

Publications
Ingrid Mertig
October 2020

2020

302. B. Göbel, I. Mertig, and O. A. Tretiakov
Beyond skyrmions: Review and perspectives of alternative magnetic quasiparticles
[Phys. Rep., in press \(2020\)](#)
301. P. K. Sivakumar, B. Göbel, E. Lesne, A. Markou, J. Gidugu, J. M. Taylor, H. Deniz, J. Jena, C. Felser, I. Mertig, and S. S. P. Parkin
Topological Hall Signatures of Two Chiral Spin Textures Hosted in a Single Tetragonal Inverse Heusler Thin Film
[ACS Nano, in press \(2020\)](#)
300. R. R. Neumann, A. Mook, J. Henk, and I. Mertig
Orbital Magnetic Moment of Magnons
[Phys. Rev. Lett. **125**, 117209 \(2020\)](#)
299. B. Zhao, B. Karpiak, D. Khokhriakov, A. Johansson, A. M. Hoque, X. Xu, Y. Jiang, I. Mertig, and S. P. Dash
Unconventional Charge-Spin Conversion in Weyl-Semimetal WTe_2
[Adv. Mater. **32**, 2000818 \(2020\)](#)
298. X.-G. Wang, L. Chotorlishvili, V. K. Dugaev, A. Ernst, I. V. Maznichenko, N. Arnold, C. Jia, J. Berakdar, I. Mertig, and J. Barnaś
The optical tweezer of skyrmions
[npj Comput. Mater. **6**, 140 \(2020\)](#)
297. C. Herschbach, D. V. Fedorov, M. Gradhand, and I. Mertig
Impact of crystalline anisotropy on the extrinsic spin Hall effect in ultrathin films
[Phys. Rev. B **102**, 104421 \(2020\)](#)
296. E. Şaşıoğlu, T. Aull, D. Kutschabsky, S. Blügel, and I. Mertig
Half-Metal–Spin-Gapless-Semiconductor Junctions as a Route to the Ideal Diode
[Phys. Rev. Appl. **14**, 014082 \(2020\)](#)
295. O. Busch, B. Göbel, and I. Mertig
Microscopic origin of the anomalous Hall effect in noncollinear kagome magnets
[Phys. Rev. Research **2**, 033112 \(2020\)](#)
294. D. C. Vaz, F. Trier, A. Dyrdał, A. Johansson, K. Garcia, A. Barthélémy, I. Mertig, J. Barnaś, A. Fert, and M. Bibes
Determining the Rashba parameter from the bilinear magnetoresistance response in a two-dimensional electron gas
[Phys. Rev. Mater. **4**, 071001\(R\) \(2020\)](#)
293. A. Mook, R. R. Neumann, A. Johansson, J. Henk, and I. Mertig
Origin of the magnetic spin Hall effect: Spin current vorticity in the Fermi sea
[Phys. Rev. Research **2**, 023065 \(2020\)](#)
292. D.-S. Park, A. D. Rata, I. V. Maznichenko, S. Ostanin, Y. L. Gan, S. Agrestini, G. J. Rees, M. Walker, J. Li, J. Herrero-Martin, G. Singh, Z. Luo, A. Bhatnagar, Y. Z. Chen, V. Tileli, P. Muralt, A. Kalaboukhov, I. Mertig, K. Dörr, A. Ernst, and N. Pryds
The emergence of magnetic ordering at complex oxide interfaces tuned by defects
[Nat. Commun. **11**, 3650 \(2020\)](#)

291. B. Göbel, A. Mook, J. Henk, and I. Mertig
Compensated Quantum and Topological Hall Effects of Electrons in Polyatomic Stripe Lattices
[phys. stat. sol. \(b\) 257, 1900518 \(2020\)](#)
290. M. M. Koch, L. Bergmann, S. Agrestini, I. Maznichenko, I. Mertig, A. Herklotz, S. Das, D. A. Rata, and K. Dörr
Thickness-Dependent Ru Exchange Spring at $La_{0.7}Sr_{0.3}MnO_3$ - $SrRuO_3$ Interface
[phys. stat. sol. \(b\) 257, 1900616 \(2020\)](#)
289. W. A. Adeagbo, I. V. Maznichenko, H. Ben Hamed, I. Mertig, A. Ernst, and W. Hergert
Electronic and Magnetic Properties of $BaFeO_3$ on the Pt(111) Surface in a Quasicrystalline Approximant Structure
[phys. stat. sol. \(b\) 257, 1900649 \(2020\)](#)
288. I. V. Maznichenko, S. Ostanin, A. Ernst, J. Henk, and I. Mertig
Formation and Tuning of 2D Electron Gas in Perovskite Heterostructures
[phys. stat. sol. \(b\) 257, 1900540 \(2020\)](#)
287. B. Göbel, C. A. Akosa, G. Tatara, and I. Mertig
Topological Hall signatures of magnetic hopfions
[Phys. Rev. Research 2, 013315 \(2020\)](#)
286. J. Jena, B. Göbel, T. Ma, V. Kumar, R. Saha, I. Mertig, C. Felser, and S. S. P. Parkin
Elliptical Bloch skyrmion chiral twins in an antiskyrmion system
[Nat. Commun. 11, 1115 \(2020\)](#)
285. T. Rauch, F. Töpler, and I. Mertig
Local spin Hall conductivity
[Phys. Rev. B 101, 064206 \(2020\)](#)

2019

284. T. Aull, E. Şaşıoğlu, I. V. Maznichenko, S. Ostanin, A. Ernst, I. Mertig, and I. Galanakis
Ab initio design of quaternary Heusler compounds for reconfigurable magnetic tunnel diodes and transistors
[Phys. Rev. Mater. 3, 124415 \(2019\)](#)
283. T. Rauch, V. A. Rogalev, M. Bauernfeind, J. Maklar, F. Reis, F. Adler, S. Moser, J. Weis, T.-L. Lee, P. K. Thakur, J. Schäfer, R. Claessen, J. Henk, and I. Mertig
Nontrivial topological valence bands of common diamond and zinc-blende semiconductors
[Phys. Rev. Mater. 3, 064203 \(2019\)](#)
282. A. Mook, R. R. Neumann, J. Henk, and I. Mertig
Spin Seebeck and spin Nernst effects of magnons in noncollinear antiferromagnetic insulators
[Phys. Rev. B 100, 100401\(R\) \(2019\)](#)
281. D. C. Vaz, P. Noël, A. Johansson, B. Göbel, F. Y. Bruno, G. Singh, S. McKeown-Walker, F. Trier, L. M. Vicente-Arche, A. Sander, S. Valencia, P. Bruneel, M. Vivek, M. Gabay, N. Bergeal, F. Baumberger, H. Okuno, A. Barthélémy, A. Fert, L. Vila, I. Mertig, J.-P. Attané, and M. Bibes
Mapping spin-charge conversion to the band structure in a topological oxide two-dimensional electron gas
[Nat. Mater. 18, 1187 \(2019\)](#)
280. A. Neroni, E. Şaşıoğlu, H. Hadipour, C. Friedrich, S. Blügel, I. Mertig, and M. Ležaić
First-principles calculation of the effective on-site Coulomb interaction parameters for Sr_2ABO_6 ($A = Cr, Mn, Fe, Co, Ni$, and $B = Mo, W$) double perovskites
[Phys. Rev. B 100, 115113 \(2019\)](#)

279. B. Göbel, A. F. Schäffer, J. Berakdar, I. Mertig, and S. S. P. Parkin
Electrical writing, deleting, reading, and moving of magnetic skyrmioniums in a racetrack device
[Sci. Rep. **9**, 12119 \(2019\)](#)
278. E. Şaşıoğlu, S. Blügel, and I. Mertig
Proposal for Reconfigurable Magnetic Tunnel Diode and Transistor
[ACS Appl. Electron. Mater. **1**, 1552 \(2019\)](#)
277. I. V. Maznichenko, S. Ostanin, A. Ernst, and I. Mertig
Tunable 2D electron gas at the LaAlO₃/SrTiO₃(001) interface
[Phys. Rev. Mater. **3**, 074006 \(2019\)](#)
276. B. Göbel, J. Henk, and I. Mertig
Forming individual magnetic biskyrmions by merging two skyrmions in a centrosymmetric nanodisk
[Sci. Rep. **9**, 9521 \(2019\)](#)
275. K. Özdoğan, I. V. Maznichenko, S. Ostanin, E. Şaşıoğlu, A. Ernst, I. Mertig, and I. Galanakis
High spin polarization in all-3d-metallic Heusler compounds: the case of Fe₂CrZ and Co₂CrZ (Z = Sc, Ti, V)
[J. Phys. D: Appl. Phys. **52**, 205003 \(2019\)](#)
274. S. K. Mahatha, A. S. Nagankeu, N. F. Hinsche, I. Mertig, K. Guilloy, P. L. Matzen, M. Bianchi, C. E. Sanders, J. A. Miwa, H. Bana, E. Travaglia, P. Lacovig, L. Bignardi, D. Lizzit, R. Larciprete, A. Baraldi, S. Lizzit, and P. Hofmann
Electron–phonon coupling in single-layer MoS₂
[Surf. Sci. **681**, 64 \(2019\)](#)
273. B. Göbel, A. Mook, J. Henk, I. Mertig, and O. A. Tretiakov
Magnetic bimerons as skyrmion analogues in in-plane magnets
[Phys. Rev. B **99**, 060407\(R\) \(2019\)](#)
272. A. Johansson, J. Henk, and I. Mertig
Chiral anomaly in type-I Weyl semimetals: Comprehensive analysis within a semiclassical Fermi surface harmonics approach
[Phys. Rev. B **99**, 075114 \(2019\)](#)
271. A. Hönemann, C. Herschbach, D. V. Fedorov, M. Gradhand, and I. Mertig
Spin and charge currents induced by the spin Hall and anomalous Hall effects upon crossing ferromagnetic/nonmagnetic interfaces
[Phys. Rev. B **99**, 024420 \(2019\)](#)
270. B. Göbel, A. Mook, J. Henk, and I. Mertig
Magnetoelectric effect and orbital magnetization in skyrmion crystals: Detection and characterization of skyrmions
[Phys. Rev. B **99**, 060406\(R\) \(2019\)](#)
269. B. Göbel, A. Mook, J. Henk, and I. Mertig
Overcoming the speed limit in skyrmion racetrack devices by suppressing the skyrmion Hall effect
[Phys. Rev. B **99**, 020405\(R\) \(2019\)](#)
268. V. Popescu, P. Kratzer, P. Entel, C. Heiliger, M. Czerner, K. Tauber, F. Töpler, C. Herschbach, D. V. Fedorov, M. Gradhand, I. Mertig, R. Kováčik, P. Mavropoulos, D. Wortmann, S. Blügel, F. Freimuth, Y. Mokrousov, S. Wimmer, D. Ködderitzsch, M. Seemann, K. Chadova, and H. Ebert
Spin caloric transport from density-functional theory
[J. Phys. D: Appl. Phys. **52**, 073001 \(2019\)](#)

