Publication list

Prof. Dr. Stefan Blügel

I. Publications in journals with scientific quality assurance

[1] P. H. Dederichs, S. Blügel, R. Zeller, and H. Akai,
Ground States of Constrained Systems: Application to Cerium Impurities,
Phys. Rev. Lett. **53**, 2512 (1984).

[2] H. Akai, M. Akai, S. Blügel, P. H. Dederichs, and R. Zeller,
Hyperfine Fields of Impurities in Ferromagnets,
J. Magn. Magn. Mater. **45**, 291 (1984).

[3] P. H. Dederichs, H. Akai, S. Blügel, A. Oswald, and R. Zeller,
Ab-initio Calculations for Impurities in Cu and Ni,
Phil. Mag. B **51**, 137 (1985).

[4] H. Akai, S. Blügel, R. Zeller, and P. H. Dederichs,
Isomer Shifts and their Relation to Charge Transfer in Dilute Fe-Alloys,
J. Magn. Magn. Mater. **54-57**, 1101 (1986).

[5] H. Akai, S. Blügel, R. Zeller, and P. H. Dederichs,
Isomer Shifts and their Relation to Charge Transfer,
Phys. Rev. Lett. **56**, 2407 (1986).

[6] S. Blügel, H. Akai, R. Zeller, and P. H. Dederichs,
Hyperfine Fields of 3d and 4d Impurities in Nickel,
Phys. Rev. B **35**, 3271 (1987).

[7] S. Blügel, M. Weinert, and P. H. Dederichs,
Ferromagnetism and Antiferromagnetism of 3d-Metal Overlayers on Metals,
Phys. Rev. Lett. **60**, 1077 (1988).

[8] E. Tamura, S. Blügel, and R. Feder,
On the Determination of Surface Antiferromagnetism by Low-Energy Electron Diffraction,
Solid State Commun. **65**, 1255 (1988).

[9] M. Stampanoni, A. Vaterlaus, D. Pescia, M. Aeschlimann, F. Meier, W. Dürr, S. Blügel,
Lack of Evidence for Ferromagnetism in the Vanadium Monolayer on Ag(001),
Phys. Rev. B **37**, 10380 (1988).

[10] S. Blügel,
Strong Ferromagnetism of 3d-Metal Overlayers on Pd(001),
Europhys. Lett. **7**, 743 (1988).

[11] S. Blügel, D. Pescia, and P. H. Dederichs,
Ferromagnetism versus c(2x2)Antiferromagnetism of the Cr(001) Surface,
Phys. Rev. B **39**, 1392 (1989).

[12] S. Blügel and P. H. Dederichs,
Ferromagnetism and Antiferromagnetism of 3d-Metal Overlayers on Noble Metal Substrates,
Europhys. Lett. **9**, 597 (1989).

[13] B. Drittler, N. Stefanou, S. Blügel, R. Zeller, and P. H. Dederichs,
Electronic Structure and Magnetic Properties of dilute Fe-Alloys with Transition Metal Impurities,
Phys. Rev. B **40**, 8203 (1989).

[14] S. Blügel, D. Drittler, R. Zeller, and P. H. Dederichs,
Magnetic Properties of 3d Transition-Metal Monolayers on Metal Substrates,
Appl. Phys. A **49**, 547 (1989).

[15] U. König, S. Blügel, G. Hörmandinger, and P. Weinberger,
Calculation of Spin- and Angle- Resolved Photoemission Spectra from Pd(001) Coated with a Monolayer of a Magnetic 3d-Metal: The antiferromagnetic configuration of V, Cr, and Mn,
Solid State Commun. **76**, 1309 (1990).

[16] S. Takizawa, S. Blügel, K. Terakura, and T. Oguchi,
Pressure Induced Phase Transition of CuPt Alloy,
Phys. Rev. B **43**, 947 (1991).

[17] U. König, S. Blügel, J. Redinger, and P. Weinberger,
Calculation of Spin- and Angle- Resolved Photoemission Spectra from Pd(001) Coated with a Monolayer of a Magnetic 3d-Metal: Fe, Co and Ni,
Phys. Rev. B **43**, 1954 (1991).

[18] K. Kobayashi, S. Blügel, H. Ishida, and K. Terakura,
Atomic Arrangement of Alkali Adatoms on Si(001) - 2 x 1,
Surf. Sci. **215**, 349 (1991).

[19] U. König, S. Blügel, G. Hörmandinger, and P. Weinberger,
Calculation of Spin- and Angle- Resolved Photoemission Spectra from Pd(001) Coated with a Monolayer of a Magnetic 3d-metal: Cr and Mn, A Comparison between the Antiferromagnetic and the Ferromagnetic Configuration,
Phys. Rev. B **43**, 14434 (1991).

[20] Y. Morikawa, K. Kobayashi, K. Terakura, and S. Blügel,
Theoretical Support to the Double-Layer Model for Potassium Adsorption on Si(001) Surface,
Phys. Rev. B **44**, 3459 (1991).

[21] W. Clemens, T. Kachel, O. Rader, E. Vescovo, S. Blügel, C. Carbone, and W. Eberhardt,
Quantum Size Effects on the Exchange Splitting in Ultrathin Co Overlayers on Cu(100),
Solid State Commun. **81**, 739 (1992).

[22] S. Blügel,
Ferromagnetism of 4d Metal Monolayers on Ag, Au, and Pd (001) Surfaces,
Europhys. Lett. **18**, 257 (1992).

[23] S. Blügel,
Two-Dimensional Ferromagnetism of 3d, 4d, and 5d Transition Metal Monolayers on Noble Metal (001) Substrates,
Phys. Rev. Lett. **68**, 851 (1992).

[24] K. Kobayashi, Y. Morikawa, K. Terakura, and S. Blügel,
Optimized Structures and Electronic Properties of Alkali-Metal (Na, K)-Adsorbed on Si(001) Surfaces,
Phys. Rev. B **45**, 3469 (1992).

[25] O. Rader, C. Carbone, W. Clemens, E. Vescovo, S. Blügel, W. Eberhardt, and W. Gudat,
Exchange-Dependent Hybridization at the Fe-Pd Interface,
Phys. Rev. B **45**, 13823 (1992).

[26] T. Kachel, C. Carbone, E. Vescovo, S. Blügel, U. Alkemper, W. Eberhardt, and W. Gudat,
Ferromagnetic Order in Ultrathin Rh Layers on Fe(100),
Phys. Rev. B **46**, 12888 (1992).

[27] S. Blügel,
Ferromagnetism of 4d and 5d Transition Metal Monolayers: Interlayer in Ag(001) versus Overlayer on Ag(001),
Solid State Commun. **84**, 621 (1992).

[28] O. Rader, C. Carbone, W. Clemens, E. Vescovo, S. Blügel, W. Eberhardt, and W. Gudat,
Growth and Magnetic Behavior of Pd on Fe(100),
Surf. Sci. **287/288**, 736 (1993).

[29] M. Wuttig, Y. Gauthier, S. Blügel,
Magnetically Driven Buckling and Stability of Ordered Surface Alloys: Cu(100) c(2 x 2) Mn,
Phys. Rev. Lett. **70**, 3619 (1993).

[30] M. Weinert, S. Blügel, and P. D. Johnson,
Comment on "Ferromagnetism of the Rh(001) Surface",
Phys. Rev. Lett. **71**, 4097 (1993).

[31] O. Rader, E. Vescovo, J. Redinger, S. Blügel, C. Carbone, W. Eberhardt, and W. Gudat,
Fe-Induced Magetization of Pd: The Role of Modified Pd Surface States,
Phys. Rev. Lett. **72**, 2247 (1994).

[32] S. Eisebitt, J.-E. Rubensson, M. Nicodemus, T. Böske, S. Blügel, W. Eberhardt, K. Radermacher S. Mantl, G. Bihlmayer,
Electronic structure of buried α-$FeSi_2$ and β-$FeSi_2$: Soft-x-ray-emission and -absorption studies compared to bandstructure calculations,
Phys. Rev. B **50**, 18330 (1994).

[33] S. Blügel,
Magnetism of 4d and 5d Transition Metal Adlayers on Ag(001): Dependence on the Adlayer Thickness,
Phys. Rev. B **51**, 2025 (1995).

[34] E. Vescovo, O. Rader, J. Redinger, S. Blügel, C. Carbone,
Two-Dimensional Spin-Polarized States of Ag on Fe(100),
Phys. Rev. B **51**, 12418 (1995).

[35] J. Redinger, R. Podloucky, S. Blügel,
Ferromagnetism of 4d and 5d Transition Metal Monolayers on Ag(111),
Phys. Rev. B **51**, 13852 (1995).

[36] M. Wuttig, S. Junghans, T. Flores, S. Blügel,
Comment on "Structure of the Mn-induced Cu(100)c(2 x 2) Mn surface",
Phys. Rev. B **53**, 7551 (1996).

[37] Ph. Ebert, B. Engels, P. Richard, K. Schroeder, S. Blügel, C. Domke, M. Heinrich, K. Urban,
Contribution of surface resonances to STM images: (110) surfaces of III-V compound semiconductors,
Phys. Rev. Lett. **77**, 2997 (1996).

[38] S. Blügel,
Magnetically stabilized surface alloys,
Appl. Phys. A **63**, 595 (1996).

[39] O. Rader, W. Gudat, C. Carbone, E. Vescovo, R. Kläsges, S. Blügel, R. Kläsges, W. Eberhardt, M. Wuttig, J. Redinger, F. J. Himpsel,
Electronic Structure of two-dimensional magnetic alloys: c(2 x2) Mn on Cu(100) and Ni(100),
Phys. Rev. B **55**, 5404 (1997).

[40] O. Rader, E. Vescovo, M. Wuttig, D. D. Sarma, S. Blügel, F. J. Himpsel, A. Kimura, K. S. An, T. Mizokawa, A. Fujimori, and C. Carbone,
Correlation satellite driven by reduced dimensionality,
Europhys. Lett. **39**, 429 (1997).

[41] W. Wolf, G. Bihlmayer, and S. Blügel,
Electronic structure of the Nowotny chimney-ladder silicide Ru_2Si_3,
Phys. Rev. B **55**, 6918 (1997).

[42] T. Asada and S. Blügel,
First Principles Calculation of Cu(100)c(2 x 2) 3d Surface Alloys Formation Energy: Improvement by Generalized Gradient Approximation,
Physica B **237-238**, 359 (1997).

[43] S. Eisebitt, J. Lüning, J.-E. Rubensson, D. Schmitz, S. Blügel, and W. Eberhardt,
Dichroism and Spin Information in Soft X-ray Emission,
Solid State Commun. **104**, 173 (1997).

[44] B. Voigtländer, V. Scheuch, H. P. Bonzel, S. Heinze and S. Blügel,
Chemical identification of atoms at multicomponent surfaces on an atomistic scale: $CoSi_2$(100),
Phys. Rev. B **55**, R13444 (1997).

[45] T. Asada and S. Blügel,
Total Energy spectra of complete sets of magnetic states for Fe films on Cu(100),
Phys. Rev. Lett. **79**, 507 (1997).

[46] Ch. Ross, M. Wuttig, Y. Gauthier, G. Bihlmayer, and S. Blügel,
Structure, Growth and Magnetism of Mn on Cu(110),
Phys. Rev. B **57**, 2607 (1998).

[47] S. Handschuh and S. Blügel,
Magnetic Exchange Coupling of 3d Metal Monolayers on Fe(001),
Solid State Commun. **105**, 633 (1998).

[48] K. Schroeder, B. Engels, P. Richard, and S. Blügel,
Re-exchange controlled Diffusion in Surfactant-mediated Epitaxial Growth: Si on As-terminated Si(111),
Phys. Rev. Lett. **80**, 2873 (1998).

[49] I. Turek, S. Blügel, and J. Kudrnovsky,
Magnetic nature of (100) surfaces of bcc RuV, RhV, and PdV binary alloys,
Phys. Rev. B **57**, R11065 (1998).

[50] B. Engels, P. Richard, K. Schroeder, S. Blügel, Ph. Ebert, and K. Urban,
Comparison between ab initio theory and scanning tunneling microscopy for (110) surfaces of III-V semiconductors,
Phys. Rev. B **58**, 7799 (1998).

[51] S. Heinze, S. Blügel, R. Pascal, M. Bode, R. Wiesendanger,
Prediction of Corrugation Reversal in STM-images of bcc-(110)-surfaces: W(110), Ta(110), Fe(110),
Phys. Rev. B **58**, 16432 (1998).

[52] I. Turek, J. Kudrnovský, S. Blügel,
Surface magnetism of disordered alloys,
Acta Physica Slovaca **48**, 6, 723-726 (1998).

[53] M. Asato, A. Settels, T. Hoshino, T. Asada, S. Blügel, R. Zeller, and P. H. Dederichs,
Full Potential KKR-calculations for Metals and Semiconductors,
Phys. Rev. B **60**, 5202 (1999).

[54] S. Heinze, X. Nie, S. Blügel, and M. Weinert,
Electric Field Induced Changes in STM Images of Metal Surfaces,
Chem. Phys. Lett. **315**, 167 (1999).

[55] S. Heinze, R. Abt, S. Blügel, G. Gilarowski, and H. Niehus,
STM-Images of transition-metal structures buried below noblemetal surfaces,
Phys. Rev. Lett. **83**, 4808 (1999).

[56] D. Wortmann, S. Heinze, G. Bihlmayer, and S. Blügel,
Interpreting STM-images of the MnCu/Cu(100) surface alloy,
Phys. Rev. B **62**, 2862 (2000).

[57] G. Bihlmayer, Ph. Kurz, and S. Blügel,
Overlayers, interlayers, and surface alloys of Mn on a Cu(111) surface,
Phys. Rev. B **62**, 4726 (2000).

[58] S. Heinze, M. Bode, A. Kubetzka, O. Pietzsch, X. Nie, S. Blügel, and R. Wiesendanger, *Real-Space Imaging of Antiferromagnetism on the Atomic Scale,* Science **288**, 1805 (2000).

[59] C. Pampuch, O. Rader, T. Kachel, W. Gudat, C. Carbone, R. Kläsges, G. Bihlmayer, S. Blügel, and W. Eberhardt, *One-dimensional spin-polarized quantum-wire states in Au on Ni(110),* Phys. Rev. Lett. **85**, 2561 (2000).

[60] G. Bihlmayer, T. Asada, and S. Blügel, *Electronic and magnetic structure of the (001)-surfaces of V, Cr, and V/Cr,* Phys. Rev. B **62**, R11937 (2000).

[61] Ph. Kurz, G. Bihlmayer, K. Hirai, and S. Blügel, *Three-dimensional spin structure on a two-dimensional lattice,* Phys. Rev. Lett. **86**, 1106 (2001).

[62] S. Clarke, G. Bihlmayer, S. Blügel, *Chemical Effects in Rare Gas Adsorption,* Phys. Rev. B **63**, 085416 (2001).

[63] Ph. Kurz, G. Bihlmayer, S. Blügel, K. Hirai, T. Asada, *Comment on "Ultrathin Mn films on Cu(111) substrates: Frustrated antiferromagnetic order",* Phys. Rev. B **63**, 096401 (2001).

[64] D. Wortmann, S. Heinze, Ph. Kurz, G. Bihlmayer, S. Blügel, *Resolving Complex Atomic-Scale Spin-Structures by SP-STM,* Phys. Rev. Lett. **86**, 4132 (2001).

[65] S. Link, H. A. Dürr, G. Bihlmayer, S. Blügel, W. Eberhardt, E. V. Chulkov, V. M. Silkin, P. M. Echenique, *Elektron dynamics of image potential states on the clean and oxygem covered Pt(111) surface,* Phys. Rev. B **63**, 115420 (2001).

[66] H.-J. Kim, E. Vescovo, S. Heinze, S. Blügel, *Surface electronic structure of Fe(110): the importance of surface resonances,* Surf. Sci. **478**, 193 (2001).

