Publications
Ingrid Mertig
January 2025

2025

356. E. Şaşıoğlu, M. Tas, S. Ghosh, W. Beida, B. Sanyal, S. Blügel, I. Mertig, and I. Galanakis
Spin gapped metals: A novel class of materials for multifunctional spintronic devices
J. Magn. Magn. Mater. **615**, 172792 (2025)

355. B. Göbel, L. Schimpf, and I. Mertig
Topological orbital Hall effect caused by skyrmions and antiferromagnetic skyrmions
Commun. Phys **8**, 17 (2025)

2024

354. B. Göbel and I. Mertig
Orbital Hall Effect Accompanying Quantum Hall Effect: Landau Levels Cause Orbital Polarized Edge Currents
Phys. Rev. Lett. **133**, 146301 (2024)

353. I. Ribeiro de Assis, I. Mertig, and B. Göbel
Circular motion of noncollinear spin textures in Corbino disks: Dynamics of Néel- versus Bloch-type skyrmions and skyrmioniums
Phys. Rev. B **110**, 064404 (2024)s

352. P. Bodewei, E. Şaşıoğlu, N.F. Hinsche, and I. Mertig
Computational design of tunnel diodes with negative differential resistance and ultrahigh peak-to-valley current ratio based on two-dimensional cold metals: The case of $NbSi_2N_4/HfSi_2N_4/NbSi_2N_4$ lateral heterojunction diode
Phys. Rev. Appl.7 **22**, 014004 (2024)

351. H. R Ramezani, E. Şaşıoğlu, H. Hadipour, H. Rahimpour Soleimani, C. Friedrich, S. Blügel, and I. Mertig
Nonconventional screening of Coulomb interaction in two-dimensional semiconductors and metals: A comprehensive constrained random phase approximation study of MX_2 (M=Mo, W, Nb, Ta; X=S, Se, Te)
Phys. Rev. B **109**, 125108 (2024)

350. R. Saha, H. L. Meyerheim, B. Göbel, I. Mertig, and S. S. P. Parkin
High-temperature Néel skyrmions in Fe_3GaTe_2 stabilized by Fe intercalation into the van der Waals gap
npj Spintronics **2**, 21 (2024)

349. I. V. Maznichenko, S. Ostanin, D. Maryenko, V. K. Dugaev, E. Ya. Sherman, P. Buczek, I. Mertig, M. Kawasaki, and A. Ernst
Emerging Two-Dimensional Conductivity at the Interface between Mott and Band Insulators
Phys. Rev. Lett. **132**, 216201 (2024)

348. R. R. Neumann, J. Henk, I. Mertig, and A. Mook
Electrical activity of topological chiral edge magnons
Phys. Rev. B **109**, L180412 (2024)

347. G. Lazrak, B. Göbel, A. Barthélémy, I. Mertig, A. Johansson, and M. Bibes
Boosting the Edelstein effect of two-dimensional electron gases by ferromagnetic exchange
Phys. Rev. Research **6**, 023074 (2024)

346. O. Busch, F. Ziolkowski, B. Göbel, I. Mertig, and J. Henk
Ultrafast orbital Hall effect in metallic nanoribbons
Phys. Rev. Research **6**, 013208 (2024)

345. K. Özdoğan, I. Maznichenko, S. Ostanin, E. Şaşıoğlu, A. Ernst, I. Mertig, and I. Galanakis
Corrigendum: high spin polarization in all-3d-metallic Heusler compounds: the case of Fe_2CrZ and Co_2CrZ (Z = Sc, Ti, V) (2019 J. Phys: D. Appl. Phys.52205003)
J. Phys. D: Appl. Phys. **57**, 049501 (2024)

2023

344. S. Leiva-Montecinos, J. Henk, I. Mertig, and A. Johansson
Spin and orbital Edelstein effect in a bilayer system with Rashba interaction
Phys. Rev. Research **5**, 043294 (2023)