267. A. Hönemann, C. Herschbach, D. V. Fedorov, M. Gradhand, and I. Mertig
Absence of strong skew scattering in crystals with multi-sheeted Fermi surfaces
[J. Phys.: Condens. Matter **31**, 085803 \(2019\)](#)
266. A. Mook, J. Henk, and I. Mertig
Thermal Hall effect in noncollinear coplanar insulating antiferromagnets
[Phys. Rev. B **99**, 014427 \(2019\)](#)
265. S. Das, A. D. Rata, I. V. Maznichenko, S. Agrestini, E. Pippel, N. Gauquelin, J. Verbeeck, K. Chen, S. M. Valvidares, H. Babu Vasili, J. Herrero-Martin, E. Pellegrin, K. Nenkov, A. Herklotz, A. Ernst, I. Mertig, Z. Hu, and K. Dörr
Low-field switching of noncollinear spin texture at $La_{0.7}Sr_{0.3}MnO_3$ - $SrRuO_3$ interfaces
[Phys. Rev. B **99**, 024416 \(2019\)](#)
264. S. Ostanin, V. Borisov, D. V. Fedorov, E. I. Salamatov, A. Ernst, and I. Mertig
Role of tetrahedrally coordinated dopants in palladium hydrides on their superconductivity and inverse isotope effect
[J. Phys.: Condens. Matter **31**, 075703 \(2019\)](#)

2018

263. H. Hadipour, E. Şaşıoğlu, F. Bagherpour, C. Friedrich, S. Blügel, and I. Mertig
Screening of long-range Coulomb interaction in graphene nanoribbons: Armchair versus zigzag edges
[Phys. Rev. B **98**, 205123 \(2018\)](#)
262. D.-S. Park, G. J. Rees, H. Wang, D. Rata, A. J. Morris, I. V. Maznichenko, S. Ostanin, A. Bhatnagar, C.-J. Choi, R. D. B. Jónsson, K. Kaufmann, R. Kashtiban, M. Walker, C.-T. Chiang, E. B. Thorsteinsson, Z. Luo, I.-S. Park, J. V. Hanna, I. Mertig, K. Dörr, H. P. Gíslason, and C. F. McConville
Electromagnetic Functionalization of Wide-Bandgap Dielectric Oxides by Boron Interstitial Doping
[Adv. Mater. **30**, 1802025 \(2018\)](#)
261. A. F. Schäffer, L. Chotorlishvili, I. V. Maznichenko, A. Ernst, K. Dörr, I. Mertig, and J. Berakdar
Element specific hysteresis of $La_{0.7}Sr_{0.3}MnO_3$ - $SrRuO_3$ (LSMO-SRO) heterostructures
[APL Mater. **6**, 076103 \(2018\)](#)
260. I. V. Maznichenko, S. Ostanin, V. K. Dugaev, I. Mertig, and A. Ernst
Impact of long-range disorder on the two-dimensional electron gas formation at a $LaAlO_3/SrTiO_3$ interface
[Phys. Rev. Mater. **2**, 074003 \(2018\)](#)
259. B. Göbel, A. Mook, J. Henk, and I. Mertig
The family of topological Hall effects for electrons in skyrmion crystals
[Eur. Phys. J. B **91**, 179 \(2018\)](#)
258. A. Mook, B. Göbel, J. Henk, and I. Mertig
Taking an electron-magnon duality shortcut from electron to magnon transport
[Phys. Rev. B **97**, 140401\(R\) \(2018\)](#)
257. A. Johansson, J. Henk, and I. Mertig
Edelstein effect in Weyl semimetals
[Phys. Rev. B **97**, 085417 \(2018\)](#)
256. L. Peters, E. Şaşıoğlu, I. Mertig, and M. I. Katsnelson
Ab initio study of the Coulomb interaction in Nb_xCo clusters: Strong on-site versus weak nonlocal screening
[Phys. Rev. B **97**, 045121 \(2018\)](#)

2017

255. T. Rauch, H. Nguyen Minh, J. Henk, and I. Mertig
Model for ferromagnetic Weyl and nodal line semimetals: Topological invariants, surface states, anomalous and spin Hall effect
[Phys. Rev. B **96**, 235103 \(2017\)](#)
254. E. Şaşıoğlu, H. Hadipour, C. Friedrich, S. Blügel, and I. Mertig
Strength of effective Coulomb interactions and origin of ferromagnetism in hydrogenated graphene
[Phys. Rev. B **95**, 060408\(R\) \(2017\)](#)
253. B. Göbel, A. Mook, J. Henk, and I. Mertig
Antiferromagnetic skyrmion crystals: Generation, topological Hall, and topological spin Hall effect
[Phys. Rev. B **96**, 060406\(R\) \(2017\)](#)
252. T. Rauch, S. Achilles, J. Henk, and I. Mertig
Multiple topological nontrivial phases in strained $Hg_xCd_{1-x}Te$
[Phys. Rev. B **96**, 035124 \(2017\)](#)
251. B. Göbel, A. Mook, J. Henk, and I. Mertig
Signatures of lattice geometry in quantum and topological Hall effect
[New J. Phys. **19**, 063042 \(2017\)](#)
250. F. Rittweger, N. F. Hinsche, and I. Mertig
Phonon limited electronic transport in Pb
[J. Phys.: Condens. Matter **29**, 355501 \(2017\)](#)
249. V. Borisov, S. Ostanin, and I. Mertig
Multiferroic properties of the $PbTiO_3/La_{2/3}Sr_{1/3}MnO_3$ interface studied from first principles
[J. Phys.: Condens. Matter **29**, 175801 \(2017\)](#)
248. V. A. Rogalev, T. Rauch, M. R. Scholz, F. Reis, L. Dudy, A. Fleszar, M.-A. Husanu, V. N. Strocov, J. Henk, I. Mertig, J. Schäfer, and R. Claessen
Double band inversion in α -Sn: Appearance of topological surface states and the role of orbital composition
[Phys. Rev. B **95**, 161117\(R\) \(2017\)](#)
247. B. Göbel, A. Mook, J. Henk, and I. Mertig
Unconventional topological Hall effect in skyrmion crystals caused by the topology of the lattice
[Phys. Rev. B **95**, 094413 \(2017\)](#)
246. P. Xu, W. Han, P. M. Rice, J. Jeong, M. G. Samant, K. Mohseni, H. L. Meyerheim, S. Ostanin, I. V. Maznichenko, I. Mertig, E. K. U. Gross, A. Ernst, and S. S. P. Parkin
Reversible Formation of 2D Electron Gas at the $LaFeO_3/SrTiO_3$ Interface via Control of Oxygen Vacancies
[Adv. Mater. **29**, 1604447 \(2017\)](#)
245. A. Mook, J. Henk, and I. Mertig
Magnon nodal-line semimetals and drumhead surface states in anisotropic pyrochlore ferromagnets
[Phys. Rev. B **95**, 014418 \(2017\)](#)
244. A. Mook, B. Göbel, J. Henk, and I. Mertig
Magnon transport in noncollinear spin textures: Anisotropies and topological magnon Hall effects
[Phys. Rev. B **95**, 020401\(R\) \(2017\)](#)

2016

243. A. Mook, J. Henk, and I. Mertig
Spin dynamics simulations of topological magnon insulators: From transverse current correlation functions to the family of magnon Hall effects
[Phys. Rev. B **94**, 174444 \(2016\)](#)
242. F. Töpler, A. Hönemann, K. Tauber, D. V. Fedorov, M. Gradhand, I. Mertig, and A. Fert
Nonlocal anomalous Hall effect in ternary alloys based on noble metals
[Phys. Rev. B **94**, 140413\(R\) \(2016\)](#)
241. D. Thonig, T. Rauch, H. Mirhosseini, J. Henk, I. Mertig, H. Wortelen, B. Engelkamp, A. B. Schmidt, and M. Donath
Existence of topological nontrivial surface states in strained transition metals: W, Ta, Mo, and Nb
[Phys. Rev. B **94**, 155132 \(2016\)](#)
240. A. Mook, J. Henk, and I. Mertig
Tunable Magnon Weyl Points in Ferromagnetic Pyrochlores
[Phys. Rev. Lett. **117**, 157204 \(2016\)](#)
239. M. Lorenz, M. S. Ramachandra Rao, T. Venkatesan, E. Fortunato, P. Barquinha, R. Branquinho, D. Salgueiro, R. Martins, E. Carlos, A. Liu, F. K. Shan, M. Grundmann, H. Boschker, J. Mukherjee, M. Priyadarshini, N. DasGupta, D. J. Rogers, F. H. Teherani, E. V. Sandana, P. Bove, K. Rietwyk, A. Zaban, A. Veziridis, A. Weidenkaff, M. Muralidhar, M. Murakami, S. Abel, J. Fompeyrine, J. Zuniga-Perez, R. Ramesh, N. A. Spaldin, S. Ostanin, V. Borisov, I. Mertig, V. Lazenka, G. Srinivasan, W. Prellier, M. Uchida, M. Kawasaki, R. Pentcheva, P. Gegenwart, F. Miletto Granozio, J. Fontcuberta, and N. Pryds
The 2016 oxide electronic materials and oxide interfaces roadmap
[J. Phys. D: Appl. Phys. **49**, 433001 \(2016\)](#)
238. A. Mook, J. Henk, and I. Mertig
Topological magnon insulators: Chern numbers and surface magnons
[Proc. SPIE **9931**, 993134 \(2016\)](#)
237. A. Johansson, J. Henk, and I. Mertig
Theoretical aspects of the Edelstein effect for anisotropic two-dimensional electron gas and topological insulators
[Phys. Rev. B **93**, 195440 \(2016\)](#)
236. T. Rauch, S. Achilles, J. Henk, and I. Mertig
*Erratum: Spin Chirality Tuning and Topological Semimetals in Strained $HgTe_xS_{1-x}$ [Phys. Rev. Lett. **114**, 236805 (2015)]*
[Phys. Rev. Lett. **116**, 199901 \(2016\)](#)
235. T. Dankwort, A.-L. Hansen, M. Winkler, U. Schürmann, J. D. Koenig, D. C. Johnson, N. F. Hinsche, P. Zahn, I. Mertig, W. Bensch, and L. Kienle
Nanostructure, thermoelectric properties, and transport theory of V_2VI_3 and $V_2VI_3/IV-VI$ based superlattices and nanomaterials
[phys. stat. sol. \(a\) **213**, 662 \(2016\)](#)
234. A. Sukhov, L. Chotorlishvili, A. Ernst, X. Zubizarreta, S. Ostanin, I. Mertig, E. K. U. Gross, and J. Berakdar
Swift thermal steering of domain walls in ferromagnetic MnBi stripes
[Sci. Rep. **6**, 24411 \(2016\)](#)
233. N. F. Hinsche, F. Rittweger, M. Hölzer, P. Zahn, A. Ernst, and I. Mertig
Ab initio description of the thermoelectric properties of heterostructures in the diffusive limit of transport
[phys. stat. sol. \(a\) **213**, 672 \(2016\)](#)

