and thermodynamic stability of the lithium alanates LiAlH ₄ and Li ₃ AlH ₆ [Phys. Rev. B 69 , 134117 (2004)] (1 page)	059902(E)
O. M. Løvvik, Susanne M. Opalka, Hendrik W. Brinks, and Bjørn C. Hauback	
Erratum: Bonding and classification of nanolayered ternary carbides [Phys. Rev. B 70 , 092102 (2004)] (1 page)	059903(E)
Zhimei Sun, Denis Music, Rajeev Ahuja, Sa Li, and Jochen M. Schneider	
Publisher's Note: Doping phase diagram of Y _{1-x} Ca _{x} Ba ₂ (Cu _{1-y} Zn _{y}) ₃ O _{7-δ} from transport measurements: Tracking the pseudogap below T_c [Phys. Rev. B 71 , 054502 (2005)] (1 page)	059904(E)
S. H. Naqib, J. R. Cooper, J. L. Tallon, R. S. Islam, and R. A. Chakalov	
Erratum: Synchrotron x-ray powder diffraction study of the structural phase transition in CaBr ₂ [Phys. Rev. B 70 , 144102 (2004)] (1 page)	059905(E)
Brendan J. Kennedy and Christopher J. Howard	