343. E. Gürbüz, M. Tas, E. Şaşıoğlu, I. Mertig, B. Sanyal, and I. Galanakis
First-principles prediction of energy bandgaps in 18-valence electron semiconducting half-Heusler compounds: Exploring the role of exchange and correlation
J. Appl. Phys. **134**, 205703 (2023)

342. S. Mallik, B. Göbel, H. Witt, L. M. Vicente-Arche, S. Varotto, J. Bréhin, G. Ménard, G. Saïz, D. Tamsaout, A. F. Santander-Syro, F. Fortuna, F. Bertran, P. Le Fèvre, J. Rault, I. Boventer, I. Mertig, A. Barthélémy, N. Bergeal, A. Johansson, and M. Bibes
Electronic band structure of superconducting $KTaO_3$ (111) interfaces
APL Mater. **11**, 121108 (2023)

341. O. Busch, F. Ziolkowski, I. Mertig, and J. Henk
Ultrafast dynamics of electrons excited by femtosecond laser pulses: Spin polarization and spin-polarized currents
Phys. Rev. B **108**, 184401 (2023)

340. I. Ribeiro de Assis, I. Mertig, and B. Göbel
Skyrmion motion in magnetic anisotropy gradients: Acceleration caused by deformation
Phys. Rev. B **108**, 144438 (2023)

339. O. Busch, I. Mertig, and B. Göbel
Orbital Hall effect and orbital edge states caused by s electrons
Phys. Rev. Research **5**, 043052 (2023)

338. N. Li, R. R. Neumann, S. K. Guang, Q. Huang, J. Liu, K. Xia, X. Y. Yue, Y. Sun, Y. Y. Wang, Q. J. Li, Y. Jiang, J. Fang, Z. Jiang, X. Zhao, A. Mook, J. Henk, I. Mertig, H. D. Zhou, and X. F. Sun
Magnon-polaron driven thermal Hall effect in a Heisenberg-Kitaev antiferromagnet
Phys. Rev. B **108**, L140402 (2023)

337. O. Busch, F. Ziolkowski, I. Mertig, and J. Henk
Ultrafast dynamics of orbital angular momentum of electrons induced by femtosecond laser pulses: Generation and transfer across interfaces
Phys. Rev. B **108**, 104408 (2023)

336. B. K. Hazra, B. Pal, J.-C. Jeon, R. R. Neumann, B. Göbel, B. Grover, H. Deniz, A. Styervoyedov, H. Meyerheim, I. Mertig, S.-H. Yang, and S. S. P. Parkin
Generation of out-of-plane polarized spin current by spin swapping
Nat. Commun. **14**, 4549 (2023)

335. I. V. Maznichenko, P. Buczek, I. Mertig, and S. Ostanin
Spin textures induced in n-doped solid electrolytes
J. Phys. D: Appl. Phys. **56**, 405305 (2023)

334. E. Gürbüz, S. Ghosh, E. Şaşıoğlu, I. Galanakis, I. Mertig, and B. Sanyal
Spin-polarized two-dimensional electron/hole gas at the interface of nonmagnetic semiconducting half-Heusler compounds: Modified Slater-Pauling rule for half-metallicity at the interface
Phys. Rev. Mater. **7**, 054405 (2023)

333. B. H. Rimmler, B. K. Hazra, B. Pal, K. Mohseni, J. M. Taylor, A. Bedoya-Pinto, H. Deniz, M. Tangi, I. Kostanovskiy, C. Luo, R. R. Neumann, A. Ernst, F. Radu, I. Mertig, H. L. Meyerheim, and S. S. P. Parkin
Atomic Displacements Enabling the Observation of the Anomalous Hall Effect in a Non-Collinear Antiferromagnet
Adv. Mater. **35**, 2209616 (2023)