232. F. Munoz, M. G. Vergniory, T. Rauch, J. Henk, E. V. Chulkov, I. Mertig, S. Botti, M. A. L. Marques, and A. H. Romero
Topological Crystalline Insulator in a New Bi Semiconducting Phase
[Sci. Rep. **6**, 21790 \(2016\)](#)
231. I. V. Maznichenko, S. Ostanin, L. V. Bekenov, V. N. Antonov, I. Mertig, and A. Ernst
Impact of oxygen doping and oxidation state of iron on the electronic and magnetic properties of BaFeO_{3-δ}
[Phys. Rev. B **93**, 024411 \(2016\)](#)

2015

230. A. Johansson, C. Herschbach, D. V. Fedorov, J. Henk, and I. Mertig
Spin Hall effect in two-dimensional systems within the relativistic phase shift model
[Phys. Rev. B **92**, 184401 \(2015\)](#)
229. M. Geilhufe, S. Achilles, M. A. Köbis, M. Arnold, I. Mertig, W. Hergert, and A. Ernst
Numerical solution of the relativistic single-site scattering problem for the Coulomb and the Mathieu potential
[J. Phys.: Condens. Matter **27**, 435202 \(2015\)](#)
228. M. Hoffmann, V. S. Borisov, S. Ostanin, I. Mertig, W. Hergert, and A. Ernst
Magnetic properties of defect-free and oxygen-deficient cubic SrCoO_{3-δ}
[Phys. Rev. B **92**, 094427 \(2015\)](#)
227. M. Hoffmann, S. Borek, I. V. Maznichenko, S. Ostanin, G. Fischer, M. Geilhufe, W. Hergert, I. Mertig, A. Ernst, and A. Chassé
Study of electronic and magnetic properties and related x-ray absorption spectroscopy of ultrathin Co films on BaTiO₃
[J. Phys.: Condens. Matter **27**, 426003 \(2015\)](#)
226. V. S. Borisov, S. Ostanin, S. Achilles, J. Henk, and I. Mertig
Spin-dependent transport in a multiferroic tunnel junction: Theory for Co/PbTiO₃/Co
[Phys. Rev. B **92**, 075137 \(2015\)](#)
225. A. Quindeau, V. Borisov, I. Fina, S. Ostanin, E. Pippel, I. Mertig, D. Hesse, and M. Alexe
Origin of tunnel electroresistance effect in PbTiO₃-based multiferroic tunnel junctions
[Phys. Rev. B **92**, 035130 \(2015\)](#)
224. K. Chadova, D. V. Fedorov, C. Herschbach, M. Gradhand, I. Mertig, D. Ködderitzsch, and H. Ebert
Separation of the individual contributions to the spin Hall effect in dilute alloys within the first-principles Kubo-Středa approach
[Phys. Rev. B **92**, 045120 \(2015\)](#)
223. A. Mook, J. Henk, and I. Mertig
Topologically nontrivial magnons at an interface of two kagome ferromagnets
[Phys. Rev. B **91**, 224411 \(2015\)](#)
222. T. Rauch, S. Achilles, J. Henk, and I. Mertig
Spin Chirality Tuning and Topological Semimetals in Strained HgTe_xS_{1-x}
[Phys. Rev. Lett. **114**, 236805 \(2015\)](#)
221. K. Tauber, A. Hönemann, D. V. Fedorov, M. Gradhand, and I. Mertig
Enhancement of the anomalous Hall effect in ternary alloys
[Phys. Rev. B **91**, 220404\(R\) \(2015\)](#)
220. V. Borisov, S. Ostanin, and I. Mertig
Two-dimensional electron gas and its electric control at the interface between ferroelectric and antiferromagnetic insulator studied from first principles
[Phys. Chem. Chem. Phys. **17**, 12812 \(2015\)](#)

219. A. Mook, J. Henk, and I. Mertig
Magnon waveguide with nanoscale confinement constructed from topological magnon insulators
[Phys. Rev. B **91**, 174409 \(2015\)](#)
218. N. F. Hinsche, S. Zastrow, J. Gooth, L. Pudewill, R. Zierold, F. Rittweger, T. Rauch, J. Henk, K. Nielsch, and I. Mertig
Impact of the Topological Surface State on the Thermoelectric Transport in Sb₂Te₃ Thin Films
[ACS Nano **9**, 4406 \(2015\)](#)
217. N. F. Hinsche, M. Hölzer, A. Ernst, I. Mertig, and P. Zahn
Ab Initio Description of Thermoelectric Properties Based on the Boltzmann Theory
 In: *Thermoelectric Bi₂Te₃ Nanomaterials*
 Edited by: O. Eibl, K. Nielsch, N. Peranio, and F. Völklein;
 Wiley VCH, ISBN 978-3-527-33489-6 (2015)

2014

216. B. Zimmermann, K. Chadova, D. Ködderitzsch, S. Blügel, H. Ebert, D. V. Fedorov, N. H. Long, P. Mavropoulos, I. Mertig, Y. Mokrousov, and M. Gradhand
Skew scattering in dilute ferromagnetic alloys
[Phys. Rev. B **90**, 220403\(R\) \(2014\)](#)
215. C. Herschbach, D. V. Fedorov, M. Gradhand, and I. Mertig
Colossal spin Hall effect in ultrathin metallic films
[Phys. Rev. B **90**, 180406\(R\) \(2014\)](#)
214. F. Muñoz, M. Flieger, J. Henk, and I. Mertig
Reorganization of a topological surface state: Theory for Bi₂Te₃(111) covered by noble metals
[Phys. Rev. B **90**, 125159 \(2014\)](#)
213. H. L. Meyerheim, A. Ernst, K. Mohseni, C. Tusche, W. A. Adeagbo, I. V. Maznichenko, W. Hergert, G. R. Castro, J. Rubio-Zuazo, A. Morgante, N. Jedrecy, I. Mertig, and J. Kirschner
Wurtzite structure in ultrathin ZnO films on Fe(110): Surface x-ray diffraction and ab initio calculations
[Phys. Rev. B **90**, 085423 \(2014\)](#)
212. A. Mook, J. Henk, and I. Mertig
Edge states in topological magnon insulators
[Phys. Rev. B **90**, 024412 \(2014\)](#)
211. A. Johansson, C. Herschbach, D. V. Fedorov, M. Gradhand, and I. Mertig
Validity of the relativistic phase shift model for the extrinsic spin Hall effect in dilute metal alloys
[J. Phys.: Condens. Matter **26**, 274207 \(2014\)](#)
210. D. Thonig, S. Reißaus, I. Mertig, and J. Henk
Thermal string excitations in artificial spin-ice square dipolar arrays
[J. Phys.: Condens. Matter **26**, 266006 \(2014\)](#)
209. M. G. Vergniory, M. M. Otrokov, D. Thonig, M. Hoffmann, I. V. Maznichenko, M. Geilhufe, X. Zubizarreta, S. Ostanin, A. Marmodoro, J. Henk, W. Hergert, I. Mertig, E. V. Chulkov, and A. Ernst
Exchange interaction and its tuning in magnetic binary chalcogenides
[Phys. Rev. B **89**, 165202 \(2014\)](#)

208. A. Mook, J. Henk, and I. Mertig
Magnon Hall effect and topology in kagome lattices: A theoretical investigation
[Phys. Rev. B **89**, 134409 \(2014\)](#)
207. V. S. Borisov, S. Ostanin, I. V. Maznichenko, A. Ernst, and I. Mertig
Magnetoelectric properties of the Co/PbZr_xTi_{1-x}O₃ (001) interface studied from first principles
[Phys. Rev. B **89**, 054436 \(2014\)](#)
206. F. Rittweger, N. F. Hinsche, P. Zahn, and I. Mertig
Signature of the topological surface state in the thermoelectric properties of Bi₂Te₃
[Phys. Rev. B **89**, 035439 \(2014\)](#)
205. T. Rauch, M. Flieger, J. Henk, I. Mertig, and A. Ernst
Dual Topological Character of Chalcogenides: Theory for Bi₂Te₃
[Phys. Rev. Lett. **112**, 016802 \(2014\)](#)