[67] S. Heinze, G. Bihlmayer, and S. Blügel, *First-Principles Interpretation of Scanning Tunneling Microscopy applied to Transition-Metal Surfaces: Buried CuIr/Cu(100) Surface Alloys,* Phys. Stat. Sol. (A) **187**, 215 (2001).

[68] S. Heinze, Ph. Kurz, D. Wortmann, G. Bihlmayer, and S. Blügel, *Complex Magnetism in Ultra-Thin Films: Atomic-Scale Spin Structures and Resolution by the Spin-Polarized Scanning Tunneling Microscope,* Appl. Phys. A **75**, 25 (2002).

[69] D. Wortmann, H. Ishida, and S. Blügel,
An ab initio Green-function formulation of the transfer matrix: Application to complex bandstructures,
Phys. Rev. B **65**, 165103 (2002).

[70] K. Schroeder, A. Antons, R. Berger, and S. Blügel,
Surfactant mediated heteroepitaxy versus homoepitaxy: Kinetics for group-IV adatoms on As-passivated Si(111),
Phys. Rev. Lett. **88**, 046101 (2002).

[71] I. Galanakis, G. Bihlmayer, V. Bellini, N. Papanikolaou, R. Zeller, S. Blügel and P. H. Dederichs,
Broken bond counting rule for the surface energies of noble metals,
Europhys. Lett. **58**, 751 (2002).

[72] D. Wortmann, Ph. Kurz, S. Heinze, K. Hirai, G. Bihlmayer and S. Blügel,
Resolving noncollinear magnetism by spin-polarized scanning tunnelling microscopy,
J. Magn. Magn. Mater. **240**, 57-63, (2002).

[73] M. Bode, S. Heinze, M. Hennefarth, O. Pietzsch, A. Kubetzka, M. Getzlaff, R. Wiesendanger, X. Nie, G. Bihlmayer, and S. Blügel,
Structural, electronic, and magnetic properties of a Mn monolayer on W(110),
Phys. Rev. B **66**, 014425 (2002).

[74] D. Wortmann, H. Ishida, and S. Blügel,
An embedded Green-function approach to the ballistic electron transport through an interface,
Phys. Rev. B **66**, 075113 (2002).

[75] A. Hirnet, K. Schroeder, S. Blügel, X. Torrelles, M. Albrecht, B. Jenichen, M. Gierer, and W. Moritz,
A novel Sb induced reconstruction of the (113) surface of Ge,
Phys. Rev. Lett. **88**, 226102 (2002).

[76] A. Antons, K. Schroeder, B. Voigtländer, V. Cherepanov, R. Berger, S. Blügel,
Element Specific Surface Reconstructions of Islands During Surfactant-Mediated Growth on Si(111),
Phys. Rev. Lett. **89**, 236101 (2002).

[77] M. Bode, S. Heinze, A. Kubetzka, O. Pietzsch, X. Nie, G. Bihlmayer, S. Blügel, and R. Wiesendanger,
Magnetization-direction-dependent local electronic structure probed by scanning tunneling spectroscopy,
Phys. Rev. Lett. **89**, 237205 (2002).

[78] Ph. Kurz, G. Bihlmayer and S. Blügel,
Magnetism and electronic structure of hcp Gd and the Gd(0001) surface,
J. Phys.: Condens. Matter **14**, 6353 (2002).

[79] Y. Cao, J. Zheng-Kuan, A. Antons, K. Schroeder, S. Blügel,
Relaxation of small molecules, an ab initio study,
Communications in Theoretical Physics **37**, 597 (2002).

[80] Y. Cao, J. Zheng-Kuan, A. Antons, K. Schroeder, S. Blügel,
Stable structure of Sb monolayer on a strained Ge(111) substrate,
Chinese Physics Letters **19**, 259 (2002).

[81] K. Schroeder, A. Antons, R. Berger, S. Blügel,
Ad-atom kinetics on surfactant-covered Si(111), ab initio calculations,
Phase Transitions **75**, 1-2, 91-99 (2002).

[82] Ph. Kurz, G. Bihlmayer, K. Hirai, S. Blügel,
Itinerant magnets on a triangular Cu(111) lattice,
Phase Transitions **75**, 1-2, 101-112 (2002).

[83] A. Antons, Y. Cao, K. Schroeder, R. Berger, W. Kromen, S. Blügel,
Strain-induced surface structures on Sb-covered Ge(111): Epitaxial Ge films on Si(111):Sb,
Europhys. Lett. **62**, 547 (2003).

[84] M. Bode, S. Heinze, A. Kubetzka, O. Pietzsch, X. Nie, G. Bihlmayer, S. Blügel, and R. Wiesendanger,
Spin-Orbit Induced Local Band Structure Variations revealed by Scanning Tunneling Spectroscopy,
J. Phys.: Condens. Matter **15**, 679 (2003).

[85] I. Turek, J. Kudrnovsky, G. Bihlmayer, and S. Blügel,
Ab initio theory of exchange interactions and the Curie temperature of Gd metal,
J. Phys.: Condens. Matter **15**, 2771 (2003).

[86] C. Busse, S. Baud, G. Bihlmayer, C. Polop, T. Michely, and S. Blügel,
Tunneling voltage dependent heights of faulted and unfaulted Ir islands on Ir(111),
Phys. Rev. B **68**, 201401(R) (2003).

[87] J. Klijn, L. Sacharow, Ch. Meyer, S. Blügel, M. Morgenstern, and R. Wiesendanger,
STM measurements on the InAs(110) surface directly compared with surface electronic structure calculations,
Phys. Rev. B **68**, 205327 (2003).

[88] I. Turek, J. Kudrnovsky, M. Divis, P. Franek, G. Bihlmayer, and S. Blügel,
A first-principles study of electronic structure and exchange interactions in bcc Europium,
Phys. Rev. B **68**, 224431 (2003).

[89] K. von Bergmann, M. Bode, A. Kubetzka, M. Heide, S. Blügel, R. Wiesendanger,
Spin-polarized electron scattering at single oxygen adsorbates on a magnetic surface,
Phys. Rev. Lett. **92**, 046801 (2004).

[90] Ph. Kurz, F. Förster, L. Nordström, G. Bihlmayer, and S. Blügel,
Ab initio treatment of non-collinear magnets with the full-potential linearized augmented planewave method,
Phys. Rev. B **69**, 024415 (2004).

[91] L. Sacharow, M. Morgenstern, G. Bihlmayer, and S. Blügel,
High spin polarization at the interface between a Fe monolayer and InAs(110),

Phys. Rev. B **69**, 085317 (2004).

[92] J. L. F. Da Silva, K. Schroeder, S. Blügel,
First-principles investigation of the multilayer relaxation of stepped Cu surfaces,
Phys. Rev. B **69**, 245411 (2004).

[93] J. Wiebe, L. Sacharow, S. Blügel, M. Morgenstern, A. Wachowiak, G. Bihlmayer, S. Blügel, and R. Wiesendanger,
Scanning Tunneling Spectroscopy on Cobalt(0001): Spectroscopy Signature of Stacking Faults and Dislocation Lines,
Phys. Rev. B **70**, 035404 (2004).

[94] S. Di Napoli, A. M. Llois, G. Bihlmayer, S. Blügel, M. Alouani and H. Dreyssé,
Magnetic structure and transport properties of noncollinear $LaMn_2X_2$ (X=Ge, Si) systems,
Phys. Rev. B **70**, 174418 (2004).

[95] S. Baud, C. Ramseyer, G. Bihlmayer, S. Blügel, C. Barreteau, M. C. Desjonquères, and D. Spanjaard,
Comparative study of ab initio and tight-binding electronic structure calculations applied to Platinum surfaces,
Phys. Rev. B **70**, 235423 (2004).

[96] Yu. M. Koroteev, G. Bihlmayer, J. E. Gayone, E. V. Chulkov, S. Blügel, P. M. Echenique, and Ph. Hofmann,
Strong Spin-Orbit Splitting on Bi Surfaces,
Phys. Rev. Lett. **93**, 046403 (2004).

[97] J. L. F. Da Silva, K. Schroeder, S. Blügel,
Trend for the multilayer relaxation sequence of stepped Cu surfaces,
Phys. Rev. B **70**, 245432 (2004).

[98] S. di Napoli, G. Bihlmayer, S. Blügel, M. Alouani, H. Dreyssé, A. M. Llois,
Noncollinear magnetism in $LaMn_2Ge_2$ and $LaMn_2Si_2$ compounds,
J. Magn. Magn. Mat. **272-276**, Suppl. 1, e265 - e266 (2004).

[99] D. Wortmann, G. Bihlmayer, and S. Blügel,
Ab initio calculations of interface effects in tunneling through MgO barriers on Fe(100),
J. Phys.: Condens. Matter **16**, 5819 (2004).

[100] J. I. Pascual, G. Bihlmayer, Yu. M. Koroteev, H.-P. Rust, G. Ceballos, M. Hansmann, K. Horn, E. V. Chulkov, S. Blügel, P. M. Echenique, and Ph. Hofmann,
Role of Spin in Quasiparticle Interference,
Phys. Rev. Lett. **93**, 196802 (2004).

[101] O. Krupin, G. Bihlmayer, K. Starke, J. E. Prieto, K. M. Döbrich, S. Blügel, G. Kaindl,
Rashba Effect at Magnetic Metal Surfaces,
Phys. Rev. B **71**, 201403 (2005).

[102] I. Galanakis, M. Ležaić, G. Bihlmayer and S. Blügel,
Interface properties of the NiMnSb/InP and NiMnSb/GaAs contacts,
Phys. Rev. B **71**, 214431 (2005).

[103] A. Kubetzka, P. Ferriani, M. Bode, S. Heinze, G. Bihlmayer, K. v. Bergmann, O. Pietzsch, S. Blügel, R. Wiesendanger,
Revealing Antiferromagnetic Order of the Fe Monolayer on W(001): First-Principles Calculations and Spin-Polarized Scanning Tunneling Microscopy,
Phys. Rev. Lett. **94**, 087204 (2005).

[104] O. Rader, M. Ležaić, S. Blügel, A. Fujimori, A. Kimura, N. Kamakura, A. Kakizaki, S. Miyanishi, H. Akinaga,
Spin-polarized surface state of MnSb(0001),
New J. Phys. **7**, 111 (2005).

[105] P. Ferriani, S. Heinze, G. Bihlmayer and S. Blügel,
New trend of magnetic order of 3d transition-metal monolayers on W(001),
Phys. Rev. B **72**, 024452 (2005).

[106] J. L. F. Da Silva, K. Schroeder, and S. Blügel,
First-principles investigation of the role of registry relaxations on stepped Cu(100) surfaces,
Phys. Rev. B **72**, 033405 (2005).

[107] V. Caciuc, S. Blügel, and H. Hölscher,
Ab initio investigation of NC-AFM image contrast on InAs(110) surface,
Phys. Rev. B **72**, 035423 (2005).

[108] Y. Mokrousov, G. Bihlmayer and S. Blügel,
A full-potential linearized augmented plane-wave method for one-dimensional systems: gold nanowire and iron monowires in a gold tube,
Phys. Rev. B **72**, 045402 (2005).

[109] M. Bowen, A. Barthélémy, M. Bibes, E. Jacquet, J. P. Contour, A. Fert, D. Wortmann and S. Blügel,
Half-metallicity proven using fully spin-polarized tunneling,
J. Phys.: Condens. Matter **17**, L405 (2005).

[110] M. Ležaić, I. Galanakis, G. Bihlmayer, and S. Blügel,
Structural and magnetic properties of the (001) and (111) surfaces of the half-metal NiMnSb,
J. Phys.: Condens. Matter **17**, 3121 (2005).

[111] P. Mavropoulos, M. Ležaić, and S. Blügel,
Half-metallic ferromagnets in tunneling magnetoresistance junctions,
Phys. Rev. B **72**, 174428 (2005).

[112] J. Wiebe, F. Meier, K. Hashimoto, G. Bihlmayer, S. Blügel, P. Ferriani, S. Heinze, and R. Wiesendanger,
An Unoccupied Surface State on Pt(111) Studied by Scanning Tunneling Spectroscopy,
Phys. Rev. B **72**, 193406 (2005).

[113] S. Lounis, P. Mavropoulos, S. Blügel and P. H. Dederichs,
Non-collinear Korringa-Kohn-Rostocker Green function method: Application to 3d nanostructures on Ni(001),
Phys. Rev. B **72**, 224437 (2005).

[114] W. Welnic, A. Pamungkas, R. Detemple, Ch. Steimer, S. Blügel, and M. Wuttig,
Unravelling the interplay of local structure and physical properties in phase-change materials,
Nature Materials **5**, 56 (2006).

[115] P. Mavropoulos, S. Lounis, R. Zeller, and S. Blügel,
Fe clusters on Ni and Cu substrates: Size, shape and orientation dependence of the spin moment,
Appl. Phys. A **82**, 103 (2006).

[116] S. Baud, Ch. Ramseyer, G. Bihlmayer and S. Blügel,
Relaxation effects on the magnetism of decorated step edges: Co/Pt(664),
Phys. Rev. B **73**, 104427 (2006).

[117] V. Caciuc, H. Hölscher, S. Blügel, and H. Fuchs,
Atomic-scale sharpening of silicon tips in non-contact atomic force microscopy,
Phys. Rev. Lett. **96**, 016101 (2006).

[118] J. L. F. Da Silva, K. Schroeder, S. Blügel,
Linear scaling of the interlayer relaxations of the vicinal Cu(p, p, p-2) surfaces with the number of atom-rows in the terraces,
Surf. Sci. **600**, 3008 (2006).

[119] G. Bihlmayer, Yu. M. Koroteev, P. M. Echenique, E. V. Chulkov, S. Blügel,
The Rashba-effect at metallic surfaces,
Surf. Sci. **600**, 3888 (2006).

[120] S. Baud, G. Bihlmayer, S. Blügel, and Ch. Ramseyer,
First-principles investigation of Co wires at Pt(111) step-edges,
Surf. Sci. **600,** 4301 (2006).

[121] M. Ležaić, P. Mavropoulos, G. Bihlmayer and S. Blügel,
Scanning tunneling microscopy of surfaces of half-metals: an ab initio study,
J. Phys. D: Appl. Phys. **39**, 797 (2006).

[122] J. L. F. Da Silva, C. Barreteau, K. Schroeder, S. Blügel,
All-electron first-principles investigations of the energetics of vicinal Cu surfaces,
Phys. Rev. B **73**, 125402 (2006).

[123] Y. Mokrousov, G. Bihlmayer, S. Heinze and S. Blügel,
Giant magneto-crystalline anisotropies of 4d transition-metal monowires,
Phys. Rev. Lett. **96**, 147201 (2006).

[124] K. v. Bergmann, S. Heinze, M. Bode, E. Y. Vedmedenko, G. Bihlmayer, S. Blügel, R. Wiesendanger,
Observation of a complex nano-scale magnetic structure in a hexagonal Fe monolayer,
Phys. Rev. Lett. **96**, 167203 (2006).

[125] L. Chioncel, P. Mavropoulos, M. Ležaić, S. Blügel, E. Arrigoni, M. I. Katsnelson, and A. I. Lichtenstein,
Half-Metallic Ferromagnetism Induced by Dynamic Electron Correlations in VAs,

Phys. Rev. Lett. **96**, 197203 (2006).

[126] S. Lounis, P. Mavropoulos, P. H. Dederichs, and S. Blügel,
Surface-state scattering by adatoms on noble metals: Ab initio calculations using the Korringa-Kohn-Rostoker Green function method,
Phys. Rev. B **73**, 195421 (2006).

[127] T. Ohwaki, D. Wortmann, H. Ishida, S. Blügel, K. Terakura,
Spin-polarized field-emission from Ni(001) and Ni(111) surfaces,
Phys. Rev. B **73**, 235424 (2006).