332. D.-S. Park, A. D. Rata, R. T. Dahm, K. Chu, Y. Gan, I. Maznichenko, S. Ostanin, F. Trier, H. Baik, W. S. Choi, C.-J. Choi, Y. H. Kim, G. J. Rees, H. P. Gíslason, P. A. Buczek, I. Mertig, M. A. Ionescu, A. Ernst, K. Dörr, P. Muralt, and N. Pryds
Controlled Electronic and Magnetic Landscape in Self-Assembled Complex Oxide Heterostructures
Adv. Mater. **35**, 2300200 (2023)

331. I. Ribeiro de Assis, I. Mertig, and B. Göbel
Biskyrmion-based artificial neuron
Neuromorph. Comput. Eng. **3**, 014012 (2023)

330. E. Şaşıoğlu and I. Mertig
Theoretical Prediction of Semiconductor-Free Negative Differential Resistance Tunnel Diodes with High Peak-to-Valley Current Ratios Based on Two-Dimensional Cold Metals
ACS Appl. Nano Mater. **6**, 3758 (2023)

329. F. Ziolkowski, O. Busch, I. Mertig, and J. Henk
Ultrafast spin dynamics: complementing theoretical analyses by quantum state measures
J. Phys.: Condens. Matter **35**, 125501 (2023)

2022

328. M. Tas, E. Şaşıoğlu, S. Blügel, I. Mertig, and I. Galanakis
Ab initio calculation of the Hubbard U and Hund exchange J in local moment magnets: The case of Mn-based full Heusler compounds
Phys. Rev. Mater. **6**, 114401 (2022)

327. S. Varotto, A. Johansson, B. Göbel, L. M. Vicente-Arche, S. Mallik, J. Bréhin, R. Salazar, F. Bertran, P. Le Fèvre, N. Bergeal, J. Rault, I. Mertig, and M. Bibes
Direct visualization of Rashba-split bands and spin/orbital-charge interconversion at $KTaO_3$ interfaces
Nat. Commun. **13**, 6165 (2022)

326. A. Melnikov, L. Brandt, N. Liebing, M. Ribow, I. Mertig, and G. Woltersdorf
Ultrafast spin transport and control of spin current pulse shape in metallic multilayers
Phys. Rev. B **106**, 104417 (2022)

325. A. D. Rata, J. Herrero-Martin, I. V. Maznichenko, F. M. Chiabrera, R. T. Dahm, S. Ostanin, D. Lee, B. Jalan, P. Buczek, I. Mertig, A. Ernst, A. M. Ionescu, K. Dörr, N. Pryds, and D.-S. Park
Defect-induced magnetism in homoepitaxial $SrTiO_3$
APL Mater. **10**, 091108 (2022)

324. T. Aull, E. Şaşıoğlu, N.F. Hinsche, and I. Mertig
Ab Initio Study of Magnetic Tunnel Junctions Based on Half-Metallic and Spin-Gapless Semiconducting Heusler Compounds: Reconfigurable Diode and Inverse Tunnel-Magnetoresistance Effect
Phys. Rev. Appl. **18**, 034024 (2022)

323. R. Saha, H. L. Meyerheim, B. Göbel, B. K. Hazra, H. Deniz, K. Mohseni, V. Antonov, A. Ernst, D. Knyazev, A. Bedoya-Pinto, I. Mertig, and S. S. P. Parkin
Observation of Néel-type skyrmions in acentric self-intercalated $Cr_{1+\delta}Te_2$
Nat. Commun. **13**, 3965 (2022)

322. B. Pal, B. K. Hazra, B. Göbel, J.-C. Jeon, A. K. Pandeya, A. Chakraborty, O. Busch, A. K. Srivastava, H. Deniz, J. M. Taylor, H. Meyerheim, I. Mertig, S.-H. Yang, and S. S. P. Parkin
Setting of the magnetic structure of chiral kagome antiferromagnets by a seeded spin-orbit torque
Sci. Adv. **8**, eabo5930 (2022)

321. I. V. Maznichenko, P. Buczek, I. Mertig, and S. Ostanin
Charge-to-spin conversion in the quasi-two-dimensional electron gas emerging at the hydrogen-doped interface between $LiNbO_3$ and $LaAlO_3$
Phys. Rev. Mater. **6**, 064001 (2022)