2013

204. T. Rauch, M. Flieger, J. Henk, and I. Mertig
Nontrivial interface states confined between two topological insulators
[Phys. Rev. B **88**, 245120 \(2013\)](#)
203. T. Miyamachi, T. Schuh, T. Märkl, C. Bresch, T. Balashov, A. Stöhr, C. Karlewski, S. André, M. Marthaler, M. Hoffmann, M. Geilhufe, S. Ostanin, W. Hergert, I. Mertig, G. Schön, A. Ernst, and W. Wulfhekel
Stabilizing the magnetic moment of single holmium atoms by symmetry
[Nature **503**, 242 \(2013\)](#)
202. S. Achilles, M. Czerner, J. Henk, I. Mertig, and C. Heiliger
Nonequilibrium Green's functions and Korringa-Kohn-Rostoker method: Open planar junctions
[Phys. Rev. B **88**, 125411 \(2013\)](#)
201. V. V. Maslyuk, S. Achilles, L. Sandratskii, M. Brandbyge, and I. Mertig
Thermopower switching by magnetic field: First-principles calculations
[Phys. Rev. B **88**, 081403\(R\) \(2013\)](#)
200. C. Herschbach, D. V. Fedorov, I. Mertig, M. Gradhand, K. Chadova, H. Ebert, and D. Ködderitzsch
Insight into the skew-scattering mechanism of the spin Hall effect: Potential scattering versus spin-orbit scattering
[Phys. Rev. B **88**, 205102 \(2013\)](#)
199. H. L. Meyerheim, A. Ernst, K. Mohseni, I. V. Maznichenko, J. Henk, S. Ostanin, N. Jedrecy, F. Klimenta, J. Zegenhagen, C. Schlueter, I. Mertig, and J. Kirschner
Tuning the Structure of Ultrathin BaTiO₃ Films on Me(001) (Me=Fe, Pd, Pt) Surfaces
[Phys. Rev. Lett. **111**, 105501 \(2013\)](#)
198. D. V. Fedorov, C. Herschbach, A. Johansson, S. Ostanin, I. Mertig, M. Gradhand, K. Chadova, D. Ködderitzsch, and H. Ebert
Analysis of the giant spin Hall effect in Cu(Bi) alloys
[Phys. Rev. B **88**, 085116 \(2013\)](#)
197. P. Barone, T. Rauch, D. di Sante, J. Henk, I. Mertig, and S. Picozzi
Pressure-induced topological phase transitions in rocksalt chalcogenides
[Phys. Rev. B **88**, 045207 \(2013\)](#)
196. D. V. Fedorov, G. Fahsold, K. Singer, V. Greim, A. Pucci, P. Zahn, and I. Mertig
*Erratum: Mobility of conduction electrons in ultrathin Fe and Cu films on Si(111) [Phys. Rev. B **75**, 245427 (2007)]*
[Phys. Rev. B **87**, 079909\(E\) \(2013\)](#)

195. V. V. Maslyuk, I. Mertig, O. V. Farberovich, A. Tarantul, and B. Tsukerblat
Electronic and Spin Structures of Polyoxometalate V_{15} from a First-Principles Non-Collinear Molecular-Magnetism Approach
[Eur. J. Inorg. Chem. **2013**, 1897 \(2013\)](#)
194. K. Tauber, D. V. Fedorov, M. Gradhand, and I. Mertig
Spin Hall and spin Nernst effect in dilute ternary alloys
[Phys. Rev. B **87**, 161114\(R\) \(2013\)](#)
193. D. V. Fedorov, M. Gradhand, S. Ostanin, I. V. Maznichenko, A. Ernst, J. Fabian, and I. Mertig
Impact of Electron-Impurity Scattering on the Spin Relaxation Time in Graphene: A First-Principles Study
[Phys. Rev. Lett. **110**, 156602 \(2013\)](#)
192. N. F. Hinsche, I. Mertig, and P. Zahn
Lorenz Function of Bi_2Te_3/Sb_2Te_3 Superlattices
[J. Electron. Mater. **42**, 1406 \(2013\)](#)

2012

191. M. Gradhand, D. V. Fedorov, P. Zahn, I. Mertig, Y. Otani, Y. Niimi, L. Vila, and A. Fert
Perfect Alloys for Spin Hall Current-Induced Magnetization Switching
[SPIN **2**, 1250010 \(2012\)](#)
190. C. Etz, I. V. Maznichenko, D. Böttcher, J. Henk, A. N. Yaresko, W. Hergert, I. I. Mazin, I. Mertig, and A. Ernst
Indications of weak electronic correlations in $SrRuO_3$ from first-principles calculations
[Phys. Rev. B **86**, 064441 \(2012\)](#)
189. N. F. Hinsche, B. Yu. Yavorsky, M. Gradhand, M. Czerner, M. Winkler, J. König, H. Böttner, I. Mertig, and P. Zahn
Thermoelectric transport in Bi_2Te_3/Sb_2Te_3 superlattices
[Phys. Rev. B **86**, 085323 \(2012\)](#)
188. J. Henk, M. Flieger, I. V. Maznichenko, I. Mertig, A. Ernst, S. V. Eremeev, and E. V. Chulkov
Topological Character and Magnetism of the Dirac State in Mn-Doped Bi_2Te_3
[Phys. Rev. Lett. **109**, 076801 \(2012\)](#)
187. F. Pientka, M. Gradhand, D. V. Fedorov, I. Mertig, and B. L. Györfy
Gauge freedom for degenerate Bloch states
[Phys. Rev. B **86**, 054413 \(2012\)](#)
186. K. Tauber, M. Gradhand, D. V. Fedorov, and I. Mertig
Extrinsic Spin Nernst Effect from First Principles
[Phys. Rev. Lett. **109**, 026601 \(2012\)](#)
185. N. F. Hinsche, I. Mertig, and P. Zahn
Thermoelectric transport in strained Si and Si/Ge heterostructures
[J. Phys.: Condens. Matter **24**, 275501 \(2012\)](#)
184. J. de Boor, D. S. Kim, X. Ao, M. Becker, N. F. Hinsche, I. Mertig, P. Zahn, and V. Schmidt
Thermoelectric properties of porous silicon
[Appl. Phys. A **107**, 789 \(2012\)](#)
183. C. Herschbach, M. Gradhand, D. V. Fedorov, and I. Mertig
Enhancement of the spin Hall angle by quantum confinement
[Phys. Rev. B **85**, 195133 \(2012\)](#)

182. M. Gradhand, D. V. Fedorov, F. Pientka, P. Zahn, I. Mertig, and B. L. Györfly
First-principle calculations of the Berry curvature of Bloch states for charge and spin transport of electrons
[J. Phys.: Condens. Matter **24**, 213202 \(2012\)](#)
181. S. Borek, I. Maznichenko, G. Fischer, W. Hergert, I. Mertig, A. Ernst, S. Ostanin, and A. Chassé
First-principles calculation of x-ray absorption spectra and x-ray magnetic circular dichroism of ultrathin Fe films on BaTiO₃(001)
[Phys. Rev. B **85**, 134432 \(2012\)](#)
180. H. L. Meyerheim, A. Ernst, K. Mohseni, I. V. Maznichenko, S. Ostanin, F. Klimenta, N. Jedrecy, W. Feng, I. Mertig, R. Felici, and J. Kirschner
BaTiO₃(001)-(2 x 1): Surface Structure and Spin Density
[Phys. Rev. Lett. **108**, 215502 \(2012\)](#)
179. M. Fechner, P. Zahn, S. Ostanin, M. Bibes, and I. Mertig
Switching Magnetization by 180° with an Electric Field
[Phys. Rev. Lett. **108**, 197206 \(2012\)](#)
178. J. Henk, A. Ernst, S. V. Ereameev, E. V. Chulkov, I. V. Maznichenko, and I. Mertig
Complex spin texture in the pure and Mn-doped topological insulator Bi₂Te₃
[Phys. Rev. Lett. **108**, 206801 \(2012\)](#)
177. V. S. Borisov, I. V. Maznichenko, D. Böttcher, S. Ostanin, A. Ernst, J. Henk, and I. Mertig
Magnetic exchange interactions and antiferromagnetism of ATcO₃ (A=Ca, Sr, Ba) studied from first principles
[Phys. Rev. B **85**, 134410 \(2012\)](#)
176. A. Höfer, M. Fechner, K. Duncker, M. Hölzer, I. Mertig, and W. Widdra
Persistence of Surface Domain Structures for a Bulk Ferroelectric above T_C
[Phys. Rev. Lett. **108**, 087602 \(2012\)](#)

2011

175. P. Zahn, N. F. Hinsche, B. Yu. Yavorsky, and I. Mertig
Bi₂Te₃: implications of the rhombohedral k-space texture on the evaluation of the in-plane/out-of-plane conductivity anisotropy
[J. Phys.: Condens. Matter **23**, 505504 \(2011\)](#)
174. N. F. Hinsche, B. Yu. Yavorsky, I. Mertig, and P. Zahn
Influence of strain on anisotropic thermoelectric transport in Bi₂Te₃ and Sb₂Te₃
[Phys. Rev. B **84**, 165214 \(2011\)](#)
173. B. Yu. Yavorsky, N. F. Hinsche, I. Mertig, and P. Zahn
Electronic structure and transport anisotropy of Bi₂Te₃ and Sb₂Te₃
[Phys. Rev. B **84**, 165208 \(2011\)](#)
172. M. M. Otrokov, A. Ernst, V. V. Tugushev, S. Ostanin, P. Buczek, L. M. Sandratskii, G. Fischer, W. Hergert, I. Mertig, V. M. Kuznetsov, and E. V. Chulkov
Ab initio study of the magnetic ordering in Si/Mn dilute alloys
[Phys. Rev. B **84**, 144431 \(2011\)](#)
171. L. V. Bekenov, V. N. Antonov, S. Ostanin, A. N. Yaresko, I. V. Maznichenko, W. Hergert, I. Mertig, and A. Ernst
Electronic and magnetic properties of (Zn_{1-x}V_x)O diluted magnetic semiconductors elucidated from x-ray magnetic circular dichroism at V L_{2,3} edges and first-principles calculations
[Phys. Rev. B **84**, 134421 \(2011\)](#)