[128] C. Friedrich, A. Schindlmayr, S. Blügel, T. Kotani,
Elimination of the linearization error in GW calculations based on the linearized augmented-plane-wave method,
Phys. Rev. B **74**, 045104 (2006).

[129] M. Ležaić, P. Mavropoulos, J. Enkovaara, G. Bihlmayer and S. Blügel,
Thermal collapse of spin-polarization in half-metallic ferromagnets,
Phys. Rev. Lett. **97**, 026404 (2006).

[130] S. Picozzi, K. Yamauchi, G. Bihlmayer, S. Blügel,
First-principles stabilization of an unconventional collinear magnetic ordering in distorted manganites,
Phys. Rev. B **74**, 094402 (2006).

[131] P. Moras, L. Ferrari, C. Spezzani, S. Gardonio, M. Ležaić, P. Mavropoulos, S. Blügel, and C. Carbone,
Probing quasiparticle states bound by disparate periodic potentials,
Phys. Rev. Lett. **97**, 206802 (2006).

[132] Y. Mokrousov, N. Atodiresei, G. Bihlmayer, S. Blügel,
Magnetic anisotropy energies of metal-benzene sandwiches,
Int. J. Quantum Chem. **106**, 3208 (2006).

[133] O. Andreyev, Yu. M. Koroteev, M. Sánchez Albaneda, M. Cinchetti, G. Bihlmayer, E. V. Chulkov, J. Lange, F. Steeb, M. Bauer, P. M. Echenique, S. Blügel, M. Aeschlimann,
Spin-resolved two-photon photoemission study of the surface resonance state on Co/Cu(001),
Phys. Rev. B **74**, 195416 (2006).

[134] S. R. Woodford, A. Bringer, and S. Blügel,
Interpreting magnetization from Faraday rotation in birefringent, magnetic media,
J. Appl. Phys. **101**, 053912 (2007).

[135] P. A. Loukakos, M. Lisowski, G. Bihlmayer, S. Blügel, M. Wolf, U. Bovensiepen,
Dynamics of the self-energy of the Gd(0001) surface state probed by femtosecond photoemission spectroscopy,
Phys. Rev. Lett. **98**, 097401 (2007).

[136] M. Bowen, J.-L. Maurice, A. Barthélémy, M. Bibes, D. Imhoff, V. Bellini, R. Bertacco, D. Wortmann, P. Seneor, E. Jacquet, A. Vaurès, J. Humbert, J. P. Contour, C. Colliex,

S. Blügel and P. H. Dederichs,
Using half-metallic manganite interfaces to reveal insights into spintronics,
J. Phys.: Condens. Matter **19**, 315208 (2007).

[137] S. Di Napoli, A. M. Lois, G. Bihlmayer, and S. Blügel,
Magnetic order in RMn_2Ge_2 (R=Y,Ca) compounds and their solid solutions with $LaMn_2Ge_2$,
Phys. Rev. B **75**, 104406 (2007).

[138] Y. Mokrousov, G. Bihlmayer, S. Blügel and S. Heinze,
Magnetic order and exchange interactions in monoatomic 3d transitionmetal chains,
Phys. Rev. B **75**, 104413 (2007).

[139] M. Bode, M. Heide, K. von Bergmann, S. Heinze, G. Bihlmayer, A. Kubetzka,
O. Pietzsch, S. Blügel, R. Wiesendanger,
Chiral magnetic order at surfaces driven by inversion asymmetry,
Nature **447**, 190 (2007).

[140] M. Ležaić, P. Mavropoulos and S. Blügel,
First-principles prediction of high Curie temperature for ferromagnetic bcc-Co and bcc-FeCo alloys and its relevance to tunnelling magnetoresistance,
Appl. Phys. Lett. **90**, 082504 (2007).

[141] S. Lounis, P. Mavropoulos, R. Zeller, P. H. Dederichs, and S. Blügel,
Noncollinear magnetism of Cr and Mn nanoclusters on Ni(111): Changing the magnetic configuration atom by atom,
Phys. Rev. B **75**, 174436 (2007).

[142] G. Bihlmayer, S. Blügel and E. V. Chulkov,
Enhanced Rashba spin-orbit splitting in Bi/Ag(111) and Pb/Ag(111) surface alloys,
Phys. Rev. B **75**, 195414 (2007).

[143] M. De Santis, Y. Gauthier, H. C. N. Tolentino, G. Bihlmayer, S. Blügel, V. Langlais,
Structure and magnetic properties of Mn/Pt(110)-(1×2): A joint x-ray diffraction and theoretical study,
Phys. Rev. B **75**, 205432 (2007).

[144] P. Ferriani, I. Turek, S. Heinze, G. Bihlmayer, and S. Blügel,
Magnetic Phase Control in Monolayer Films by Substrate Tuning,
Phys. Rev. Lett. **99**, 187203 (2007).

[145] K. M. Döbrich, G. Bihlmayer, K. Starke, J. E. Prieto, K. Rossnagel, H. Koh, E. Rotenberg,
S. Blügel, G. Kaindl,
Electronic band structure and Fermi surface of ferromagnetic Tb: Experiment and theory,
Phys. Rev. B **76**, 035123 (2007).

[146] J. Enkovaara, D. Wortmann, S. Blügel,
Spin-polarized tunneling between an antiferromagnet and a ferromagnet: First-principles calculations and transport theory,
Phys. Rev. B **76**, 054437 (2007).

[147] N. Atodiresei, V. Caciuc, K. Schroeder, S. Blügel,
First-principles investigation of terephthalic acid on Cu(110),
Phys. Rev. B **76**, 115433 (2007).

[148] M.-H. Liu, G. Bihlmayer, S. Blügel, Ch.-R. Chang,
Intrinsic spin-Hall accumulation in honeycomb lattices: Band structure effects,
Phys. Rev. B **76**, 121301(R) (2007).

[149] A. Hanuschkin, D. Wortmann, S. Blügel,
Image potential and field states at Ag(100) and Fe(110) surfaces,
Phys. Rev. B **76**, 165417 (2007).

[150] K. v. Bergmann, S. Heinze, M. Bode, G. Bihlmayer, S. Blügel, R. Wiesendanger,
Complex magnetism of the Fe monolayer on Ir(111),
New J. Phys. **9**, 396 (2007).

[151] Y. Mokrousov, N. Atodiresei, G. Bihlmayer, S. Heinze, S. Blügel,
Interplay of structure and spin-orbit strength in magnetism of metal-benzene sandwiches: from single molecules to infinite wires,
Nanotechnology **18**, 495402 (2007).

[152] N. Atodiresei, V. Caciuc, H. Hölscher, S. Blügel,
Ab initio modeling of noncontact atomic force microscopy imagingof benzene on Cu(110) surface,
Int. J. Quantum Chem. **108**, 2803 (2008).

[153] N. Atodiresei, P. H. Dederichs, Y. Mokrousov, L. Bergqvist, G. Bihlmayer, S. Blügel,
Controlling the magnetization direction in molecules via their oxidation state,
Phys. Rev. Lett. **100**, 117207 (2008).

[154] Yu. M. Koroteev, G. Bihlmayer, E. V. Chulkov, S. Blügel,
First-principles investigation of structural and electronic properties of ultrathin Bi films,
Phys. Rev. B **77**, 045428 (2008).

[155] K. Yamauchi, F. Freimuth, S. Blügel, E. Dagotto, S. Picozzi,
Magnetically-induced ferroelectricity in orthorhombic manganites: microscopic origin and chemical trends,
Phys. Rev. B **78**, 014403 (2008).

[156] F. Freimuth, Y. Mokrousov, D. Wortmann, S. Heinze, S. Blügel,
Maximally Localized Wannier Functions within the FLAPW formalism,
Phys. Rev. B **78**, 035120 (2008).

[157] N. Atodiresei, V. Caciuc, S. Blügel, H. Hölscher,
Manipulation of benzene on Cu(110) by dynamic force microscopy: An ab initio study,
Phys. Rev. B **78**, 045411 (2008).

[158] S. Lounis, M. Reif, P. Mavropoulos, L. Glaser, P. H. Dederichs, M. Martins, S. Blügel, W. Wurth,
Non-collinear magnetism of Cr nanostructures on Fe3ML/Cu(001): First principles and experimental investigations,
Europhys. Lett. **81**, 47004 (2008).

[159] P. Ferriani, K. von Bergmann, E. Y. Vedmedenko, S. Heinze, M. Bode, M. Heide, G. Bihlmayer, A. Kubetzka, S. Blügel, R. Wiesendanger,
Atomic-Scale Spin Spiral with Unique Rotational Sense: Mn Monolayer on W(001),
Phys. Rev. Lett. **101**, 027201 (2008).

[160] P. H. Zhou, P. Moras, L. Ferrari, G. Bihlmayer, S. Blügel, C. Carbone,
One-Dimensional 3d Electronic Bands of Monatomic Cu Chains,
Phys. Rev. Lett. **101**, 036807 (2008).

[161] M. Heide, G. Bihlmayer, S. Blügel,
Dzyaloshinskii-Moriya interaction accounting for the orientation of magnetic domains in ultrathin films: Fe/W(110),
Phys. Rev. B **78**, 140403(R) (2008).

[162] S. Lounis, P. H. Dederichs, S. Blügel,
Magnetism of Nanowires Driven by Novel Even-Odd Effects,
Phys. Rev. Lett. **101**, 107204 (2008).

[163] A. Thiess, Y. Mokrousov, S. Blügel, S. Heinze,
Theory and application of chain formation in break junctions,
Nano Letters **8**, 2144 (2008).

[164] O. Krupin, G. Bihlmayer, K. M. Döbrich, J. E. Prieto, K. Starke, S. Gorovikov, S. Blügel, S. Kevan, G. Kaindl,
Rashba effect at the surfaces of rare-earth metals and their monoxides,
New J. Phys. **11,** 013035 (2009).

[165] A. Weismann, M. Wenderoth, S. Lounis, P. Zahn, N. Quaas, R. G. Ulbrich, P. H. Dederichs, S. Blügel,
Seeing the Fermi-surface in Real Space by Nanoscale Electron Focusing,
Science **323,** 1190 (2009).
and
Advanced Functional Materials **19**, 10 (2009).

[166] P. Ferriani, K. von Bergmann, E. Y. Vedmedenko, S. Heinze, M. Bode, M. Heide, G. Bihlmayer, S. Blügel, R. Wiesendanger,
Erratum: Atomic-Scale Spin Spiral with a Unique Rotational Sense: Mn Monolayer on W(001),
Phys. Rev. Lett. **102**, 019901(E) (2009).

[167] N. Atodiresei, V. Caciuc, P. Lazic, S. Blügel,
Chemical versus van der Waals Interaction: The Role of the Heteroatom in the Flat Absorption of Aromatic Molecules C6H6, C5NH5, and C4N2H4 on the Cu(110) Surface,
Phys. Rev. Lett. **102,** 136809 (2009).

[168] C. Friedrich, A. Schindlmayr, S. Blügel,
Efficient calculation of the Coulomb matrix and its expansion around k=0 within the FLAPW method,
Computer Physics Communications **180**, 347 (2009).

[169] M. Heide, G. Bihlmayer, S. Blügel,
Describing Dzyaloshinskii-Moriya spirals from first principles,
Physica B: Condensed Matter **404,** 2678 (2009).

[170] B. Hardrat, A. Al-Zubi, P. Ferriani, S. Blügel, G. Bihlmayer, S. Heinze,
Complex Magnetism of Iron Monolayers on Hexagonal Transition Metal Surfaces from First Principles,
Phys. Rev. B **79**, 094411 (2009).

[171] C. Lennartz, N. Atodiresei, L. Müller-Meskamp, S. Karthäuser, R. Waser, S. Blügel,
Cu-adatom-mediated bonding in close-packed benzoate/Cu (110)-Systems,
Langmuir **25**, 856 – 864 (2009).

[172] P. Mavropoulos, M. Lezaic, S. Blügel,
Ferromagnetism in nitrogen-doped MgO: Density-functional calculations,
Phys. Rev. B **80**, 184403 (2009).

[173] P. Moras, D. Topwal, P. M. Sheverdyaeva, L. Ferrari, J. Fujii, G. Bihlmayer, S. Blügel, C. Carbone,
Influence of the substrate bands on the sp-levels topology of Ag films on Ge(111),
Phys. Rev. B **80**, 205418 (2009).

[174] A. Thiess, Y. Mokrousov, S. Heinze, S. Blügel,
Magnetically Hindered Chain Formation in Transition-Metal Break Junctions,
Phys. Rev. Lett. **103**, 217201 (2009).

[175] P. Lazic, M. Alaei, N. Atodiresei, V. Caciuc, R. Brako, S. Blügel,
Density functional theory with nonlocal correlation: A key to the solution of the CO adsorption puzzle,
Phys. Rev. B **81**, 045401 (2010).

[176] P. Lazic, N. Atodiresei, M. Alaei, V. Caciuc, S. Blügel, R. Brako,
JuNoLo – Jülich nonlocal code for parallel post-processing evaluation of vdW-DF correlation energy,
Computer Physics Communications **181**, 2, 371-379 (2010).

[177] E. Sasioglu, A. Schindlmayr, C. Friedrich, F. Freimuth, S. Blügel,
Wannier-function approach to spin excitations in solids,
Phys. Rev. B **81**, 054434 (2010).

[178] P. Mavropoulos, S. Lounis, S. Blügel,
Exchange coupling in transition-metal nanoclusters on Cu(001) and Cu(111) surfaces,
Physica Status Solidi B, **247**, 5, 1187–1196 (2010).

[179] L. Zhou, J. Wiebe, S. Lounis, E. Vedmedenko, F. Meier, S. Blügel, P. H. Dederichs, R. Wiesendanger,
Strength and directionality of surface Ruderman-Kittel-Kasuya-Yosida interaction mapped on the atomic scale,
Nature Physics **6**, 187 (2010).

[180] G. Bihlmayer, Y. M. Koroteev, E. V. Chulkov, S. Blügel,
Surface- and edge-states in ultrathin Bi-Sb films,

New Journal of Physics **12**, 065006 (2010).

[181] C. Friedrich, S. Blügel, A. Schindlmayr,
Efficient implementation of the GW approximation within the all-electron FLAPW method,
Phys. Rev. B **81**, 125102 (2010).

[182] J. Brede, N. Atodiresei, S. Kuck, P. Lazic, V. Caciuc, Y. Morikawa, G. Hoffmann, S. Blügel, R. Wiesendanger,
Spin- and Energy-Dependent Tunneling through a Single Molecule with Intramolecular Spatial Resolution,
Phys. Rev. Lett. **105**, 047204 (2010).

[183] N. Atodiresei, J. Brede, P. Lazic, V. Caciuc, G. Hoffmann, R. Wiesendanger, S. Blügel,
Design of the Local Spin Polarization at the Organic-Ferromagnetic Interface,
Phys. Rev. Lett. **105**, 066601 (2010).

[184] M. C. Lennartz, V. Caciuc, N. Atodiresei, S. Karthäuser, S. Blügel,
Electronic Mapping of Molecular Orbitals at the Molecule-Metal Interface,
Phys. Rev. Lett. **105**, 066801 (2010).

[185] C. Clavero, M. Bode, G. Bihlmayer, S. Blügel, R. A. Lukaszew,
Island-assisted interface alloying and magnetic polarization at submonolayer V/Cr(001) interfaces,
Phys. Rev. B **82**, 085445 (2010).

[186] A. Schindlmayr, C. Friedrich, E. Sasioglu, S. Blügel,
First-principles calculation of electronic excitations in solids with SPEX,
Zeitschrift für physikalische Chemie **224**, 357-368 (2010).

[187] P. Moras, D. Wortmann, G. Bihlmayer, L. Ferrari, G. Alejandro, P. H. Zhou, D. Topwal, P. M. Sheverdyaeva, S. Blügel, C. Carbone,
Probing the electronic transmission across a buried metal/metal interface,
Phys. Rev. B **82**, 155427 (2010).