320. M. A. Wahada, E. Şaşıoğlu, W. Hoppe, X. Zhou, H. Deniz, R. Rouzegar, T. Kampfrath, I. Mertig, S. S. P. Parkin, and G. Woltersdorf
Atomic Scale Control of Spin Current Transmission at Interfaces
Nano Lett. **22**, 3539 (2022)

319. J. Jena, B. Göbel, T. Hirosawa, S. A. Díaz, D. Wolf, T. Hinokihara, V. Kumar, I. Mertig, C. Felser, A. Lubk, D. Loss, and S. S. P. Parkin
Observation of fractional spin textures in a Heusler material
Nat. Commun. **13**, 2348 (2022)

318. R. R. Neumann, A. Mook, J. Henk, and I. Mertig
Thermal Hall Effect of Magnons in Collinear Antiferromagnetic Insulators: Signatures of Magnetic and Topological Phase Transitions
Phys. Rev. Lett. **128**, 117201 (2022)

317. F. Calavalle, M. Suárez-Rodríguez, B. Martín-García, A. Johansson, D. C. Vaz, H. Yang, I. V. Maznichenko, S. Ostanin, A. Mateo-Alonso, A. Chuvilin, I. Mertig, M. Gobbi, F. Casanova, and L. E. Hueso
Gate-tuneable and chirality-dependent charge-to-spin conversion in tellurium nanowires
Nat. Mater. **21**, 526 (2022)

316. D. V. Fedorov, M. Gradhand, K. Tauber, G. E. W. Bauer, and I. Mertig
Seebeck effect in nanomagnets
J. Phys.: Condens. Matter **34**, 085801 (2022)

2021

315. T. Aull, I. V. Maznichenko, S. Ostanin, E. Şaşıoğlu, and I. Mertig
Externally controlled and switchable two-dimensional electron gas at the Rashba interface between ferroelectrics and heavy d metals
Phys. Rev. Research **3**, 043110 (2021)

314. O. Busch, B. Göbel, and I. Mertig
Spin Hall effect in noncollinear kagome antiferromagnets
Phys. Rev. B **104**, 184423 (2021)

313. B. Göbel and I. Mertig
Quaternary-Digital Data Storage Based on Magnetic Bubbles in Anisotropic Materials
Phys. Rev. Appl. **15**, 064052 (2021)

312. I. V. Maznichenko, S. Ostanin, I. Mertig, and P. Buczek
Emergent quasi-two-dimensional electron gas between $Li_{1\pm x}NbO_3$ and $LaAlO_3$ and its prospectively switchable magnetism
Phys. Rev. Mater. **5**, 114001 (2021)

311. L. Nádvorník, M. Borchert, L. Brandt, R. Schlitz, K. A. de Mare, K. Výborný, I. Mertig, G. Jakob, M. Kläui, S. T. B. Goennenwein, M. Wolf, G. Woltersdorf, and T. Kampfrath
Broadband Terahertz Probes of Anisotropic Magnetoresistance Disentangle Extrinsic and Intrinsic Contributions
Phys. Rev. X **11**, 021030 (2021)

310. A. Johansson, B. Göbel, J. Henk, M. Bibes, and I. Mertig
Spin and orbital Edelstein effects in a two-dimensional electron gas: Theory and application to $SrTiO_3$ interfaces
Phys. Rev. Research **3**, 013275 (2021)

309. M. Raju, A. P. Petrović, A. Yagil, K. S. Denisov, N. K. Duong, B. Göbel, E. Şaşıoğlu, O. M. Auslaender, I. Mertig, I. V. Rozhansky, and C. Panagopoulos
Colossal topological Hall effect at the transition between isolated and lattice-phase interfacial skyrmions
Nat. Commun. **12**, 2758 (2021)