170. M. Hölzer, M. Fechner, S. Ostanin, and I. Mertig
Ab initio study of magnetoelectricity in Fe/BaTiO₃: the effects of n-doped perovskite interfaces
[J. Phys.: Condens. Matter **23**, 455902 \(2011\)](#)
169. M. Gradhand, D. V. Fedorov, F. Pientka, P. Zahn, I. Mertig, and B. L. Györfly
Calculating the Berry curvature of Bloch electrons using the KKR method
[Phys. Rev. B **84**, 075113 \(2011\)](#)
168. S. Achilles, M. Czerner, and I. Mertig
Tailoring magnetoresistance through rotating Ni particles
[Phys. Rev. B **84**, 054418 \(2011\)](#)
167. N. F. Hinsche, I. Mertig, and P. Zahn
Effect of strain on the thermoelectric properties of silicon: an ab initio study
[J. Phys.: Condens. Matter **23**, 295502 \(2011\)](#)
166. M. Polok, D. V. Fedorov, A. Bagrets, P. Zahn, and I. Mertig
Evaluation of conduction eigenchannels of an adatom probed by an STM tip
[Phys. Rev. B **83**, 245426 \(2011\)](#)
165. L. Gerhard, T. K. Yamada, T. Balashov, A. F. Takacs, R. J. H. Wesselink, M. Däne, M. Fechner, S. Ostanin, A. Ernst, I. Mertig, and W. Wulfhekel
Electrical control of the magnetic state of Fe
[IEEE Trans. Magnetism **47**, 1619 \(2011\)](#)
164. P. Bose, P. Zahn, I. Mertig, and J. Henk
Correlating transmission and local electronic structure in planar junctions: A tool for analyzing transport calculations
[Phys. Rev. B **83**, 174451 \(2011\)](#)
163. S. Lounis, P. Zahn, A. Weismann, M. Wenderoth, R. G. Ulbrich, I. Mertig, P. H. Dederichs, and S. Blügel
Theory of real space imaging of Fermi surface parts
[Phys. Rev. B **83**, 035427 \(2011\)](#)
162. M. Gradhand, D. V. Fedorov, P. Zahn, and I. Mertig
Skew scattering mechanism by an ab initio approach: extrinsic spin Hall effect in noble metals
[Solid State Phenom. **168-169**, 27 \(2011\)](#)
161. K. Kummer, D. V. Vyalikh, A. Blüher, V. Sivkov, V. V. Maslyuk, T. Bredow, I. Mertig, M. Mertig, and S. L. Molodtsov
Real-time study of the modification of the peptide bond by atomic calcium
[J. Phys. Chem. B **115**, 2401 \(2011\)](#)
160. H. L. Meyerheim, F. Klimenta, A. Ernst, K. Mohseni, S. Ostanin, M. Fechner, S. Parihar, I. V. Maznichenko, I. Mertig, and J. Kirschner
Structural secrets of multiferroic interfaces
[Phys. Rev. Lett. **106**, 087203 \(2011\)](#)
159. S. Lowitzer, M. Gradhand, D. Ködderitzsch, D. V. Fedorov, I. Mertig, and H. Ebert
Extrinsic and Intrinsic Contributions to the Spin Hall Effect of Alloys
[Phys. Rev. Lett. **106**, 056601 \(2011\)](#)
158. M. M. Otrokov, A. Ernst, S. Ostanin, G. Fischer, P. Buzcek, L. M. Sandratskii, W. Hergert, I. Mertig, V. M. Kuznetsov, and E. V. Chulkov
Intralayer magnetic ordering in Ge/Mn digital alloys
[Phys. Rev. B **83**, 155203 \(2011\)](#)

157. R. Thamankar, H. L. Meyerheim, A. Ernst, S. Ostanin, I. V. Maznichenko, E. Soyka, I. Mertig, and J. Kirschner
Tilting, bending, and non-terminal sites in CO/Cu(001)
[Phys. Rev. Lett. **106**, 106101 \(2011\)](#)

2010

156. N. F. Hinsche, M. Fechner, P. Bose, S. Ostanin, J. Henk, I. Mertig, and P. Zahn
Strong influence of complex band structure on tunneling electroresistance: A combined model and ab initio study
[Phys. Rev. B **82**, 214110 \(2010\)](#)
155. L. Gerhard, T. K. Yamada, T. Balashov, A. F. Takács, R. J. H. Wesselink, M. Däne. M. Fechner, S. Ostanin, A. Ernst, I. Mertig, and W. Wulfhekel
Magnetoelectric coupling at metal surfaces
[Nat. Nano. **5**, 792 \(2010\)](#)
154. S. Abdelouahed, A. Ernst, J. Henk, I. V. Maznichenko, and I. Mertig
Spin-split electronic states in graphene: Effects due to lattice deformation, Rashba effect, and adatoms by first principles
[Phys. Rev. B **82**, 125424 \(2010\)](#)
153. V. Yu. Aristov, O. V. Molodtsova, V. V. Maslyuk, D. V. Vylikh, T. Bredow, I. Mertig, A. B. Preobrajenski, and M. Knupfer
Electronic properties of potassium-doped FePc
[Org. Electron. **11**, 1461 \(2010\)](#)
152. M. Czerner, B. Yavorsky, and I. Mertig
The role of noncollinear magnetic order and magnetic anisotropy for the transport properties through nanowires
[phys. stat. sol. \(b\) **247**, 2594 \(2010\)](#)
151. P. Bose, P. Zahn, J. Henk, and I. Mertig
Tailoring tunnel magnetoresistance by ultrathin Cr and Co interlayers: A first-principles investigation of Fe/MgO/Fe junctions
[Phys. Rev. B **82**, 014412 \(2010\)](#)
150. M. Gradhand, D. V. Fedorov, P. Zahn, and I. Mertig
Spin Hall angle versus spin diffusion length: Tailored by impurities
[Phys. Rev. B **81**, 245109 \(2010\)](#)
149. M. Hölzer, M. Fechner, S. Ostanin, and I. Mertig
Effect of interfacial Cr on magnetoelectricity of Fe₂/CrO₂/BaTiO₃(001)
[Phys. Rev. B **81**, 214428 \(2010\)](#)
148. M. Gradhand, D. V. Fedorov, P. Zahn, and I. Mertig
Extrinsic spin Hall effect from first principles
[Phys. Rev. Lett. **104**, 186403 \(2010\)](#)
147. M. Ziese, I. Vrejoiu, E. Pippel, P. Esquinazi, D. Hesse, C. Etz, J. Henk, A. Ernst, I. V. Maznichenko, W. Hergert, and I. Mertig
Tailoring magnetic interlayer coupling in La_{0.7}Sr_{0.3}MnO₃/SrRuO₃ superlattices
[Phys. Rev. Lett. **104**, 167203 \(2010\)](#)
146. A. Tange, C. L. Gao, B. Yu. Yavorsky, I. V. Maznichenko, C. Etz, A. Ernst, W. Hergert, I. Mertig, W. Wulfhekel, and J. Kirschner
Electronic structure and spin polarization of the Fe(001)-p(1×1)O surface
[Phys. Rev. B **81**, 195410 \(2010\)](#)

145. V. V. Maslyuk, S. Achilles, and I. Mertig
Spin-polarized transport and thermopower of organometallic nanocontacts
[Solid State Commun. **150**, 505 \(2010\)](#)
144. M. Fechner, S. Ostanin, and I. Mertig
Magnetoelectric coupling at biferroic interface studied from first principles
[J. Phys.: Conf. Ser. **200**, 072027 \(2010\)](#)
143. M. Fechner, I. V. Maznichenko, S. Ostanin, A. Ernst, J. Henk, and I. Mertig
Ab initio study of magnetoelectricity in composite multiferroics
[phys. stat. sol. \(b\) **247**, 1600 \(2010\)](#)
142. M. Hortamani, L. M. Sandratskii, and I. Mertig
Does a Heisenberg Hamiltonian describe magnetic interactions in a MnSi film properly?
[J. Magn. Magn. Mater. **322**, 1082 \(2010\)](#)
141. M. Czerner, G. Rodary, S. Wedekind, D. V. Fedorov, D. Sander, I. Mertig, and J. Kirschner
Electronic picture of spin-polarized tunneling with a Cr tip
[J. Magn. Magn. Mater. **322**, 1416 \(2010\)](#)
140. H. Mirhosseini, I. V. Maznichenko, S. Abdelouahed, S. Ostanin, A. Ernst, I. Mertig, and J. Henk
Toward a ferroelectric control of Rashba spin-orbit coupling: Bi on BaTiO₃(001) from first principles
[Phys. Rev. B **81**, 073406 \(2010\)](#)
139. M. Gradhand, D. V. Fedorov, P. Zahn, and I. Mertig
Fully relativistic ab initio treatment of spin-flip scattering caused by impurities
[Phys. Rev. B **81**, 020403\(R\) \(2010\)](#)

2009

138. M. Hortamani, L. Sandratskii, P. Zahn, and I. Mertig
Physical origin of the incommensurate spin spiral structure in Mn₃Si
[J. Appl. Phys. **105**, 07E506 \(2009\)](#)
137. M. Hortamani, L. Sandratskii, P. Kratzer, and I. Mertig
Searching for Si-based spintronics by first principles calculations
[New J. Phys. **11**, 125009 \(2009\)](#)
136. M. Gradhand, M. Czerner, D. V. Fedorov, P. Zahn, B. Yu. Yavorsky, L. Szunyogh, and I. Mertig
Spin polarization on Fermi surfaces of metals by the KKR method
[Phys. Rev. B **80**, 224413 \(2009\)](#)
135. K. Kummer, V. N. Sivkov, D. V. Vyalikh, V. V. Maslyuk, A. Blüher, S. V. Nekipelov, T. Bredow, I. Mertig, M. Mertig, and S. L. Molodtsov
Oscillator strength of the peptide bond π^ resonances at all relevant x-ray absorption edges*
[Phys. Rev. B **80**, 155433 \(2009\)](#)
134. I. V. Maznichenko, A. Ernst, M. Bouhassoune, J. Henk, M. Däne, M. Lüders, P. Bruno, W. Hergert, I. Mertig, Z. Szotek, and W. M. Temmerman
Structural phase transitions and fundamental band gaps of Mg_xZn_{1-x}O alloys from first principles
[Phys. Rev. B **80**, 144101 \(2009\)](#)
133. M. Fechner, S. Ostanin, and I. Mertig
Effect of oxidation of the ultrathin Fe electrode material on the strength of magnetoelectric coupling in composite multiferroics
[Phys. Rev. B **80**, 094405 \(2009\)](#)