[188] T. Ono, M. Heide, N. Atodiresei, P. Baumeister, S. Tsukamoto, S. Blügel,
Real-space electronic structure calculations with full-potential all-electron precision for transition metals,
Phys. Rev. B **82**, 205115 (2010).

[189] F. Freimuth, S. Blügel, Y. Mokrousov,
Anisotropic Spin Hall Effect From First Principles,
Phys. Rev. Lett. **105**, 246602 (2010).

[190] A. Al-Zubi, G. Bihlmayer, S. Blügel,
Magnetism of 3d transition-metal monolayers on Rh(100),
Phys. Rev. B **83**, 024407 (2011).

[191] S. Lounis, P. Zahn, A. Weismann, M. Wenderoth, R. G. Ulbrich, I. Mertig, P. H. Dederichs, S. Blügel,
Theory of real space imaging of Fermi surface parts,
Phys. Rev. B **83**, 035427 (2011).

[192] M. Betzinger, C. Friedrich, S. Blügel, A. Görling,
Local exact exchange potentials within the all-electron FLAPW method and a comparison with pseudopotential results,
Phys. Rev. B **83**, 045105 (2011).

[193] F. Meier, S. Lounis, J. Wiebe, L. Zhou, S. Heers, P. Mavropoulos, P. H. Dederichs, S. Blügel, R. Wiesendanger,
Spin polarization of platinum (111) induced by the proximity to cobalt nanostripes,
Phys. Rev. B **83**, 075407 (2011).

[194] C. Friedrich, M. C. T. D. Müller, S. Blügel,
Band convergence and linearization error correction of all-electron GW calculations: The extreme case of zinc oxide,
Phys. Rev. B **83**, 081101 (2011).

[195] M. Lezaic, P. Mavropoulos, S. Blügel, H. Ebert,
Complex magnetic behavior and high spin polarization in Fe3−xMnxSi alloys,
Phys. Rev. B **83**, 094434 (2011).

[196] M. Heide, G. Bihlmayer, S. Blügel,
Non-planar Dzyaloshinskii spirals and magnetic domain walls in non-centrosymmetric systems with orthorhombic anisotropy,
Journal of Nanoscience and Nanotechnology **11**, 3005 (2011).

[197] V. Caciuc, M. C. Lennartz, N. Atodiresei, S. Karthäuser, S. Blügel,
Fine tuning of the electronic structure of π -conjugated molecules for molecular electronics,
Nanotechnology **22**, 145701 (2011).

[198] H. Zhang, F. Freimuth, S. Blügel, Y. Mokrousov,
Role of Spin-Flip Transitions in the Anomalous Hall Effect of FePt Alloy,
Phys. Rev. Lett. **106**, 117202 (2011).

[199] D. Wortmann, S. Blügel,
Influence of the electronic structure on tunneling through ferroelectric insulators: Application to $BaTiO_3$ and $PbTiO3_3$,
Phys. Rev. B **83**, 155114 (2011).

[200] T. O. Wehling, E. Sasioglu, C. Friedrich, A. I. Lichtenstein, M. I. Katsnelson, S. Blügel,
Strength of Effective Coulomb Interactions in Graphene and Graphite,
Phys. Rev. Lett. **106**, 236805 (2011).

[201] C. Busse, P. Lazic, R. Djemour, J. Coraux, T. Gerber, N. Atodiresei, V. Caciuc, R. Brako, A. T. N'Diaye, S. Blügel, J. Zegenhagen, T. Michely,
Graphene on Ir(111): Physisorption with Chemical Modulation,
Phys. Rev. Lett. **107**, 036101 (2011).

[202] P. Kowalzik, N. Atodiresei, M. Gingras, V. Caciuc, S. Blügel, R. Waser, S. Karthäuser,
Single Electron Tunneling through a Tailored Arylthio-coronene,
Journal of Physical Chemistry C **115**, 18, 9204 (2011).

[203] H. Zhang, S. Blügel, Y. Mokrousov,
Anisotropic intrinsic anomalous Hall effect in ordered 3dPt alloys,
Phys. Rev. B **84**, 024401 (2011).

[204] C. Friedrich, M. C. T. D. Müller, S. Blügel,
Erratum: Band convergence and linearization error correction of all-electron GW calculations: The extreme case of zinc oxide [Phys. Rev. B 83, 081101(R) (2011)],
Phys. Rev. B **84**, 039906 (2011).

[205] K. M. Seemann, F. Freimuth, H. Zhang, S. Blügel, Y. Mokrousov, D. E. Bürgler, C. M. Schneider,
Origin of the Planar Hall Effect in Nanocrystalline Co(60)Fe(20)B(20),
Phys. Rev. Lett. **107**, 086603 (2011).

[206] R. Sakuma, C. Friedrich, T. Miyake, S. Blügel, F. Aryasetiawan,
GW calculations including spin-orbit coupling: Application to Hg chalcogenides,
Phys. Rev. B **84**, 085144 (2011).

[207] J. Weischenberg, F. Freimuth, J. Sinova, S. Blügel, Y. Mokrousov,
Ab Initio Theory of the Scattering-Independent Anomalous Hall Effect,
Phys. Rev. Lett. **107**, 106601 (2011).

[208] D. Bauer, P. Mavropoulos, S. Lounis, S. Blügel,
Thermally activated magnetization reversal in monatomic magnetic chains on surfaces studied by classical atomistic spin-dynamics simulations,
J. Phys.: Condens. Matter **23**, 394204 (2011).

[209] I. Slipukhina, P. Mavropoulos, S. Blügel, M. Lezaic,
Ferromagnetic Spin Coupling of 2p Impurities in Band Insulators Stabilized by an Intersite Coulomb Interaction: Nitrogen-Doped MgO,
Phys. Rev. Lett. **107**, 137203 (2011).

[210] H. Bentmann, T. Kuzumaki, G. Bihlmayer, S. Blügel, E. V. Chulkov, F. Reinert, K. Sakamoto,
Spin orientation and sign of the Rashba splitting in Bi/Cu(111),
Phys. Rev. B **84**, 115426 (2011).

[211] S. Tsukamoto, Y. Egami, K. Hirose, S. Blügel,
Stabilized scattering wave-function calculations using the Lippmann-Schwinger equation for long conductor systems,
Phys. Rev. B **84**, 115443 (2011).

[212] M. Schlipf, M. Betzinger, C. Friedrich, M. Lezaic, S. Blügel,
HSE hybrid functional within the FLAPW method and its application to GdN,
Phys. Rev. B **84**, 125142 (2011).

[213] A. Al-Zubi, G. Bihlmayer, S. Blügel,
Modeling magnetism of hexagonal Fe monolayers on 4d substrates,
Physica Status Solidi B **248**, 2242 (2011).

[214] T. Hirahara, G. Bihlmayer, Y. Sakamoto, M. Yamada, H. Miyazaki, S.-I. Kimura, S. Blügel, S. Hasegawa,

Interfacing 2D and 3D topological insulators: Bi(111) bilayer on Bi2Te3,
Phys. Rev. Lett. **107**, 166801 (2011).

[215] S. Heinze, K. von Bergmann, M. Menzel, J. Brede, A. Kubetzka, R. Wiesendanger, G. Bihlmayer, and S. Blügel,
Spontaneous atomic-scale magnetic skyrmion lattice in two dimensions,
Nature Physics **7**, 713 (2011).

[216] N. Atodiresei, V. Caciuc, P. Lazic, S. Blügel,
Engineering the magnetic properties of hybrid organic-ferromagnetic interfaces by molecular chemical functionalization,
Phys. Rev. B **84**, 172402 (2011).

[217] D. Popova, A. Bringer, S. Blügel,
Theory of the inverse Faraday effect in view of ultrafast magnetization experiments,
Phys. Rev. B **84**, 214421 (2011).

[218] P. Kowalzik, N. Atodiresei, M. Gingras, V. Caciuc, N. Schnaebele, J.-M. Raimundo, S. Blügel, R. Waser, S. Karthäuser,
Arylthio-substituted coronenes as tailored building blocks for molecular electronics,
Physical Chemistry Chemical Physics **14**, 1635-1641 (2012).

[219] H. Zhang, C. Lazo, S. Blügel, S. Heinze, Y. Mokrousov,
Electrically Tunable Quantum Anomalous Hall Effect in Graphene Decorated by 5d Transition-Metal Adatoms,
Phys. Rev. Lett. **108**, 056802 (2012).

[220] K. M. Seemann, F. Garcia-Sanchez, F. Kronast, J. Miguel, A. Kakay, C. M. Schneider, R. Hertel, F. Freimuth, Y. Mokrousov, S. Blügel,
Disentangling the Physical Contributions to the Electrical Resistance in Magnetic Domain Walls: A Multiscale Study,
Phys. Rev. Lett. **108**, 077201 (2012).

[221] D. Popova, A. Bringer, S. Blügel,
Theoretical investigation of the inverse Faraday effect via a stimulated Raman scattering process,
Phys. Rev. B **85**, 094419 (2012).

[222] K. Rahmanizadeh, G. Bihlmayer, M. Luysberg, S. Blügel,
First-principles study of intermixing and polarization at the DyScO3/SrTiO3 interface,
Phys. Rev. B **85**, 205103 (2012).

[223] E. Di Napoli, S. Blügel, P. Bientinesi,
Correlations in sequences of generalized eigenproblems arising in Density Functional Theory,
Computer Physics Communications **183**, 1674-1682 (2012).

[224] A. Thiess, R. Zeller, M. Bolten, P. H. Dederichs, S. Blügel,
Massively parallel density functional calculations for thousands of atoms: KKRnano,
Phys. Rev. B **85**, 235103 (2012).

[225] M. Betzinger, C. Friedrich, A. Görling, S. Blügel,
Precise response functions in all-electron methods: Application to the optimized-effective-potential approach,
Phys. Rev. B **85**, 245124 (2012).

[226] S. Tsukamoto, V. Caciuc, N. Atodiresei, S. Blügel,
Tuning the electron transport of molecular junctions by chemically functionalizing anchoring groups: First-principles study,
Phys. Rev. B **85**, 245435 (2012).

[227] S. Di Napoli, A. Thiess, S. Blügel, Y. Mokrousov,
Modelling impurity-assisted chain creation in noble-metal break junctions,
J. Phys.: Condens. Matter **24**, 135501 (2012).

[228] C. Friedrich, M. Betzinger, M. Schlipf, S. Blügel, A. Schindlmayr,
Hybrid functionals and GW approximation in the FLAPW method,
J. Phys.: Condens. Matter **24**, 293201 (2012).

[229] A. A. Khajetoorians, J. Wiebe, B. Chilian, S. Lounis, S. Blügel, R. Wiesendanger,
Atom-by-atom engineering and magnetometry of tailored nanomagnets,
Nature Physics **8**, 497 (2012).

[230] M. Menzel, Y. Mokrousov, R. Wieser, K. von Bergmann, E. Vedmedenko, S. Blügel, S. Heinze, A. Kubetzka, R. Wiesendanger,
Information transfer by vector spin chirality in finite magnetic chains,
Phys. Rev. Lett. **108**, 197204 (2012).

[231] S. Lounis, A. Bringer, S. Blügel,
Magnetic Adatom Induced Skyrmion-Like Spin Texture in Surface Electron Waves,
Phys. Rev. Lett. **108**, 207202 (2012).

[232] E. Sasioglu, C. Friedrich, S. Blügel,
Strength of the Effective Coulomb Interaction at Metal and Insulator Surfaces,
Phys. Rev. Lett. **109**, 146401 (2012).

[233] H. Zhang, F. Freimuth, G. Bihlmayer, S. Blügel, Y. Mokrousov,
Topological phases of Bi(111) bilayer in an external exchange field,
Phys. Rev. B **86**, 035104 (2012).

[234] D. Topwal, U. Manju, D. Pacilé, M. Papagno, D. Wortmann, G. Bihlmayer, S. Blügel, C. Carbone,
Quantum electron confinement in closely matched metals: Au films on Ag(111),
Phys. Rev. B **86**, 085419 (2012).

[235] M. Callsen, N. Atodiresei, V. Caciuc, S. Blügel,
Semiempirical van der Waals interactions versus ab initio nonlocal correlation effects in the thiophene-Cu(111) system,
Phys. Rev. B **86**, 085439 (2012).

[236] S. Blizak, G. Bihlmayer, S. Blügel,
Ab initio investigations of magnetic properties of FeCo monolayer alloy films on Rh(001),
Phys. Rev. B **86**, 094436 (2012).

[237] S. Heers, P. Mavropoulos, S. Lounis, R. Zeller, S. Blügel,
Lifetime reduction of surface states at Cu, Ag, and Au(111) caused by impurity scattering,
Phys. Rev. B **86**, 125444 (2012).

[238] H. Sims, W. H. Butler, M. Richter, K. Koepernik, E. Sasioglu, C. Friedrich, S. Blügel,
Theoretical investigation into the possibility of very large moments in Fe16N2,
Phys. Rev. B **86**, 174422 (2012).

[239] C. Pauly, G. Bihlmayer, M. Liebmann, M. Grob, A. Georgi, D. Subramaniam, M. Scholz, J. Sánchez-Barriga, A. Varykhalov, S. Blügel, O. Rader, M. Morgenstern,
Probing two topological surface bands of Sb_2Te_3 by spin-polarized photoemission spectroscopy,
Phys. Rev. B **86**, 235106 (2012).

[240] M. Meinert, C. Friedrich, G. Reiss, S. Blügel,
GW study of the half-metallic Heusler compounds Co_2MnSi and Co_2FeSi,
Phys. Rev. B **86**, 245115 (2012).

[241] V. Caciuc, N. Atodiresei, M. Callsen, P. Lazic, S. Blügel,
Ab initio and semi-empirical van der Waals study of graphene–boron nitride interaction from a molecular point of view,
J. Phys.: Condens. Matter **24**, 424214 (2012).

[242] P. Lazic, N. Atodiresei, V. Caciuc, R. Brako, B. Gumhalter, S. Blügel,
Rationale for switching to nonlocal functionals in density functional theory,
J. Phys.: Condens. Matter **24**, 424215 (2012).

[243] W. Zhang, A. Thiess, P. Zalden, R. Zeller, P. H. Dederichs, J.-Y. Raty, M. Wuttig, S. Blügel, R. Mazzarello,
Role of vacancies in metal-insulator transitions of crystalline phase-change materials,
Nature Materials **11**, 952 (2012).

[244] B. Zimmermann, P. Mavropoulos, S. Heers, N. H. Long, S. Blügel, Y. Mokrousov,
Anisotropy of Spin Relaxation in Metals,
Phys. Rev. Lett. **109**, 236603 (2012).

[245] E. Sasioglu, C. Friedrich, S. Blügel,
Strong magnon softening in tetragonal FeCo compounds,
Phys. Rev. B **87**, 020410 (2013).

[246] A. Herdt, L. Plucinski, G. Bihlmayer, G. Mussler, S. Döring, J. Krumrain, D. Grützmacher, S. Blügel, C. M. Schneider,
Spin-polarization limit in Bi_2Te_3 Dirac cone studied by angle- and spin-resolved photoemission experiments and ab initio calculations,
Phys. Rev. B **87**, 035127 (2013).

[247] R. Decker, J. Brede, N. Atodiresei, V. Caciuc, S. Blügel, R. Wiesendanger,
Atomic-scale magnetism of cobalt-intercalated grapheme,
Phys. Rev. B **87**, 041403 (2013).

[248] J. Weischenberg, F. Freimuth, S. Blügel, Y. Mokrousov,
Scattering-independent anomalous Nernst effect in ferromagnets,
Phys. Rev. B **87**, 060406 (2013).