308. Y. Yekta, H. Hadipour, E. Şaşıoğlu, C. Friedrich, S. A. Jafari, S. Blügel, and I. Mertig
Strength of effective Coulomb interaction in two-dimensional transition-metal halides MX_2 and MX_3 (M=Ti, V, Cr, Mn, Fe, Co, Ni; X=Cl, Br, I)
Phys. Rev. Mater. **5**, 034001 (2021)

307. O. Gueckstock, L. Nádvorník, M. Gradhand, T. S. Seifert, G. Bierhance, R. Rouzegar, M. Wolf, M. Vafaee, J. Cramer, M. A. Syskaki, G. Woltersdorf, I. Mertig, G. Jakob, M. Kläui, and T. Kampfrath
Terahertz Spin-to-Charge Conversion by Interfacial Skew Scattering in Metallic Bilayers
Adv. Mater. **33**, 2006281 (2021)

306. B. Göbel and I. Mertig
Skyrmion ratchet propagation: utilizing the skyrmion Hall effect in AC racetrack storage devices
Sci. Rep. **11**, 3020 (2021)

305. F. Töpler, J. Henk, and I. Mertig
Ultrafast spin dynamics in inhomogeneous systems: a density-matrix approach applied to Co/Cu interfaces
New J. Phys. **23**, 033042 (2021)

304. T. Aull, E. Şaşıoğlu, and I. Mertig
First principles design of Ohmic spin diodes based on quaternary Heusler compounds
Appl. Phys. Lett. **118**, 052405 (2021)

303. B. Göbel, I. Mertig, and O. A. Tretiakov
Beyond skyrmions: Review and perspectives of alternative magnetic quasiparticles
Phys. Rep. **895**, 1 (2021)

2020

302. J. Jena, B. Göbel, V. Kumar, I. Mertig, C. Felser, and S. Parkin
Evolution and competition between chiral spin textures in nanostripes with D_{2d} symmetry
Sci. Adv. **6**, eabc0723 (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 **14**, 13463 (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 $LaAlO_3/SrTiO_3$(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 Fe_2CrZ and Co_2CrZ (Z = Sc,Ti,V)
J. Phys. D: Appl. Phys. **52**, 205003 (2019)

274. S. K. Mahatha, A. S.Ngankeu, 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 MoS_2
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 $BaFeO_{3-\delta}$
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 $SrCoO_{3-\delta}$
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 $BaTiO_3$
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/$PbTiO_3$/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 $PbTiO_3$-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 Sb_2Te_3 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 Bi_2Te_3 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 Bi_2Te_3(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/$PbZr_xTi_{1-x}O_3$ (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 Bi_2Te_3
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 Bi_2Te_3
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 $BaTiO_3$ 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. Györffy
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. Györffy
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 $BaTiO_3(001)$
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
$BaTiO_3(001)$-(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. Eremeev, E. V. Chulkov, I. V. Maznichenko, and I. Mertig
Complex spin texture in the pure and Mn-doped topological insulator Bi_2Te_3
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 $ATcO_3$ (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
Bi_2Te_3: 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 Bi_2Te_3 and Sb_2Te_3
Phys. Rev. B **84**, 165214 (2011)

173. B. Yu. Yavorsky, N. F. Hinsche, I. Mertig, and P. Zahn
Electronic structure and transport anisotropy of Bi_2Te_3 and Sb_2Te_3
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 digital 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 $Fe/BaTiO_3$: 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. Györffy
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. Magnetics **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. Vyalikh, 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 $Fe_2/CrO_2/BaTiO_3(001)$
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 $La_{0.7}Sr_{0.3}MnO_3/SrRuO_3$ 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 $BaTiO_3$(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 Mn_3Si
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 phtalocyanine: 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 TiO_2: 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 Cu_3Ni_3 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. Rücker, 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 Vl. 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 Vl. 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, Vl. 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, Vl. N. Antonov, and P. Ziesche
Calculation of effective optical masses in Copper and Silver
In: Proc. 16th Symposium Electronic Structure
Edidted 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