132. P. Bose, P. Zahn, J. Henk, and I. Mertig
Tailoring TMR ratios by ultrathin magnetic interlayers: A first-principles investigation of Fe/MgO/Fe
[MRS Proceedings **1183**, 1183-FF07-02 \(2009\)](#)
131. T. Balashov, T. Schuh, A. F. Takács, A. Ernst, S. Ostanin, J. Henk, I. Mertig, P. Bruno, T. Miyamachi, S. Suga, and W. Wulfhekel
Magnetic Anisotropy and Magnetization Dynamics of Individual Atoms and Clusters of Fe and Co on Pt(111)
[Phys. Rev. Lett. **102**, 257203 \(2009\)](#)
130. H. L. Meyerheim, C. Tusche, A. Ernst, S. Ostanin, I. V. Maznichenko, K. Mohseni, N. Jedrecy, J. Zegenhagen, J. Roy, I. Mertig, and J. Kirschner
Wurtzite-type CoO nanocrystals in ultrathin ZnCoO films
[Phys. Rev. Lett. **102**, 156102 \(2009\)](#)
129. D. V. Vyalikh, V. V. Maslyuk, A. Blüher, A. Kade, K. Kummer, Yu. S. Dedkov, T. Bredow, I. Mertig, M. Mertig, and S. L. Molodtsov
Charge transport in proteins probed by resonant photoemission
[Phys. Rev. Lett. **102**, 098101 \(2009\)](#)
128. D. V. Fedorov, P. Zahn, M. Gradhand, and I. Mertig
*Erratum: First-principles calculations of spin relaxation times of conduction electrons in Cu with nonmagnetic impurities [Phys. Rev. B **77**, 092406 (2008)]*
[Phys. Rev. B **79**, 059901\(E\) \(2009\)](#)
127. I. V. Maznichenko, S. Ostanin, A. Ernst, and I. Mertig
First-principles study of manganese-stabilized hafnia
[J. Magn. Magn. Mater. **321**, 913 \(2009\)](#)
126. V. V. Maslyuk, V. Y. Aristov, O. V. Molodtsova, D. V. Vyalikh, V. M. Zhilin, Y. A. Ossipyan, T. Bredow, I. Mertig, and M. Knupfer
The electronic structure of cobalt phthalocyanine
[Appl. Phys. A **94**, 485 \(2009\)](#)

2008

125. M. Fechner, I. V. Maznichenko, S. Ostanin, A. Ernst, J. Henk, P. Bruno, and I. Mertig
Magnetic phase transition in two-phase multiferroics predicted from first principles
[Phys. Rev. B **78**, 212406 \(2008\)](#)
124. P. Bose, A. Ernst, I. Mertig, and J. Henk
Large reduction of the magnetoresistance in Fe/MgO/Fe tunnel junctions due to small oxygen concentrations at a single FeO interface layer: A first-principles study
[Phys. Rev. B **78**, 092403 \(2008\)](#)
123. M. Hortamani, L. Sandratskii, P. Kratzer, I. Mertig, and M. Scheffler
Exchange interactions and critical temperature of bulk and thin films of MnSi: A density functional theory study
[Phys. Rev. B **78**, 104402 \(2008\)](#)
122. K. Tao, V. S. Stepanyuk, P. Bruno, D. I. Bazhanov, V. V. Maslyuk, M. Brandbyge, and I. Mertig
Manipulating magnetism and conductance of an adatom-molecule junction on a metal surface: An ab initio study
[Phys. Rev. B **78**, 014426 \(2008\)](#)
121. C. Heiliger, P. Zahn, B. Yu. Yavorsky, and I. Mertig
Thickness dependence of the tunneling current in the coherent limit of transport
[Phys. Rev. B **77**, 224407 \(2008\)](#)

120. M. Gradhand, C. Heiliger, P. Zahn, and I. Mertig
Tunneling magnetoresistance with amorphous electrodes
[Phys. Rev. B **77**, 134403 \(2008\)](#)
119. M. Czerner, B. Yu. Yavorsky, and I. Mertig
Fully relaxed magnetic structure of transition metal nanowires: First-principles calculations
[Phys. Rev. B **77**, 104411 \(2008\)](#)
118. M. Fechner, S. Ostanin, and I. Mertig
Effect of the surface polarization in polar perovskites studied from first principles
[Phys. Rev. B **77**, 094112 \(2008\)](#)
117. D. V. Fedorov, P. Zahn, M. Gradhand, and I. Mertig
First-principles calculations of spin relaxation times of conduction electrons in Cu with nonmagnetic impurities
[Phys. Rev. B **77**, 092406 \(2008\)](#)
116. T. Bredow, C. Tegenkamp, H. Pfnür, J. Meyer, V. V. Maslyuk, and I. Mertig
Ferrocene-1,1'-dithiol as molecular wire between Ag electrodes: The role of surface defects
[J. Chem. Phys. **128**, 064704 \(2008\)](#)
115. C. Heiliger, M. Czerner, B. Yu. Yavorsky, I. Mertig, and M. D. Stiles
Implementation of a nonequilibrium Green's function method to calculate spin-transfer torque
[J. Appl. Phys. **103**, 07A709 \(2008\)](#)
114. M. Czerner, B. Yu. Yavorsky, and I. Mertig
Magnetic order in geometrically constrained domain walls
[J. Appl. Phys. **103**, 07F304 \(2008\)](#)
113. V. V. Maslyuk, I. Mertig, T. Bredow, M. Mertig, D. V. Vyalikh, and S. L. Molodtsov
Electronic structure of bacterial surface protein layers
[Phys. Rev. B **77**, 045419 \(2008\)](#)
112. V. Yu. Aristov, O. V. Molodtsova, V. V. Maslyuk, D. V. Vyalikh, V. M. Zhilin, Yu. A. Ossipyan, T. Bredow, I. Mertig, and M. Knupfer
Electronic structure of the organic semiconductor copper phthalocyanine: Experiment and theory
[J. Chem. Phys. **128**, 034703 \(2008\)](#)

2007

111. C. Heiliger, M. Gradhand, P. Zahn, and I. Mertig
Tunneling magnetoresistance on the subnanometer scale
[Phys. Rev. Lett. **99**, 066804 \(2007\)](#)
110. D. V. Fedorov, G. Fahsold, A. Pucci, P. Zahn, and I. Mertig
Mobility of conduction electrons in ultrathin Fe and Cu films on Si(111)
[Phys. Rev. B **75**, 245427 \(2007\)](#)
109. A. Bagrets, N. Papanikolaou, and I. Mertig
Conduction eigenchannels of atomic-sized contacts: Ab initio KKR Green's function formalism
[Phys. Rev. B **75**, 235448 \(2007\)](#)
108. C. Heiliger, P. Zahn, and I. Mertig
Influence of interface oxidation on the TMR ratio of Fe/MgO/Fe tunnel junctions
[J. Magn. Magn. Mater. **316**, 478 \(2007\)](#)
107. P. Zahn and I. Mertig
Theory of enhanced magnetoresistance
In: *The handbook of modern magnetism and advanced magnetic material*
Edited by: H. Kronmüller and S. Parkin; John Wiley & Sons, Ltd (2007)

106. P. Bose, I. Mertig, and J. Henk
Oscillatory tunneling magnetoresistance caused by antiferromagnetic Mn layers
[Phys. Rev. B **75**, 100402\(R\) \(2007\)](#)
105. D. V. Fedorov, P. Zahn, and I. Mertig
Manifestation of quantum confinement in transport properties of ultrathin metallic films
[Thin Solid Films **515**, 6921 \(2007\)](#)
104. S. Ostanin, A. Ernst, L. M. Sandratskii, P. Bruno, M. Däne, I. D. Hughes, J. B. Staunton, W. Hergert, I. Mertig, and J. Kudrnovsky
Mn-stabilized zirconia: From imitation diamonds to a new potential high- T_C ferromagnetic spintronics material
[Phys. Rev. Lett. **98**, 016101 \(2007\)](#)

2006

103. B. Yu. Yavorsky and I. Mertig
Noncollinear interface magnetism and ballistic transport in Fe/FeO/MgO/Fe tunnel junctions: Ab initio calculations using the KKR method
[Phys. Rev. B **74**, 174402 \(2006\)](#)
102. C. Heiliger, P. Zahn, and I. Mertig
Microscopic origin of magnetoresistance
[Mater. Today **9**, 46 \(2006\)](#)
101. C. Heiliger, P. Zahn, and I. Mertig
How many Fe layers cause TMR?
[MRS Proceedings **941**, 0941-Q01-02 \(2006\)](#)
100. C. Heiliger, P. Zahn, and I. Mertig
Which states contribute to the tunneling current for large barrier thicknesses?
[MRS Proceedings **941**, 0941-Q03-05 \(2006\)](#)
99. M. Czerner, A. Bagrets, V. S. Stepanyuk, A. L. Klavsyuk, and I. Mertig
Parity oscillation and relaxation in monatomic copper wires
[Phys. Rev. B **74**, 115108 \(2006\)](#)
98. V. V. Maslyuk, A. Bagrets, V. Meded, A. Arnold, F. Evers, M. Brandbyge, T. Bredow, and I. Mertig
Organometallic benzene-vanadium wire: A one-dimensional half-metallic ferromagnet
[Phys. Rev. Lett. **97**, 097201 \(2006\)](#)
97. C. Heiliger, P. Zahn, B. Yu. Yavorsky, and I. Mertig
Interface structure and bias dependence of Fe/MgO/Fe tunnel junctions: Ab initio calculations
[Phys. Rev. B **73**, 214441 \(2006\)](#)
96. C. Heiliger, F. Heyroth, F. Syrowatka, H. S. Leipner, I. Maznichenko, K. Kokko, W. Hergert, and I. Mertig
Orientation-dependent electron-energy-loss spectroscopy of TiO₂: A comparison of theory and experiment
[Phys. Rev. B **73**, 045129 \(2006\)](#)
95. A. Bagrets, N. Papanikolaou, and I. Mertig
Ab initio approach to the ballistic transport through single atoms
[Phys. Rev. B **73**, 045428 \(2006\)](#)