[249] K. V. Raman, A. M. Kamerbeek, A. Mukherjee, N. Atodiresei, T. K. Sen, P. Lazić, V. Caciuc, R. Michel, D. Stalke, S. K. Mandal, S. Blügel, M. Münzenberg, J. S. Moodera,
Interface-engineered templates for molecular spin memory devices,
Nature **493**, 509 - 513 (2013).

[250] I. A. Nechaev, R. C. Hatch, M. Bianchi, D. Guan, C. Friedrich, I. Aguilera, J. L. Mi, B. B. Iversen, S. Blügel, Ph. Hofmann, E. V. Chulkov,
Evidence for a direct band gap in the topological insulator Bi2Se3 from theory and experiment,
Phys. Rev. B **87**, 121111(R) (2013).

[251] T. Kampfrath, M. Battiato, P. Maldonado, G. Eilers, J. Nötzold, S. Mährlein, V. Zbarsky, F. Freimuth, Y. Mokrousov, S. Blügel, M. Wolf, I. Radu, P. M. Oppeneer, M. Münzenberg,
Terahertz spin current pulses controlled by magnetic heterostructures,
Nature Nanotechnology **8**, 256 (2013).

[252] K. Garello, I. M. Miron, C. O. Avci, F. Freimuth, Y. Mokrousov, S. Blügel, S. Auffret, O. Boulle, G. Gaudin and P. Gambardella,
Symmetry and magnitude of spin–orbit torques in ferromagnetic heterostructures,
Nature Nanotechnology **8**, 587 (2013).

[253] S. Holzberger, T. Schuh, S. Blügel, S. Lounis, W. Wulfhekel,
Parity Effect in the Ground state Localization of Antiferromagnetic Chains Coupled to a Ferromagnet,
Phys. Rev. Lett. **110**, 157206 (2013).

[254] H. Sims, E. R. Ylvisaker, E. Sasioglu, C. Friedrich, S. Blügel, W. E. Pickett,
Effect of local electron-electron correlation in hydrogen-like impurities in Ge,
Phys. Rev. B **87**, 195120 (2013).

[255] I. P. Rusinov, I. A. Nechaev, S. V. Eremeev, C. Friedrich, S. Blügel, E. V. Chulkov,
Many-body effects on the Rashba-type spin splitting in bulk bismuth tellurohalides,
Phys. Rev. B **87**, 205103 (2013).

[256] H. Zhang, F. Freimuth, G. Bihlmayer, M. Ležaić, S. Blügel, Y. Mokrousov,
Engineering quantum anomalous Hall phases with orbital and spin degrees of freedom,
Phys. Rev. B **87**, 205132 (2013).

[257] H. L. Nguyen, P. Mavropoulos, B. Zimmermann, S. Heers, D. Bauer, S. Blügel, Y. Mokrousov,
Spin relaxation and the Elliott-Yafet parameter in W(001) ultrathin films: Surface states, anisotropy, and oscillation effects,
Phys. Rev. B **87**, 224420 (2013).

[258] Y. Li, D. Subramaniam, N. Atodiresei, P. Lazić, V. Caciuc, C. Pauly, A. Georgi, C. Busse, M. Liebmann, S. Blügel, M. Pratzer, M. Morgenstern, R. Mazzarello,
Absence of Edge States in Covalently Bonded Zigzag Edges of Graphene on Ir(111),
Advanced Materials **25**, 1967 (2013).

[259] H. Harutyunyan, M. Callsen, T. Allmers, V. Caciuc, S. Blügel, N. Atodiresei, D. Wegner, *Hybridisation at the organic–metal interface: a surface-scientific analogue of Hückel's rule?*
Chemical Communications **49**, 5993 (2013).

[260] S. Di Napoli, A. Weichselbaum, P. Roura-Bas, A. A. Aligia, Y. Mokrousov, S. Blügel, *Non-Fermi-Liquid Behavior in Transport Through Co-Doped Au Chains,*
Phys. Rev. Lett. **110**, 196402 (2013).

[261] I. Aguilera, C. Friedrich, G. Bihlmayer, S. Blügel, *GW study of topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3: Beyond the perturbative one-shot approach,*
Phys. Rev. B **88**, 045206 (2013).

[262] A. Jakobsson, E. Sasioglu, P. Mavropoulos, M. Lezaic, B. Sanyal, G. Bihlmayer, S. Blügel, *Tuning the Curie temperature of FeCo compounds by tetragonal distortion,*
Appl. Phys. Lett. **103**, 102404 (2013).

[263] M. Callsen, V. Caciuc, N. Kiselev, N. Atodiresei, S. Blügel, *Magnetic Hardening Induced by Nonmagnetic Organic Molecules,*
Phys. Rev. Lett. **111**, 106805 (2013).

[264] S. Fahrendorf, N. Atodiresei, C. Besson, V. Caciuc, F. Matthes, S. Blügel, P. Kögerler, D. Bürgler, C. M. Schneider, *Accessing 4f-states in single-molecule spintronics,*
Nature Communications **4**, 2425 (2013).

[265] C. Friedrich, M. Betzinger, S. Blügel, *Comment on "Nonanalyticity of the optimized effective potential with finite basis sets",*
Phys. Rev. A **88**, 046501 (2013).

[266] M. Betzinger, C. Friedrich, S. Blügel, *Precise response functions in all-electron methods: Generalization to nonspherical perturbations and application to NiO,*
Phys. Rev. B **88**, 075130 (2013).

[267] M. Schlipf, M. Betzinger, M. Ležaić, C. Friedrich, S. Blügel, *Structural, electronic, and magnetic properties of the europium chalcogenides: A hybrid-functional DFT study,*
Phys. Rev. B **88**, 094433 (2013).

[268] S. Tsukamoto, V. Caciuc, N. Atodiresei, S. Blügel, *Tuning electron transport through molecular junctions by chemical modification of the molecular core: First-principles study,*
Phys. Rev. B **88**, 125436 (2013).

[269] E. Sasioglu, I. Galanakis, C. Friedrich, S. Blügel, *Ab initio calculation of the effective on-site Coulomb interaction parameters for half-metallic magnets,*
Phys. Rev. B **88**, 134402 (2013).

[270] M. Ležaić, P. Mavropoulos, G. Bihlmayer, S. Blügel,
Exchange interactions and local-moment fluctuation corrections in ferromagnets at finite temperatures based on noncollinear density-functional calculations,
Phys. Rev. B **88**, 134403 (2013).

[271] A. Jacobsson, B. Sanyal, M. Ležaić, S. Blügel,
Exchange parameters and adiabatic magnon energies from spin-spiral calculations,
Phys. Rev. B **88**, 134427 (2013).

[272] N. H. Long, P. Mavropoulos, S. Heers, B. Zimmermann, Y. Mokrousov, S. Blügel,
Spin-flip hot spots in ultrathin films of monovalent metals: Enhancement and anisotropy of the Elliott-Yafet parameter,
Phys. Rev. B **88**, 144408 (2013).

[273] I. Aguilera, C. Friedrich, S. Blügel,
Spin-orbit coupling in quasiparticle studies of topological insulators,
Phys. Rev. B **88**, 165136 (2013).

[274] F. Y. Bruno, K. Rushchanskii, S. Valencia, Y. Dumont, C. Carrétéro, E. Jacquet, R. Abrudan, S. Blügel, M. Ležaić, M. Bibes, A. Barthélémy,
Rationalizing strain engineering effects in rare-earth nickelates,
Phys. Rev. B **88**, 195108 (2013).

[275] S. Schumacher, T. O. Wehling, P. Lazić, S. Runte, D. F. Förster, C. Busse, M. Petrović, M. Kralj, S. Blügel, N. Atodiresei, V. Caciuc, T. Michely,
The Backside of Graphene: Manipulating Adsorption by Intercalation,
Nano Letters **13**, 5013 - 5019 (2013).

[276] G. Michalicek, M. Betzinger, C. Friedrich, S. Blügel,
Elimination of the linearization error and improved basis-set convergence within the FLAPW method,
Computer Physics Communications **184**, 2670 - 2679 (2013).

[277] T. Schena, G. Bihlmayer, S. Blügel,
First-principles studies of FeS_2 using many-body perturbation theory in the G_0W_0 approximation,
Phys. Rev. B **88**, 235203 (2013).

[278] S. K. Panda, I. Dasgupta, E. Şaşıoğlu, S. Blügel, D. D. Sarma,
NiS - An unusual self-doped, nearly compensated antiferromagnetic metal,
Scientific Reports **3**, 2995 (2013).

[279] L. Plucinski, A. Herdt, S. Fahrendorf, G. Bihlmayer, G. Mussler, S. Döring, J. Kampmeier, F. C. Matthes, D. E. Bürgler, D. Grützmacher, S. Blügel, C. M. Schneider,
Electronic structure, surface morphology, and topologically protected surface states of Sb2Te3 thin films grown on Si(111),
Journal of Applied Physics **113**, 053706 (2013).

[280] L. El-Kareh, P. Mehring, V. Caciuc, N. Atodiresei, A. Beimborn, S. Blügel, C. Westphal,
Self-assembled monolayers of methylselenolate on the Au(111) surface: A combined STM and DFT study,

Surface Science **619**, 67 - 70 (2014).

[281] P. Czaja, F. Freimuth, J. Weischenberg, S. Blügel, Y. Mokrousov,
Anomalous Hall effect in ferromagnets with Gaussian disorder,
Phys. Rev. B **89**, 014411 (2014).

[282] F. Freimuth, S. Blügel, Y. Mokrousov,
Berry phase theory of Dzyaloshinskii–Moriya interaction and spin–orbit torques,
J. Phys.: Condens. Matter **26**, 104202 (2014).

[283] L. El-Kareh, G. Bihlmayer, A. Buchter, H. Bentmann, S. Blügel, F. Reinert, M. Bode,
A combined experimental and theoretical study of Rashba-split surface states on the (√3 x √3) Pb/Ag(111)$_{R30°}$ surface,
New journal of physics **16**, 1-14 (2014).

[284] R. Kováčik, P. Mavropoulos, D. Wortmann, S. Blügel,
Spin-caloric transport properties of cobalt nanostructures: Spin disorder effects from first principles,
Phys. Rev. B **89**, 134417 (2014).

[285] W. Jolie, F. Craes, M. Petrović, N. Atodiresei, V. Caciuc, S. Blügel, M. Kralj, T. Michely, C. Busse,
Confinement of Dirac electrons in graphene quantum dots,
Phys. Rev. B **89**, 155435 (2014).

[286] C. Franz, F. Freimuth, A. Bauer, R. Ritz, C. Schnarr, C. Duvinage, T. Adams, S. Blügel, A. Rosch, Y. Mokrousov, C. Pfleiderer,
Real-Space and Reciprocal-Space Berry Phases in the Hall Effect of $Mn_{1-x}Fe_xSi$,
Phys. Rev. Lett. **112**, 186601 (2014).

[287] V. Kashid, T. Schena, B. Zimmermann, Y. Mokrousov, S. Blügel, V. Shah, H. G. Salunke,
Dzyaloshinskii-Moriya interaction and chiral magnetism in 3d − 5d zigzag chains: Tight-binding model and ab initio calculations,
Phys. Rev. B **90**, 054412 (2014).

[288] N. H. Long, P. Mavropoulos, B. Zimmermann, D. Bauer, S. Blügel, Y. Mokrousov,
Spin relaxation and spin Hall transport in 5d transition-metal ultrathin films,
Phys. Rev. B **90**, 064406 (2014).

[289] I. Galanakis, E. Şaşıoğlu, S. Blügel, K. Özdoğan,
Voids-driven breakdown of the local-symmetry and Slater-Pauling rule in half-metallic Heusler compounds,
Phys. Rev. B **90**, 064408 (2014).

[290] M. Michiardi, I. Aguilera, M. Bianchi, V. E. de Carvalho, L. O. Ladeira, N. G. Teixeira, E. A. Soares, C. Friedrich, S. Blügel, P. Hofmann,
Bulk band structure of Bi_2Te_3,
Phys. Rev. B **90**, 075105 (2014).

[291] S. Tsukamoto, K. Hirose, S. Blügel,
Real-space finite-difference calculation method of generalized Bloch wave functions and complex band structures with reduced computational cost,

Phys. Rev. E **90**, 013306 (2014).

[292] P. Lazić, V. Caciuc, N. Atodiresei, M. Callsen, S. Blügel,
First-principles insights into the electronic and magnetic structure of hybrid organic-metal interfaces,
J. Phys.: Condens. Matter **26**, 263001 (2014).

[293] S. Fahrendorf, F. Matthes, D. Bürgler, C. M. Schneider, N. Atodiresei, V. Caciuc, S. Blügel, C. Besson, P. Kögerler,
Structural integrity of single bis (phthalocyaninato) - Neodymium(III) molecules on metal surfaces with different reactivity,
SPIN **2014**, 1440007 (2014).

[294] K. Rahmanizadeh, D. Wortmann, G. Bihlmayer, S. Blügel,
Charge and orbital order at head-to-head domain walls in $PbTiO_3$,
Phys. Rev. B **90**, 115104 (2014).

[295] I. Galanakis, K. Özdoğan, E. Şaşıoğlu, S. Blügel,
Conditions for spin-gapless semiconducting behavior in Mn2CoAl inverse Heusler compound,
Journal of Applied Physics **115**, 093908 (2014).

[296] S. Di Napoli, A. Thiess, S. Blügel, Y. Mokrousov,
Effect of magnetism and light sp-dopants on chain creation in Ir and Pt break junctions,
J. Phys.: Condens. Matter **26**, 295302 (2014).

[297] I. Galanakis, K. Özdoğan, E. Şaşıoğlu, S. Blügel,
Effect of disorder on the magnetic properties of cubic Mn2RuxGa compounds: A first-principles study,
Journal of Applied Physics **116**, 033903 (2014).

[298] R. Decker, M. Bazarnik, N. Atodiresei, V. Caciuc, S. Blügel, R. Wiesendanger,
Local tunnel magnetoresistance of an iron intercalated graphene-based heterostructure,
J. Phys.: Condens. Matter **26**, 394004 (2014).

[299] B. Zimmermann, M. Heide, G. Bihlmayer, S. Blügel,
First-principles analysis of a homochiral cycloidal magnetic structure in a monolayer Cr on W(110),
Phys. Rev. B **90**, 115427 (2014).

[300] J. Brede, N. Atodiresei, V. Caciuc, M. Bazarnik, A. Al-Zubi, S. Blügel, R. Wiesendanger,
Long-range magnetic coupling between nanoscale organic–metal hybrids mediated by a nanoskyrmion lattice,
Nature Nanotechnology **9**, 1018 (2014).

[301] F. Freimuth, S. Blügel, Y. Mokrousov,
Spin-orbit torques in Co/Pt(111) and Mn/W(001) magnetic bilayers from first principles,
Phys. Rev. B **90**, 174423 (2014).

[302] B. Zimmermann, K. Chadova, D. Ködderitzsch, S. Blügel, H. Ebert, D. V. Fedorov, N. H. Long, P. Mavropoulos, I. Mertig, Y. Mokrousov, M. Gradhand,
Skew scattering in dilute ferromagnetic alloys,

Phys. Rev. B **90**, 220403 (2014).

[303] W. Wulfhekel, S. Blügel,
Spins on surfaces,
Surface Science **630**, (2014).

[304] S. Blizak, G. Bihlmayer, S. Blügel, S. E. H. Abaidia,
Interlayer exchange coupling between FeCo and Co ultrathin films through Rh(001) spacers,
Phys. Rev. B **91**, 014408 (2015).

[305] G. Géranton, F. Freimuth, S. Blügel, Y. Mokrousov,
Spin-orbit torques in thin films driven by electrical and thermal currents,
Phys. Rev. B **91**, 014417 (2015).

[306] R. Kovacik, P. Mavropoulos, S. Blügel,
Spin transport and spin-caloric effects in (Cr,Zn)Te half-metallic nanostructures: Effect of spin disorder at elevated temperatures from first principles,
Phys. Rev. B **91**, 014421 (2015).