2005

94. C. Heiliger, P. Zahn, B. Yu. Yavorsky, and I. Mertig
Influence of the interface structure on the bias dependence of tunneling magnetoresistance
[Phys. Rev. B **72**, 180406\(R\) \(2005\)](#)
93. N. Papanikolaou, A. Bagrets, and I. Mertig
Electronic transport through atomic size constrictions
[J. Phys.: Conf. Ser. **10**, 109 \(2005\)](#)
92. P. Zahn, J. Binder, and I. Mertig
Impurity scattering and quantum confinement in giant magnetoresistance systems: A comparative ab initio study
[Phys. Rev. B **72**, 174425 \(2005\)](#)
91. B. Yu. Yavorsky, P. Zahn, and I. Mertig
About noncollinear magnetic structures in FCC-Fe on Cu(100)
[J. Magn. Magn. Mater. **290-291**, 408 \(2005\)](#)
90. D. V. Fedorov, P. Zahn, and I. Mertig
Size effects and conductivity of ultrathin Cu films
[Thin Solid Films **473**, 346 \(2005\)](#)

2004

89. V. S. Stepanyuk, A. L. Klavsyuk, W. Hergert, A. M. Saletsky, P. Bruno, and I. Mertig
Magnetism and structure of atomic-size nanocontacts
[Phys. Rev. B **70**, 195420 \(2004\)](#)
88. B. Yu. Yavorsky, P. Zahn, and I. Mertig
Ab initio study of the magnetic structure of fcc Fe grown on a Cu(001) substrate
[Phys. Rev. B **70**, 014413 \(2004\)](#)
87. A. L. Klavsyuk, V. S. Stepanyuk, W. Hergert, A. M. Saletsky, P. Bruno, and I. Mertig
Structure and electronic states in Cu nanocontacts
[Surf. Sci. **566-568**, 944 \(2004\)](#)
86. A. Bagrets, N. Papanikolaou, and I. Mertig
Magnetoresistance of atomic-sized contacts: An ab initio study
[Phys. Rev. B **70**, 064410 \(2004\)](#)
85. P. Zahn and I. Mertig
Landauer conductance of tunnel junctions: strong impact from boundary conditions
[Philos. Mag. B **84**, 2949 \(2004\)](#)
84. V. S. Stepanyuk, P. Bruno, A. L. Klavsyuk, A. N. Baranov, W. Hergert, A. M. Saletsky, and I. Mertig
Structure and quantum effects in atomic-sized contacts
[Phys. Rev. B **69**, 033302 \(2004\)](#)

2003

83. P. Zahn, J. Binder, and I. Mertig
Impurity scattering and quantum confinement in giant magnetoresistive systems
[Phys. Rev. B **68**, 100403\(R\) \(2003\)](#)
82. B. Yu. Yavorsky, I. Mertig, and V. N. Antonov
Electronic Structure and Transport Properties of Co/Ni Superlattices
[Phase Transit. **76**, 481 \(2003\)](#)

2002

81. J. Opitz, P. Zahn, and I. Mertig
Ab initio calculated electronic structure of metallic nanowires and nanotubes
[Phys. Rev. B **66**, 245417 \(2002\)](#)
80. B. Yu. Yavorsky, I. Mertig, A. Ya. Perlov, A. N. Yaresko, and V. N. Antonov
Giant magnetoresistance due to a domain wall in Fe: Ab initio study
[Phys. Rev. B **66**, 174422 \(2002\)](#)
79. N. Papanikolaou, J. Opitz, P. Zahn, and I. Mertig
Spin-filter effect in metallic nanowires
[Phys. Rev. B **66**, 165441 \(2002\)](#)
78. M. Ye. Zhuravlev, W. Schepper, S. Heitmann, H. Vinzelberg, P. Zahn, I. Mertig, H. O. Lutz, A. V. Vedyayev, G. Reiss, and A. Hütten
Reliable prediction of giant magnetoresistance characteristics
[Phys. Rev. B **65**, 144428 \(2002\)](#)
77. P. Zahn, N. Papanikolaou, F. Erler, and I. Mertig
Evolution of Co/Cu multilayer conductivity during growth: An ab initio study
[Phys. Rev. B **65**, 134432 \(2002\)](#)
76. I. Mertig and P. Levy
Theory of GMR
In: *Spin-dependent transport in Magnetic Nanostructures*
Edited by: S. Maekawa; Gordon and Breach Publishing Group (2002)

2001

75. I. Mertig
Band calculations in Thin Film Magnetism
In: *Encyclopedia of materials: Science and technology*
Edited by: K. H. J. Buschow, R. W. Cahn, M. C. Flemings, B. Ilschner, E. J. Kramer, and S. Mahajan; Elsevier (2001)
74. J. Binder, P. Zahn, and I. Mertig
Scattering anisotropy and giant magnetoresistance in magnetic multilayers
[J. App. Phys. **89**, 7107 \(2001\)](#)
73. F. Erler, P. Zahn, and I. Mertig
Finite-size effects in giant magnetoresistance: An ab initio calculation
[Phys. Rev. B **64**, 094408 \(2001\)](#)
72. I. Riedel, P. Zahn, and I. Mertig
Ab initio calculation of the transmission coefficients from a superlattice electronic structure
[Phys. Rev. B **63**, 195403 \(2001\)](#)
71. P. Zahn and I. Mertig
c(2x2) interface alloys in Co/Cu multilayers: Influence on interlayer exchange coupling and giant magnetoresistance
[Phys. Rev. B **63**, 104412 \(2001\)](#)
70. J. Opitz, P. Zahn, J. Binder, and I. Mertig
Ab initio calculation of the interlayer exchange coupling in Fe/Au multilayers: The role of impurities at the interface
[Phys. Rev. B **63**, 094418 \(2001\)](#)

2000

69. B. Yu. Yavorsky, I. Mertig, A. Ya. Perlov, A. N. Yaresko, and V. N. Antonov
Ab initio study of the angular dependence of giant magnetoresistance in Fe/Cr superlattices
[Phys. Rev. B **62**, 9586 \(2000\)](#)
68. J. Binder, P. Zahn, and I. Mertig
Ab initio calculations of giant magnetoresistance
[J. App. Phys. **87**, 5182 \(2000\)](#)
67. J. Opitz, P. Zahn, J. Binder, and I. Mertig
Interlayer-exchange coupling in Fe/Au multilayers
[J. App. Phys. **87**, 6588 \(2000\)](#)

1999

66. I. Mertig
Theorie des Magnetowiderstandes
IFF-Ferienkurs „Magnetismus“ 1999
65. I. Mertig
Transport properties of dilute alloys
Rep. Prog. Phys. **62**, 1 (1999)

1998

64. C. Blaas, P. Weinberger, L. Szunyogh, P. M. Levy, C. B. Sommers, and I. Mertig
Giant magnetoresistance of repeated multilayers of Cu₃Ni₃ embedded in Cu(100)
Philos. Mag. B **78**, 549 (1998)
63. J. Binder, P. Zahn, I. Mertig, R. Zeller, and P. H. Dederichs
Magnetic properties of impurities and impurity pairs in magnetic multilayers
Philos. Mag. B **78**, 537 (1998)
62. J. Opitz, P. Zahn, and I. Mertig
Interlayer exchange coupling: A comparison of two theoretical concepts
Philos. Mag. B **78**, 557 (1998)
61. P. Zahn, I. Mertig, R. Zeller, and P. Dederichs
Screened KKR with hard-core potentials
Philos. Mag. B **78**, 411 (1998)
60. P. Zahn, J. Binder, I. Mertig, R. Zeller, and P. H. Dederichs
Origin of giant magnetoresistance - bulk or interface scattering
Phys. Rev. Lett. **80**, 4309 (1998)

1997

59. M. Richter, V. N. Antonov, P. Zahn, M. Divis, and I. Mertig
Ab-initio calculation of the giant magnetoresistance in uranium compounds
J. Appl. Phys. **81**, 5538 (1997)
58. P. Zahn, I. Mertig, R. Zeller, and P. H. Dederichs
Tight binding KKR - application to CoCu(001): Electronic structure and transport
MRS Proceedings **475**, 525 (1997)
57. P. Grünberg, M. Schaefer, K. Takanashi, U. Rucker, J. Nassar, and I. Mertig
Experiments on interlayer-exchange coupling
Acta Physica Polonica A **91**, 7 (1997)

56. J. Binder, P. Zahn, and I. Mertig
Inverse giant magnetoresistance in Fe/Cu/Co/Cu multilayers
J. Magn. Magn. Mater. **165**, 100 (1997)

1996

55. M. Richter, P. Zahn, M. Divis, and I. Mertig
Ab-initio calculation of giant magnetoresistance in antiferromagnetic U_2Pd_2X compounds ($X=In, Sn$)
Phys. Rev. B **54**, 11985 (1996)
54. I. Mertig
Ab initio calculation of spin-dependent transport properties
J. Appl. Phys. **79**, 5276 (1996)
53. I. Mertig
Electronic structure and physical properties
NATO ASI on Stability of Materials B **355**, 265 (1996)
52. K. Takanashi, R. Schreiber, I. Mertig, and P. Grünberg
Interlayer exchange coupling of Fe across CuAu alloys
J. Magn. Magn. Mater. **156**, 237 (1996)

1995

51. I. Mertig, P. Zahn, M. Richter, H. Eschrig, R. Zeller, and P. H. Dederichs
Ab initio calculation of residual resistivity in dilute Fe alloys and giant magnetoresistance for Fe/Cr multilayers
J. Magn. Magn. Mater. **151**, 363 (1995)
50. P. Zahn, I. Mertig, M. Richter, and H. Eschrig
Ab Initio Calculations of the Giant Magnetoresistance
Phys. Rev. Lett. **75**, 2996 (1995)
49. I. V. Solovyev, P. H. Dederichs, and I. Mertig
On the origin of orbital magnetization and magnetocrystalline anisotropy in TX ordered alloys ($T=Fe, Co$ and $X=Pd, Pt$)
Phys. Rev. B **52**, 13419 (1995)

1994

48. L. M. Sandratskii, J. Kübler, P. Zahn, and I. Mertig
Electronic structure, magnetic, and Fermi-surface properties of $UPd_2 Al_3$
Phys. Rev. B **50**, 15834 (1994)
47. I. Mertig, R. Zeller, and P. H. Dederichs
Deviations from Matthiessen's rule in dilute ternary alloys
Phys. Rev. B **49**, 11767 (1994)
46. V. S. Stepanyuk, R. Zeller, P. H. Dederichs, and I. Mertig
Electronic structure and magnetic properties of dilute Co alloys with transition-metal impurities
Phys. Rev. B **49**, 5157 (1994)

1993

45. I. Mertig, R. Zeller, and P. H. Dederichs
Ab initio calculations of residual resistivities for dilute ferromagnetic alloys: An application to giant magnetoresistance
NATO-ASI Series E **256**, 423 (1993)
44. I. Mertig
Transport-Theorie für magnetische Vielfachschichten
IFF-Ferienkurs „Magnetismus von Festkörpern und Grenzflächen“ (1993)
43. I. Mertig, R. Zeller, and P. H. Dederichs
Ab initio calculations of residual resistivities for dilute Ni-alloys
Phys. Rev. B **47**, 16178 (1993)
42. I. Mertig, R. Zeller, and P. H. Dederichs
Calculation of residual resistivities for ferromagnetic dilute alloys
Int. J. Mod. Phys. B **7**, 778 (1993)

1992

41. T. Vojta, I. Mertig, and R. Zeller
Thermopower of dilute Silver alloys
Phys. Rev. B **46**, 15761 (1992)
40. I. Mertig, R. Zeller, and P. H. Dederichs
Calculation of residual resistivities for ferromagnetic dilute alloys
In: Physics of transition metals, p.778 (1992)
Edited by: P. M. Oppener and J. Kübler
39. I. Mertig, R. Zeller, and P. H. Dederichs
Ab-initio calculations of residual resistivities for dilute Ni-alloys
MRS Proceedings **253**, 249 (1992)

1991

38. I. Mertig, R. Zeller, B. Drittler, and P. H. Dederichs
Residual resistivity of ferromagnetic Ni-alloys
In: Proc. 21st Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1991, p.218

1990

36. H. L. Skriver and I. Mertig
Electron-phonon coupling of the rare-earth metals
Phys. Rev. B **41**, 6553 (1990)
37. I. Mertig and H. L. Skriver
Resistivity anisotropy and electron-phonon coupling in hexagonal metals
In: Proc. 20th Symposium Electronic Structure
Edited by: P. Ziesche: TU Dresden, 1990, p.289

1989

35. H. L. Skriver and I. Mertig
Electron-phonon interaction in rare earth metals
In: Proc. 19th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1989, p.82

1988

34. H. L. Skriver, O. Eriksson, I. Mertig, and E. Mrosan
Electron-phonon coupling of the actinides
Phys. Rev. B **37**, 1706 (1988)
33. J. Gräfenstein, I. Mertig, E. Mrosan, and R. Zeller
Anisotropic electron-impurity scattering rates of dilute noble-metal alloys: A comparison with surface state resonance data
J. Phys. F **18**, 731 (1988)
32. J. Gräfenstein, I. Mertig, E. Mrosan, V. N. Antonov, and VI. N. Antonov
Calculated Fermi surface characteristics of the noble metals
phys. stat. sol.(b) **147**, 575 (1988)
31. J. Gräfenstein, I. Mertig, E. Mrosan, V. N. Antonov, and VI. N. Antonov
Anisotropic Fermi velocities of the noble metals
In: Proc. 18th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1988, p.202

1987

30. H. L. Skriver and I. Mertig
Electron-phonon coupling of the rare earth metals
In: Proc. 17th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1987, p.49
29. E. Mrosan and I. Mertig
Relativistic Hopfield parameter: LMTO-formulation
In: Proc. 17th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1987, p.50

1986

28. I. Mertig, E. Mrosan, V. N. Antonov, VI. N. Antonov, and P. Ziesche
Calculation of effective optical masses in Copper and Silver
phys. stat. sol. (b) **135**, K13 (1986)
27. A. Lodder, I. Mertig, R. Zeller, E. Mrosan, and P. H. Dederichs
Influence of charge transfer on ab initio calculated impurity resistivities in noble metals
phys. stat. sol. (b) **135**, 831 (1986)
26. I. Mertig, E. Mrosan, and R. Zeller
Local electron-impurity scattering rates of Cu(Al) and Cu(Ni)
In: Proc. 16th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1986, p.140

1985

25. H. L. Skriver and I. Mertig
Electron-phonon coupling of the actinide metals
Phys. Rev. B **32**, 4431 (1985)
24. I. Mertig, E. Mrosan, R. Zeller, P. H. Dederichs, and P. Ziesche
Calculation of the thermoelectric power of Ga, Ni, Rh and Pd impurities in Copper
phys. stat. sol. (b) **129**, 407 (1985)
23. I. Mertig, E. Mrosan, V. N. Antonov, VI. N. Antonov, and P. Ziesche
Calculation of effective optical masses in Copper and Silver
In: Proc. 16th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1985, p.124
22. H. L. Skriver and I. Mertig
Electron-phonon coupling in actinide metals
In: Proc. 15th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1985, p.80
21. I. Mertig and E. Mrosan
First principle calculation of the thermoelectric power of Ga, Ni, Rh and Pd impurities in Cu
In: Proc. 15th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1985, p.103
20. P. Ziesche, I. Mertig, and E. Mrosan
Residual resistivity and thermopower of dilute copper alloys
6th International Symposium:High-purity materials in Science and Technology Dresden,
1985, p.371

1983

19. I. Mertig, E. Mrosan, R. Zeller, and P. H. Dederichs
Electronic properties of dilute copper alloys: III. Influence on the de Haas-van Alphen effect
phys. stat. sol. (b) **119**, 251 (1983)
18. I. Mertig, E. Mrosan, R. Zeller, and P. H. Dederichs
Electronic properties of dilute copper alloys: II. Residual resistivity
phys. stat. sol. (b) **117**, 619 (1983)
17. I. Mertig, E. Mrosan, R. Zeller, P. H. Dederichs, and P. Ziesche
Electronic properties of dilute copper alloys: I. Theory
phys. stat. sol. (b) **117**, 335 (1983)
16. I. Mertig and E. Mrosan
Magnetoresistivity of metals: I. Application to 3d transition metal impurities in Cu
J. Phys. F **13**, 373 (1983)
15. I. Mertig, E. Mrosan, R. Zeller, and P. H. Dederichs
Electronic properties of 4d transition metal impurities in Cu
In: Proc. 13th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1983, p.3

1982

14. I. Mertig and E. Mrosan
Calculation of Fermi surface orbit integrals using a tetrahedron method: III. Fermi surface changes of Cu by alloying
J. Phys. F **12**, 1139 (1982)

13. I. Mertig, E. Mrosan, and R. Schöpke
Calculation of residual resistivity of 3d transition metal impurities in Cu using an exact solution of the linearised Boltzmann equation
J. Phys. F **12**, 1689 (1982)
12. I. Mertig and E. Mrosan
Magnetoresistivity of metals: I. Solution of the linearised Boltzmann equation using Fermi surface harmonics
J. Phys. F **12**, 3031 (1982)
11. I. Mertig, E. Mrosan, R. Zeller, and P. H. Dederichs
Anisotropic cyclotron masses and electron-phonon interaction in Silver
phys. stat. sol. (b) **109**, K17 (1982)
10. I. Mertig and E. Mrosan
Galvanomagnetic properties of 3d transition metal impurities in Cu
In: Proc. 12th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1982, p.183

1981

9. I. Mertig and E. Mrosan
Fermi surface changes of Cu by alloying of Al and Ni
In: Proc. 11th Symposium Electronic Structure
Edited by: TU Dresden, 1981, p.56

1980

8. I. Mertig, E. Mrosan, U. Fleck and H. Wonn
Calculation of Fermi surface orbit integrals using a tetrahedron method: I. Orientation dependence of cyclotron masses in Cu and Au
J. Phys. F **10**, 407 (1980)
7. I. Mertig and E. Mrosan
Calculation of Fermi surface orbit integrals using a tetrahedron method: II. Dingle temperatures for 3d transition metal impurities in Cu
J. Phys. F **10**, 417 (1980)

1979

6. I. Mertig and E. Mrosan
Calculation of cyclotron masses of copper using a tetrahedron method
phys. stat. sol. (b) **94**, K23 (1979)
5. I. Mertig and E. Mrosan
Calculation of Dingle temperatures for Ni-impurities in Copper using a tetrahedron method
phys. stat. sol. (b) **94**, K119 (1979)
4. I. Mertig and E. Mrosan
Dingle temperatures for 3d-transition metal impurities in Cu
In: Proc. 9th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1979, p.10
3. I. Mertig, E. Mrosan, U. Fleck, and H. Wonn
Orientation dependence of cyclotron masses in Cu and Au
In: Proc. 9th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1979, p.2

1978

2. H. Eschrig and I. Bergert (verheiratet Mertig)
An optimized LCAO version for band structure calculations
phys. stat. sol. (b) **90**, 621 (1978)
1. H. Eschrig and I. Bergert (verheiratet Mertig)
The LCAO concept of electronic structure
In: Proc. 8th Symposium Electronic Structure
Edited by: P. Ziesche, TU Dresden, 1978, p.179

Books:

I. Mertig, E. Mrosan, and P. Ziesche
Multiple scattering theory of point defects in metals: Electronic properties
Teubner-Verlagsgesellschaft, Leipzig, 1987