[307] D. A. Klüppelberg, M. Betzinger, S. Blügel,
Atomic force calculations within the all-electron FLAPW method: Treatment of core states and discontinuities at the muffin-tin sphere boundary,
Phys. Rev. B **91**, 035105 (2015).

[308] C. Niu, G. Bihlmayer, H. Zhang, D. Wortmann, S. Blügel, Y. Mokrousov,
Functionalized bismuth films: Giant gap quantum spin Hall and valley-polarized quantum anomalous Hall states,
Phys. Rev. B **91**, 041303 (2015).

[309] M. dos Santos Dias, B. Schweflinghaus, S. Blügel, S. Lounis,
Relativistic dynamical spin excitations of magnetic adatoms,
Phys. Rev. B **91**, 075405 (2015).

[310] R. Friedrich, V. Caciuc, N. Kiselev, N. Atodiresei, S. Blügel,
Chemically functionalized magnetic exchange interactions of hybrid organic-ferromagnetic metal interfaces,
Phys. Rev. B **91**, 115432 (2015).

[311] I. Aguilera, C. Friedrich, S. Blügel,
Electronic phase transitions of bismuth under strain from relativistic self-consistent calculations,
Phys. Rev. B **91**, 125129 (2015).

[312] T. Iffländer, S. Rolf-Pissarczyk, L. Winking, R. G. Ulbrich, A. Al-Zubi, S. Blügel, M. Wenderoth,
Local Density of States at Metal-Semiconductor Interfaces: An Atomic Scale Study,
Phys. Rev. Lett. **114**, 146804 (2015).

[313] F. Tran, P. Blaha, M. Betzinger, S. Blügel,
Comparison between exact and semilocal exchange potentials: An all-electron study for solids,

Phys. Rev. B **91**, 165121 (2015).

[314] A. Jakobsson, P. Mavropoulos, E. Şaşıoğlu, S. Blügel, M. Ležaić, B. Sanyal, I. Galanakis, *First-principles calculations of exchange interactions, spin waves, and temperature dependence of magnetization in inverse-Heusler-based spin gapless semiconductors,* Phys. Rev. B **91**, 174439 (2015).

[315] J.-P. Hanke, F. Freimuth, S. Blügel, Y. Mokrousov, *Higher-dimensional Wannier functions of multiparameter Hamiltonians,* Phys. Rev. B **91**, 184413 (2015).

[316] C. Niu, P. M. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, Y. Mokrousov, *Typological crystalline insulator and quantum anomalous Hall states in IV-VI-based monolayers and their quantum wells,* Phys. Rev. B **91**, 201401 (R) (2015).

[317] I. A. Nechaev, I. Aguilera, V. De Renzi, A. di Bona, A. Lodi Rizzini, A. M. Mio, G. Nicotra, A. Politano, S. Scalese, Z. S. Aliev, M. B. Babanly, C. Friedrich, S. Blügel, E. V. Chulkov, *Quasiparticle spectrum and plasmonic excitations in the topological insulator Sb_2 Te_3,* Phys. Rev. B **91**, 245123 (2015).

[318] J. Gayles, F. Freimuth, T. Schena, G. Lani, P. Mavropoulos, R. A. Duine, S. Blügel, J. Sinova, Y. Mokrousov, *Dzyaloshinskii-Moriya Interaction and Hall Effects in the Skyrmion Phase of Mn 1 − x Fe x Ge,* Phys. Rev. Lett. **115**, 036602 (2015).

[319] V. Kashid, V. Shah, H. G. Salunke, Y. Mokrousov, S. Blügel, *Magnetic properties of 2D nickel nanostrips: structure dependent magnetism and Stoner criterion,* J. Phys.: Condens. Matter **27**, 316002 (2015).

[320] F. Freimuth, S. Blügel, Y. Mokrousov, *Direct and inverse spin-orbit torques,* Phys. Rev. B **92**, 064415 (2015).

[321] M. Rösner, E. Şaşıoğlu, C. Friedrich, S. Blügel, T. O. Wehling, *Wannier function approach to realistic Coulomb interactions in layered materials and heterostructures,* Phys. Rev. B **92**, 085102 (2015).

[322] A. Thiess, S. Blügel, P. H. Dederichs, R. Zeller, W. R. L. Lambrecht, *Systematic study of the exchange interactions in Gd-doped GaN containing N interstitials, O interstitials, or Ga vacancies,* Phys. Rev. B **92**, 104418 (2015).

[323] F. N. Rybakov, A. B. Borisov, S. Blügel, N. Kiselev, *New Type of Stable Particlelike States in Chiral Magnets,* Phys. Rev. Lett. **115**, 117201 (2015).

[324] D. Crum, M. Bouhassoune, J. Bouaziz, B. Schweflinghaus, S. Blügel, S. Lounis, *Perpendicular reading of single confined magnetic skyrmions,*

Nature Communications **6**, 8541 (2015).

[325] R. Friedrich, V. Caciuc, N. Atodiresei, S. Blügel,
Molecular induced skyhook effect for magnetic interlayer softening,
Phys. Rev. B **92**, 195407 (2015).

[326] M. Eschbach, E. Młyńczak, J. Kellner, J. Kampmeier, M. Lanius, E. Neumann, C. Weyrich, M. Gehlmann, P. Gospodarič, S. Döring, G. Mussler, N. Demarina, M. Luysberg, G. Bihlmayer, T. Schäpers, L. Plucinski, S. Blügel, M. Morgenstern, C. M. Schneider, D. Grützmacher,
Realization of a vertical topological p–n junction in epitaxial Sb2Te3/Bi2Te3 heterostructures,
Nature Communications **6**, 8816 (2015).

[327] C. Niu, P. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, Y. Mokrousov,
Two-Dimensional Topological Crystalline Insulator and Topological Phase Transition in TlSe and TlS Monolayers,
Nano Letters **15**, 6071 - 6075 (2015).

[328] M. Betzinger, C. Friedrich, A. Görling, S. Blügel,
Precise all-electron dynamical response functions: Application to COHSEX and the RPA correlation energy,
Phys. Rev. B **92**, 245101 (2015).

[329] F. Huttmann, A. J. Martínez-Galera, V. Caciuc, N. Atodiresei, S. Schumacher, S. Standop, I. Hamada, T. O. Wehling, S. Blügel, T. Michely,
Tuning the van der Waals Interaction of Graphene with Molecules via Doping,
Phys. Rev. Lett. **115**, 236101 (2015).

[330] A. J. Martínez-Galera, U. A. Schröder, F. Huttmann, W. Jolie, F. Craes, C. Busse, V. Caciuc, N. Atodiresei, S. Blügel, T. Michely,
Oxygen orders differently under graphene: new superstructures on Ir(111),
Nanoscale **8**, 1932 (2016).

[331] K. Lejaeghere, G. Bihlmayer, T. Bjorkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, I. E. Castelli, S. J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J. K. Dewhurst, I. Di Marco, C. Draxl, M. Dulak, O. Eriksson, J. A. Flores-Livas, K. F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Granas, E. K. U. Gross, A. Gulans, F. Gygi, D. R. Hamann, P. J. Hasnip, N. A. W. Holzwarth, D. Iusan, D. B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepernik, E. Kucukbenli, Y. O. Kvashnin, I. L. M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordstrom, T. Ozaki, L. Paulatto, C. J. Pickard, W. Poelmans, M. I. J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunström, A. Tkatchenko, M. Torrent, D. Vanderbilt, M. J. van Setten, V. Van Speybroeck, J. M. Wills, J. R. Yates, G.-X. Zhang, S. Cottenier,
Reproducibility in density functional theory calculations of solids,
Science **351**, 6280 (2016).

[332] C. Carbone, P. Moras, P. M. Sheverdyaeva, D. Pacilé, M. Papagno, L. Ferrari, D. Topwal, E. Vescovo, G. Bihlmayer, F. Freimuth, Y. Mokrousov, S. Blügel,
Asymmetric band gaps in a Rashba film system,
Phys. Rev. B **93**, 125409 (2016).

[333] B. Zimmermann, P. Mavropoulos, N. H. Long, C.-R. Gerhorst, S. Blügel, Y. Mokrousov,
Fermi surfaces, spin-mixing parameter, and colossal anisotropy of spin relaxation in transition metals from ab initio theory,
Phys. Rev. B **93**, 144403 (2016).

[334] F. N. Rybakov, A. B. Borisov, S. Blügel, N. Kiselev,
New spiral state and skyrmion lattice in 3D model of chiral magnets,
New Journal of Physics **18**, 045002 (2016).

[335] A. K. Nandy, N. Kiselev, S. Blügel,
Interlayer Exchange Coupling: A General Scheme Turning Chiral Magnets into Magnetic Multilayers Carrying Atomic-Scale Skyrmions,
Phys. Rev. Lett. **116**, 177202 (2016).

[336] T. J. Huisman, R. V. Mikhaylovskiy, J. D. Costa, F. Freimuth, E. Paz, J. Ventura,
P. P. Freitas, S. Blügel, Y. Mokrousov, T. Rasing, A. V. Kimel,
Femtosecond control of electric currents in metallic ferromagnetic heterostructures,
Nature Nanotechnology **11**, 455 (2016).

[337] N. H. Long, P. Mavropoulos, B. Zimmermann, S. Blügel, Y. Mokrousov,
Giant spin Nernst effect induced by resonant scattering at surfaces of metallic films,
Phys. Rev. B **93**, 180406 (2016).

[338] M. Tas, E. Sasioglu, I. Galanakis, C. Friedrich, S. Blügel,
Quasiparticle band structure of the almost-gapless transition-metal-based Heusler semiconductors,
Phys. Rev. B **93**, 195155 (2016).

[339] B. Dupé, G. Bihlmayer, M. Böttcher, S. Blügel, S. Heinze,
Engineering skyrmions in transition-metal multilayers for spintronics,
Nature Communications **7**, 11779 (2016).

[340] A. Belabbes, G. Bihlmayer, S. Blügel, A. Manchon,
Oxygen-enabled control of Dzyaloshinskii-Moriya Interaction in ultra-thin magnetic films,
Scientific Reports **6**, 24634 (2016).

[341] M. Gehlmann, I. Aguilera, G. Bihlmayer, E. Mlynczak, M. Eschbach, S. Döring,
P. Gospodarič, S. Cramm, B. Kardynal, L. Plucinski, S. Blügel, C. M. Schneider,
Quasi 2D electronic states with high spin-polarization in centrosymmetric MoS_2 bulk crystals,
Scientific Reports **6**, 26197 (2016).

[342] R. Friedrich, V. Caciuc, N. Atodiresei, S. Blügel,
Exchange interactions of magnetic surfaces below two-dimensional materials,
Phys. Rev. B **93**, 220406 (2016).

[343] G. Geranton, B. Zimmermann, N. H. Long, P. Mavropoulos, S. Blügel, F. Freimuth,
Y. Mokrousov,
Spin-orbit torques and spin accumulation in FePt/Pt and Co/Cu thin films from first principles: The role of impurities,
Phys. Rev. B **93**, 224420 (2016).

[344] F. Freimuth, S. Blügel, Y. Mokrousov,
The inverse thermal spin–orbit torque and the relation of the Dzyaloshinskii–Moriya interaction to ground-state energy currents,
J. Phys.: Condens. Matter **28**, 316001 (2016).

[345] L. Peters, I. Di Marco, O. Grånäs, E. Şaşıoğlu, A. Altun, S. Rossen, C. Friedrich, S. Blügel, M. I. Katsnelson, A. Kirilyuk, O. Eriksson,
Correlation effects and orbital magnetism of Co clusters,
Phys. Rev. B **93**, 224428 (2016).

[346] B. Schweflinghaus, B. Zimmermann, M. Heide, G. Bihlmayer, S. Blügel,
Role of Dzyaloshinskii-Moriya interaction for magnetism in transition-metal chains at Pt step edges,
Phys. Rev. B **94**, 024403 (2016).

[347] C. Heo, N. Kiselev, A. K. Nandy, S. Blügel, T. Rasing,
Switching of chiral magnetic skyrmions by picosecond magnetic field pulses via transient topological states,
Scientific Reports **6**, 27146 (2016).

[348] J. Bouaziz, S. Lounis, S. Blügel, H. Ishida,
Microscopic theory of the residual surface resistivity of Rashba electrons,
Phys. Rev. B **94**, 045433 (2016).

[349] B. Zimmermann, N. H. Long, P. Mavropoulos, S. Blügel, Y. Mokrousov,
Influence of complex disorder on skew-scattering Hall effects in L 1 0 -ordered FePt alloy,
Phys. Rev. B **94**, 060406 (2016).

[350] M. C. T. D. Müller, C. Friedrich, S. Blügel,
Acoustic magnons in the long-wavelength limit: Investigating the Goldstone violation in many-body perturbation theory,
Phys. Rev. B **94**, 064433 (2016).

[351] E. Trushin, M. Betzinger, S. Blügel, A. Görling,
Band gaps, ionization potentials, and electron affinities of periodic electron systems via the adiabatic-connection fluctuation-dissipation theorem,
Phys. Rev. B **94**, 075123 (2016).

[352] P. Sessi, P. Rüßmann, T. Bathon, A. Barla, K. A. Kokh, O. E. Tereshchenko, K. Fauth, S. K. Mahatha, M. A. Valbuena, S. Godey, F. Glott, A. Mugarza, P. Gargiani, M. Valvidares, N. H. Long, C. Carbone, P. Mavropoulos, S. Blügel, M. Bode,
Superparamagnetism-induced mesoscopic electron focusing in topological insulators,
Phys. Rev. B **94**, 075137 (2016).

[353] K. Rahmanizadeh, G. Bihlmayer, S. Blügel,
Spin-orbit and exchange effects in the 2DEG of $BiAlO_3$ -based oxide heterostructures,
EPL **115**, 17006 (2016).

[354] C. Niu, P. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, Y. Mokrousov,
Two-dimensional topological crystalline insulator phase in quantum wells of trivial insulators,

2D Materials **3**, 025037 (2016).

[355] J.-P. Hanke, F. Freimuth, A. K. Nandy, H. Zhang, S. Blügel, Y. Mokrousov,
Role of Berry phase theory for describing orbital magnetism: From magnetic heterostructures to topological orbital ferromagnets,
Phys. Rev. B **94**, 121114 (2016).

[356] J. I. Azpiroz, M. dos Santos Dias, S. Blügel, S. Lounis,
Zero-Point Spin-Fluctuations of Single Adatoms,
Nano Letters **16**, 4305 (2016).

[357] F. Freimuth, S. Blügel, Y. Mokrousov,
Laser-induced torques in metallic ferromagnets,
Phys. Rev. B **94**, 144432 (2016).

[358] J. Sánchez-Barriga, M. G. Vergniory, D. Evtushinsky, I. Aguilera, A. Varykhalov, S. Blügel, O. Rader,
Surface Fermi arc connectivity in the type-II Weyl semimetal candidate WTe_2,
Phys. Rev. B **94**, 161401 (2016).

[359] N. H. Long, P. Mavropoulos, D. Bauer, B. Zimmermann, Y. Mokrousov, S. Blügel,
Strong spin-orbit fields and Dyakonov-Perel spin dephasing in supported metallic films,
Phys. Rev. B **94**, 180406 (2016).

[360] E. Mlynczak, M. Eschbach, S. Borek, J. Minár, J. Braun, I. Aguilera, G. Bihlmayer, S. Döring, M. Gehlmann, P. Gospodarič, S. Suga, L. Plucinski, S. Blügel, H. Ebert, C. M. Schneider,
Fermi Surface Manipulation by External Magnetic Field Demonstrated for a Prototypical Ferromagnet,
Phys. Rev. X **6**, 041048 (2016).

[361] B. Warner, F. El Hallak, N. Atodiresei, P. Seibt, H. Prüser, V. Caciuc, M. Waters, A. J. Fisher, S. Blügel, J. van Slageren, C. F. Hirjibehedin,
Sub-molecular modulation of a 4f driven Kondo resonance by surface-induced asymmetry,
Nature Communications **7**, 12785 (2016).

[362] A. Belabbes, G. Bihlmayer, F. Bechstedt, S. Blügel, A. Manchon,
Hund's Rule-Driven Dzyaloshinskii-Moriya Interaction at 3d − 5d Interfaces,
Phys. Rev. Lett. **117**, 247202 (2016).

[363] M. dos Santos Dias, J. Bouaziz, M. Bouhassoune, S. Blügel, S. Lounis,
Chirality-driven orbital magnetic moments as a new probe for topological magnetic structures,
Nature Communications **7**, 13613 (2016).

[364] S. Oyarzún, A. K. Nandy, F. Rortais, J.-C. Rojas-Sánchez, M.-T. Dau, P. Noël, P. Laczkowski, S. Pouget, H. Okuno, L. Vila, C. Vergnaud, C. Beigné, A. Marty, J.-P. Attané, S. Gambarelli, J.-M. George, H. Jaffrès, S. Blügel, M. Jamet,
Evidence for spin-to-charge conversion by Rashba coupling in metallic states at the Fe/Ge(111) interface,
Nature Communications **7**, 13857 (2016).

[365] F. H. Farwick zum Hagen, D. M. Zimmermann, C. C. Silva, C. Schlueter, N. Atodiresei, W. Jolie, A. J. Martínez-Galera, D. Dombrowski, U. A. Schröder, M. Will, P. Lazić, V. Caciuc, S. Blügel, T.-L. Lee, T. Michely, C. Busse,
Structure and Growth of Hexagonal Boron Nitride on Ir(111),
ACS Nano **10**, 11012 (2016).

[366] M. Paßens, V. Caciuc, N. Atodiresei, M. Moors, S. Blügel, R. Waser, S. Karthäuser,
Tuning the surface electronic structure of a $Pt_3Ti(111)$ electro catalyst,
Nanoscale **8**, 13924 (2016).

[367] J.-P. Hanke, F. Freimuth, S. Blügel, Y. Mokrousov,
Prototypical topological orbital ferromagnet γ-FeMn,
Scientific Reports **7**, 41078 (2017).

[368] M. Tas, E. Şaşıoğlu, C. Friedrich, S. Blügel, I. Galanakis,
Design of L 2 1 -type antiferromagnetic semiconducting full-Heusler compounds: A first principles DFT + GW study,
Journal of Applied Physics **121**, 053903 (2017.)

[369] E. Şaşıoğlu, H. Hadipour, C. Friedrich, S. Blügel, I. Mertig,
Strength of effective Coulomb interactions and origin of ferromagnetism in hydrogenated graphene,
Phys. Rev. B **95**, 060408 (2017).

[370] J. Bouaziz, M. dos Santos Dias, A. Ziane, M. Benakki, S. Blügel, S. Lounis,
Chiral magnetism of magnetic adatoms generated by Rashba electrons,
New Journal of Physics **19**, 023010 (2017).

[371] C. Niu, P. Buhl, G. Bihlmayer, D. Wortmann, Y. Dai, S. Blügel, Y. Mokrousov,
Robust dual topological character with spin-valley polarization in a monolayer of the Dirac semimetal Na 3 Bi,
Phys. Rev. B **95**, 075404 (2017).

[372] F. Huttmann, D. Klar, N. Atodiresei, C. Schmitz-Antoniak, A. Smekhova, A. J. Martínez-Galera, V. Caciuc, G. Bihlmayer, S. Blügel, T. Michely, H. Wende,
Magnetism in a graphene- 4 f − 3 d hybrid system,
Phys. Rev. B **95**, 075427 (2017).

[373] S. Tsukamoto, T. Ono, K. Hirose, S. Blügel,
Self-energy matrices for electron transport calculations within the real-space finite-difference formalism,
Phys. Rev. E **95**, 033309 (2017).

[374] T. Esat, R. Friedrich, F. Matthes, V. Caciuc, N. Atodiresei, S. Blügel, D. E. Bürgler, S. Tautz, C. M. Schneider,
Quantum interference effects in molecular spin hybrids,
Phys. Rev. B **95**, 094409 (2017).

[375] F. Freimuth, S. Blügel, Y. Mokrousov,
Charge pumping driven by the laser-induced dynamics of the exchange splitting,
Phys. Rev. B **95**, 094434 (2017).

[376] D. D. Scherer, A. C. Jacko, C. Friedrich, E. Şaşıoğlu, S. Blügel, R. Valentí, B. M. Andersen,
Interplay of nematic and magnetic orders in FeSe under pressure,
Phys. Rev. B **95**, 094504 (2017).

[377] G. Géranton, B. Zimmermann, N. H. Long, P. Mavropoulos, S. Blügel, F. Freimuth, Y. Mokrousov,
Nonlocal fieldlike spin-orbit torques in Rashba systems: Ab initio study of a Ag 2 Bi - terminated Ag(111) film grown on a ferromagnetic Fe(110) substrate,
Phys. Rev. B **95**, 134449 (2017).

[378] L. Peters, E. Şaşioğlu, S. Rossen, C. Friedrich, S. Blügel, M. I. Katsnelson,
Nonconventional screening of the Coulomb interaction in FexOy clusters: An ab initio study,
Phys. Rev. B **95**, 155119 (2017).

[379] M. Passens, V. Caciuc, N. Atodiresei, M. Feuerbacher, M. Moors, R. Dunin-Borkowski, S. Blügel, R. Waser, S. Karthäuser,
Interface-driven formation of a two-dimensional dodecagonal fullerene quasicrystal,
Nature Communications **8**, 15367 (2017).

[380] D. Go, J.-P. Hanke, P. Buhl, F. Freimuth, G. Bihlmayer, H.-W. Lee, Y. Mokrousov, S. Blügel,
Toward surface orbitronics: giant orbital magnetism from the orbital Rashba effect at the surface of sp-metals,
Scientific Reports **7**, 46742 (2017).

[381] P. Buhl, F. Freimuth, S. Blügel, Y. Mokrousov,
Topological spin Hall effect in antiferromagnetic skyrmions,
Physica Status Solidi/Rapid research letters **11**, 1700007 (2017).

[382] R. Friedrich, V. Caciuc, G. Bihlmayer, N. Atodiresei, S. Blügel,
Designing the Rashba spin texture by adsorption of inorganic molecules,
New Journal of Physics **19**, 043017 (2017).

[383] V. Heß, R. Friedrich, F. Matthes, V. Caciuc, N. Atodiresei, D. E. Bürgler, S. Blügel, C. M. Schneider,
Magnetic subunits within a single molecule–surface hybrid,
New Journal of Physics **19**, 053016 (2017).

[384] M. Hoffmann, B. Zimmermann, G. P. Müller, D. Schürhoff, N. S. Kiselev, C. Melcher, S. Blügel,
Antiskyrmions stabilized at interfaces by anisotropic Dzyaloshinskii-Moriya interactions,
Nature Communications **8**, 308 (2017).

[385] C. Niu, P. Buhl, G. Bihlmayer, D. Wortmann, Y. Dai, S. Blügel, Y. Mokrousov,
Two-dimensional topological nodal line semimetal in layered X 2 Y (X = Ca, Sr, and Ba; Y = As, Sb, and Bi),
Phys. Rev. B **95**, 235138 (2017).

[386] J. Hermenau, J. I. Azpiroz, C. Hübner, A. Sonntag, B. Baxevanis, K. T. Ton,

M. Steinbrecher, A. A. Khajetoorians, M. dos Santos Dias, S. Blügel, R. Wiesendanger, S. Lounis, J. Wiebe,
A gateway towards non-collinear spin processing using three-atom magnets with strong substrate coupling,
Nature Communications **8**, 642 (2017).

[387] M. Passens, V. Caciuc, N. Atodiresei, M. Feuerbacher, M. Moors, R. Dunin-Borkowski, S. Blügel, R. Waser, S. Karthäuser,
Interface-driven formation of a two-dimensional dodecagonal fullerene quasicrystal,
Nature Communications **8**, 15367 (2017).

[388] J. I. Azpiroz, M. dos Santos Dias, B. Schweflinghaus, S. Blügel, S. Lounis,
Tuning Paramagnetic Spin Excitations of Single Adatoms,
Phys. Rev. Lett. **119**, 017203 (2017).

[389] C. Jin, Z.-A. Li, A. Kovács, J. Caron, F. Zheng, F. N. Rybakov, N. S. Kiselev, H. Du, S. Blügel, M. Tian, Y. Zhang, M. Farle, R. Dunin-Borkowski,
Control of morphology and formation of highly geometrically confined magnetic skyrmions,
Nature Communications **8**, 15569 (2017).

[390] F. Freimuth, S. Blügel, Y. Mokrousov,
Relation of the Dzyaloshinskii-Moriya interaction to spin currents and to the spin-orbit field,
Phys. Rev. B **96**, 054403 (2017).

[391] R. Friedrich, V. Caciuc, B. Zimmermann, G. Bihlmayer, N. Atodiresei, S. Blügel,
Creating anisotropic spin-split surface states in momentum space by molecular adsorption,
Phys. Rev. B **96**, 085403 (2017).

[392] B. V. Senkovskiy, A. V. Fedorov, D. Haberer, M. Farjam, K. A. Simonov, A. B. Preobrajenski, N. Martensson, N. Atodiresei, V. Caciuc, S. Blügel, A. Rosch, N. I. Verbitskiy, M. Hell, D. V. Evtushinsky, R. German, T. Marangoni, P. H. M. van Loosdrecht, F. R. Fischer, A. Grüneis,
Semiconductor-to-Metal Transition and Quasiparticle Renormalization in Doped Graphene Nanoribbons,
Advanced electronic materials **3**, 1600490 (2017).

[393] M. Gehlmann, I. Aguilera, G. Bihlmayer, S. Nemšák, P. Nagler, P. Gospodarič, G. Zamborlini, M. Eschbach, V. Feyer, F. Kronast, E. Młyńczak, T. Korn, L. Plucinski, C. Schüller, S. Blügel, C. M. Schneider,
Direct Observation of the Band Gap Transition in Atomically Thin ReS2,
Nano Letters **17**, 5187 (2017).

[394] J. I. Azpiroz, M. dos Santos Dias, S. Blügel, S. Lounis,
Longitudinal and transverse spin relaxation times of magnetic single adatoms: An ab initio analysis,
Phys. Rev. B **96**, 144410 (2017).

[395] B. Warner, T. G. Gill, V. Caciuc, N. Atodiresei, A. Fleurence, Y. Yoshida, Y. Hasegawa, S. Blügel, Y. Yamada-Takamura, C. F. Hirjibehedin,

Guided Molecular Assembly on a Locally Reactive 2D Material,
Advanced Materials **29**, 1703929 (2017).

[396] A. Kovacs, J. Caron, A. S. Savchenko, N. Kiselev, K. Shibata, Z.-A. Li, N. Kanazawa, Y. Tokura, S. Blügel, R. Dunin-Borkowski,
Mapping the magnetization fine structure of a lattice of Bloch-type skyrmions in an FeGe thin film,
Applied Physics Letters **111**, 192410 (2017).

[397] J.-P. Hanke, F. Freimuth, C. Niu, S. Blügel, Y. Mokrousov,
Mixed Weyl semimetals and low-dissipation magnetization control in insulators by spin–orbit torques,
Nature Communications **8**, 1479 (2017).

[398] J.-P. Hanke, F. Freimuth, S. Blügel, Y. Mokrousov,
Higher-dimensional Wannier Interpolation for the Modern Theory of the Dzyaloshinskii–Moriya Interaction: Application to Co-based Trilayers,
Journal of the Physical Society of Japan **87**, 041010 (2018).

[399] H. Momida, G. Bihlmayer, S. Blügel, K. Segawa, Y. Ando, T. Oguchi,
Topological interface states in the natural heterostructure (PbSe) 5 (Bi2 Se3) 6 with Bi Pb defects,
Phys. Rev. B **97**, 035113 (2018).

[400] P. Rüßmann, A. P. Weber, F. Glott, N. Xu, M. Fanciulli, S. Muff, A. Magrez, P. Bugnon, H. Berger, M. Bode, J. H. Dil, S. Blügel, P. Mavropoulos, P. Sessi,
Universal scattering response across the type-II Weyl semimetal phase diagram,
Phys. Rev. B **97**, 075106 (2018).

[401] P. F. Bessarab, G. P. Müller, I. S. Lobanov, F. N. Rybakov, N. S. Kiselev, H. Jónsson, V. M. Uzdin, S. Blügel, L. Bergqvist, A. Delin,
Lifetime of racetrack skyrmions,
Scientific Reports **8**, 3433 (2018).

[402] H. Du, X. Zhao, F. N. Rybakov, A. B. Borisov, S. Wang, J. Tang, C. Jin, C. Wang, W. Wei, N. S. Kiselev, Y. Zhang, R. Che, S. Blügel, M. Tian,
Interaction of Individual Skyrmions in a Nanostructured Cubic Chiral Magnet,
Phys. Rev. Lett. **120**, 197203 (2018).

[403] S. Tsukamoto, T. Ono, S. Blügel,
Improvement of accuracy in the wave-function-matching method for transport calculations,
Phys. Rev. B **97**, 115450 (2018).

[404] A. Krönlein, M. Schmitt, M. Hoffmann, J. Kemmer, N. Seubert, M. Vogt, J. Küspert, M. Böhme, B. Alonazi, J. Kügel, H. A. Albrithen, M. Bode, G. Bihlmayer, S. Blügel,
Magnetic Ground State Stabilized by Three-Site Interactions: Fe/Rh (111),
Phys. Rev. Lett. **120**, 207202 (2018).

[405] C. S. Spencer, J. Gayles, N. A. Porter, S. Sugimoto, Z. Aslam, C. J. Kinane, T. R. Charlton, F. Freimuth, S. Chadov, S. Langridge, J. Sinova, C. Felser, S. Blügel, Y. Mokrousov, C. H. Marrows,

Helical magnetic structure and the anomalous and topological Hall effects in epitaxial B20 Fe 1 − y Co y Ge films,
Phys. Rev. B **97**, 214406 (2018).

[406] F. Zheng, F. N. Rybakov, A. B. Borisov, D. Song, S. Wang, Z.-A. Li, H. Du, N. S. Kiselev, J. Caron, A. Kovács, M. Tian, Y. Zhang, S. Blügel, R. E. Dunin-Borkowski,
Experimental observation of chiral magnetic bobbers in B20-type FeGe,
Nature Nanotechnology **13**, 451 (2018).

[407] F. Freimuth, S. Blügel, Y. Mokrousov,
Spin-orbit torques and tunable Dzyaloshinskii-Moriya interaction in Co/Cu/Co trilayers,
Phys. Rev. B **98**, 024419 (2018).

[408] J. Ibañez-Azpiroz, M. dos Santos Dias, S. Blügel, S. Lounis,
Spin-fluctuation and spin-relaxation effects of single adatoms from first principles,
Journal of Physics/Condensed matter **30**, 343002 (2018).

[409] J. Bouaziz, M. dos Santos Dias, F. Guimaraes, S. Blügel, S. Lounis,
Impurity-induced orbital magnetization in a Rashba electron gas,
Phys. Rev. B **98**, 125420 (2018).

[410] F. Lux, F. Freimuth, S. Blügel, Y. Mokrousov,
Engineering chiral and topological orbital magnetism of domain walls and skyrmions,
Communications Physics **1**, 60 (2018).

[411] A. P. Weber, P. Rüßmann, N. Xu, S. Muff, M. Fanciulli, A. Magrez, P. Bugnon, H. Berger, N. C. Plumb, M. Shi, S. Blügel, P. Mavropoulos, J. H. Dil,
Spin-Resolved Electronic Response to the Phase Transition in MoTe 2,
Phys. Rev. Lett. **121**, 156401 (2018).

[412] H. Jia, B. Zimmermann, S. Blügel,
First-principles investigation of chiral magnetic properties in multilayers: Rh/Co/Pt and Pd/Co/Pt,
Phys. Rev. B **98**, 144427 (2018).

[413] I. Lima Fernandes, J. Bouaziz, S. Blügel, S. Lounis,
Universality of defect-skyrmion interaction profiles,
Nature Communications **9**, 4395 (2018).

[414] G. Müller, P. F. Bessarab, S. M. Vlasov, F. Lux, N. Kiselev, S. Blügel, V. M. Uzdin, H. Jónsson,
Duplication, Collapse, and Escape of Magnetic Skyrmions Revealed Using a Systematic Saddle Point Search Method,
Phys. Rev. Lett. **121**, 197202 (2018).

[415] Z. Zanolli, C. Niu, G. Bihlmayer, Y. Mokrousov, P. Mavropoulos, M. J. Verstraete, S. Blügel,
Hybrid quantum anomalous Hall effect at graphene-oxide interfaces,
Phys. Rev. B **98**, 155404 (2018).

[416] S. Tsukamoto, T. Ono, S. Iwase, S. Blügel,

Complex band structure calculations based on the overbridging boundary matching method without using Green's functions,
Phys. Rev. B **98**, 195422 (2018).

[417] H. Hadipour, E. Sasioglu, F. Bagherpour, C. Friedrich, S. Blügel, I. Mertig,
Screening of long-range Coulomb interaction in graphene nanoribbons: Armchair versus zigzag edges,
Phys. Rev. B **98**, 205123 (2018).

[418] J. Sánchez-Barriga, I. Aguilera, L. V. Yashina, D. Y. Tsukanova, F. Freyse, A. N. Chaika, C. Callaert, A. M. Abakumov, J. Hadermann, A. Varykhalov, E. D. L. Rienks, G. Bihlmayer, S. Blügel, O. Rader,
Anomalous behavior of the electronic structure of (Bi 1 − x In x) 2 Se 3 across the quantum phase transition from topological to trivial insulator,
Phys. Rev. B **98**, 235110 (2018).

[419] B. Zimmermann, W. Legrand, D. Maccariello, N. Reyren, V. Cros, S. Blügel, A. Fert,
Dzyaloshinskii-Moriya interaction at disordered interfaces from ab initio theory: Robustness against intermixing and tunability through dusting,
Applied Physics Letters **113**, 232403 (2018).

[420] V. Caciuc, N. Atodiresei, S. Blügel,
Magnetic properties of transition metal dichalcogenides-Fe/Ir(111) interfaces from first principles,
Physical review materials **2**, 084001 (2018).

[421] K. Rushchanskii, S. Blügel, M. Ležaić,
Routes for increasing endurance and retention in HfO 2 -based resistive switching memories,
Physical review materials **2**, 115002 (2018).

[422] P. Rüßmann, S. K. Mahatha, P. Sessi, M. A. Valbuena, T. Bathon, K. Fauth, S. Godey, A. Mugarza, K. A. Kokh, O. E. Tereshchenko, P. Gargiani, M. Valvidares, E. Jiménez, N. B. Brookes, M. Bode, G. Bihlmayer, S. Blügel, P. Mavropoulos, C. Carbone, A. Barla,
Towards microscopic control of the magnetic exchange coupling at the surface of a topological insulator,
JPhys materials **1**, 015002 (2018).

[423] 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, H. Ebert,
Spin caloric transport from density-functional theory,
Journal of Physics / D Applied physics D **52**, 073001 (2019).

[424] E. Młyńczak, M. C. T. D. Müller, P. Gospodarič, T. Heider, I. Aguilera, G. Bihlmayer, M. Gehlmann, M. Jugovac, G. Zamborlini, C. Tusche, S. Suga, V. Feyer, L. Plucinski, C. Friedrich, S. Blügel, C. M. Schneider,
Kink far below the Fermi level reveals new electron-magnon scattering channel in Fe,
Nature Communications **10**, 505 (2019).

[425] K. Rushchanskii, S. Blügel, M.Ležaić,

Ab initio phase diagrams of Hf–O, Zr–O and Y–O: a comparative study,
Faraday discussions of the Chemical Society **213**, 321 (2019).

[426] X. Zhou, J.-P. Hanke, W. Feng, F. Li, G.-Y. Guo, Y. Yao, S. Blügel, Y. Mokrousov,
Spin-order dependent anomalous Hall effect and magneto-optical effect in the noncollinear antiferromagnets Mn 3 X N with X = Ga, Zn, Ag, or Ni,
Phys. Rev. B **99**, 104428 (2019).

[427] M. Redies, F. Lux, J.-P. Hanke, P. Buhl, G. Müller, N. Kiselev, S. Blügel, Y. Mokrousov,
Distinct magnetotransport and orbital fingerprints of chiral bobbers,
Phys. Rev. B **99**, 140407 (2019).

[428] B. Zimmermann, G. Bihlmayer, M. Böttcher, M. Bouhassoune, S. Lounis, J. Sinova, S. Heinze, S. Blügel, B. Dupé,
Comparison of first-principles methods to extract magnetic parameters in ultrathin films: Co/Pt(111),
Phys. Rev. B **99**, 214426 (2019).

[429] G. Müller, M. Hoffmann, C. Dißelkamp, D. Schürhoff, S. Mavros, M. Sallermann, N. S. Kiselev, H. Jónsson, S. Blügel,
Spirit: Multifunctional framework for atomistic spin simulations,
Phys. Rev. B **99**, 224414 (2019).

[430] M. Schmitt, P. Moras, G. Bihlmayer, R. Cotsakis, M. Vogt, J. Kemmer, A. Belabbes, P. M. Sheverdyaeva, A. K. Kundu, C. Carbone, S. Blügel, M. Bode,
Indirect chiral magnetic exchange through Dzyaloshinskii–Moriya-enhanced RKKY interactions in manganese oxide chains on Ir(100),
Nature Communications **10**, 2610 (2019).

[431] M. Bouhassoune, I. L. Fernandes, S. Blügel, S. Lounis,
Unoccupied surface and interface states in Pd thin films deposited on Fe/Ir(111) surface,
New Journal of Physics **21**, 063015 (2019).

[432] C. Niu, J.-P. Hanke, P. M. Buhl, H. Zhang, L. Plucinski, D. Wortmann, S. Blügel, G. Bihlmayer, Y. Mokrousov,
Mixed topological semimetals driven by orbital complexity in two-dimensional ferromagnets,
Nature Communications **10**, 3179 (2019).

[433] M. C. T. D. Müller, S. Blügel, C. Friedrich,
Electron-magnon scattering in elementary ferromagnets from first principles: Lifetime broadening and band anomalies,
Phys. Rev. B **100**, 045130 (2019).

[434] E. Sasioglu, S. Blügel, I. Mertig,
Proposal for Reconfigurable Magnetic Tunnel Diode and Transistor,
ACS applied electronic materials **1**, 1552 - 1559 (2019).

[435] M. Bornemann, S. Grytsiuk, P. F. Baumeister, M. dos Santos Dias, R. Zeller, S. Lounis, S. Blügel,
Complex magnetism of B20-MnGe: from spin-spirals, hedgehogs to monopoles,
Journal of physics/Condensed matter **31**, 485801 (2019).

[436] A. Neroni, E. Şaşıoğlu, H. Hadipour, C. Friedrich, S. Blügel, I. Mertig, M. Ležaić,
First-principles calculation of the effective on-site Coulomb interaction parameters for Sr2 ABO6 (A = Cr, Mn, Fe, Co, Ni, and B = Mo, W) double perovskites,
Phys. Rev. B **100**, 115113 (2019).

[437] V. Caciuc, N. Atodiresei, S. Blügel,
Ab initio study of magnetic nanopatterning of a hybrid transition metal dichalcogenides/Ir(111) system via magnetic clusters,
Physical review materials **3**, 094002 (2019).

[438] I. Aguilera, C. Friedrich, S. Blügel,
Many-body corrected tight-binding Hamiltonians for an accurate quasiparticle description of topological insulators of the Bi 2 Se 3 family,
Phys. Rev. B **100**, 155147 (2019).

[439] A. Al-Zubi, G. Bihlmayer, S. Blügel,
Electronic Structure of oxygen deficient SrTiO3 and Sr2TiO4,
Crystals **9**, 580 (2019).

[440] S. Grytsiuk, M. Hoffmann, J.-P. Hanke, P. Mavropoulos, Y. Mokrousov, G. Bihlmayer, S. Blügel,
Ab initio analysis of magnetic properties of the prototype B20 chiral magnet FeGe,
Phys. Rev. B **100**, 214406 (2019).

[441] W. Feng, J.-P. Hanke, X. Zhou, G.-Y. Guo, S. Blügel, Y. Mokrousov, Y. Yao,
Topological magneto-optical effects and their quantization in noncoplanar antiferromagnets,
Nature Communications **11**, 118 (2020).

[442] G. Pizzi, V. Vitale, R. Arita, S. Blügel, F. Freimuth, G. Géranton, M. Gibertini, D. Gresch, C. Johnson, T. Koretsune, J. Ibanez, H. Lee, J.-M. Lihm, D. Marchand, A. Marrazzo, Y. Mokrousov, J. I. Mustafa, Y. Nohara, Y. Nomura, L. Paulatto, S. Ponce, T. Ponweiser, J. Qiao, F. Thöle, S. S. Tsirkin, M. Wierzbowska, N. Marzari, D. Vanderbilt, I. Souza, A. A. Mostofi, J. R. Yates,
Wannier90 as a community code: new features and applications,
Journal of physics/Condensed matter **32**, 165902 (2020).

[443] L.-C. Zhang, Y. A. Onykiienko, P. M. Buhl, Y. V. Tymoshenko, P. Čermák, A. Schneidewind, J. R. Stewart, A. Henschel, M. Schmidt, S. Blügel, D. S. Inosov, Y. Mokrousov,
Magnonic Weyl states in Cu2OSeO3,
Physical review research **2**, 013063 (2020).

[444] S. Grytsiuk, J.-P. Hanke, M. Hoffmann, J. Bouaziz, O. Gomonay, G. Bihlmayer, S. Lounis, Y. Mokrousov, S. Blügel,
Topological–chiral magnetic interactions driven by emergent orbital magnetism,
Nature Communications **11**, 511 (2020).

[445] H. Jia, B. Zimmermann, G. Michalicek, G. Bihlmayer, S. Blügel,
Electric dipole moment as descriptor for interfacial Dzyaloshinskii-Moriya interaction,
Physical review materials **4**, 024405 (2020).

[446] X. Zhou, J.-P. Hanke, W. Feng, S. Blügel, Y. Mokrousov, Y. Yao,
Giant anomalous Nernst effect in noncollinear antiferromagnetic Mn-based antiperovskite nitrides,
Physical review materials **4**, 024408 (2020).

[447] F. Lux, F. Freimuth, S. Blügel, Y. Mokrousov,
Chiral Hall Effect in Noncollinear Magnets from a Cyclic Cohomology Approach,
Phys. Rev. Lett. **124**, 096602 (2020).

[448] M. Hoffmann, S. Blügel,
Systematic derivation of realistic spin models for beyond-Heisenberg solids,
Phys. Rev. B **101**, 024418 (2020).

[449] G. Bihlmayer, J. Sassmannshausen, A. Kubetzka, S. Blügel, K. von Bergmann, R. Wiesendanger,
Plumbene on a Magnetic Substrate: A Combined Scanning Tunneling Microscopy and Density Functional Theory Study,
Phys. Rev. Lett. **124**, 126401 (2020).

[450] A. Varykhalov, F. Freyse, I. Aguilera, M. Battiato, M. Krivenkov, D. Marchenko, G. Bihlmayer, S. Blügel, O. Rader, J. Sánchez-Barriga,
Effective mass enhancement and ultrafast electron dynamics of Au(111) surface state coupled to a quantum well,
Physical review research **2**, 013343 (2020).

[451] G. Müller, F. N. Rybakov, H. Jónsson, S. Blügel, N.Kiselev,
Coupled quasimonopoles in chiral magnets,
Phys. Rev. B **101**, 184405 (2020).

[452] S. Tsukamoto, V. Caciuc, N. Atodiresei, S.Blügel,
Spin-polarized electron transmission through B-doped graphene nanoribbons with Fe functionalization: a first-principles study,
New journal of Physics **22**, 063022 (2020).

[453] M. Hoffmann, G. P. Müller, S. Blügel,
Atomistic Perspective of Long Lifetimes of Small Skyrmions at Room Temperature,
Phys. Rev. Lett. **124**, 247201 (2020).

[454] K. Samanta, M. Lezaic, M. Merte, F. Freimuth, S. Blügel, Y. Mokrousov,
Crystal Hall and crystal magneto-optical effect in thin films of SrRuO 3,
Journal of Applied Physics **127**, 213904 (2020).

[455] E. Sasioglu, T. Aull, D. Kutschabsky, S. Blügel, I. Mertig,
Half-Metal–Spin-Gapless-Semiconductor Junctions as a Route to the Ideal Diode,
Phys. Rev. Applied **14**, 014082 (2020).

[456] S. Tsukamoto, V. Caciuc, N. Atodiresei, S. Blügel,
Spin-polarized electron transmission through B-doped graphene nanoribbons with Fe functionalization: a first-principles study,
New Journal of Physics **22**, 063022 (2020).

[457] H. Jia, B. Zimmermann, M. Hoffmann, M. Sallermann, G. Bihlmayer, S. Blügel,
Material systems for FM-/AFM-coupled skyrmions in Co/Pt-based multilayers,
Physical review materials **4**, 094407 (2020).

[458] M. Bosnar, V. Caciuc, N. Atodiresei, I. Lončarić, S. Blügel,
Se intercalation between Pt Se 2 and the Pt surface during synthesis of Pt Se 2 by direct selenization of Pt(111),
Phys. Rev. B **102**, 115427 (2020).

[459] D. Go, F. Freimuth, J.-P. Hanke, F. Xue, O. Gomonay, K.-J. Lee, S. Blügel, P. M. Haney, H.-W. Lee, Y. Mokrousov,
Theory of current-induced angular momentum transfer dynamics in spin-orbit coupled systems,
Physical review research **2**, 033401 (2020).

[460] V. Kuchkin, B. Barton-Singer, F. N. Rybakov, S. Blügel, B. J. Schroers, N. S. Kiselev,
Magnetic skyrmions, chiral kinks, and holomorphic functions,
Phys. Rev. B **102**, 144422 (2020).

[461] A. Kosma, P. Rüßmann, S. Blügel, P. Mavropoulos,
Strong spin-orbit torque effect on magnetic defects due to topological surface state electrons in Bi 2 Te 3,
Phys. Rev. B **102**, 144424 (2020.

[462] G. Chen, A. Mascaraque, H. Jia, B. Zimmermann, M. Robertson, R. L. Conte, M. Hoffmann, M. A. González Barrio, H. Ding, R. Wiesendanger, E. G. Michel, S. Blügel, A. K. Schmid, K. Liu,
Large Dzyaloshinskii-Moriya interaction induced by chemisorbed oxygen on a ferromagnet surface,
Science advances **6**, eaba4924 (2020).

[463] A. S. Kebaili, S. Blizak, G. Bihlmayer, S. Blügel,
Magnetic properties of ultra-thin (Fe, Co) films coupled by Ir(001) spacers,
Physica B **596**, 412395 (2020).

[464] T. R. F. Peixoto, H. Bentmann, P. Rüßmann, A.-V. Tcakaev, M. Winnerlein, S. Schreyeck, S. Schatz, R. C. Vidal, F. Stier, V. Zabolotnyy, R. J. Green, C. H. Min, C. I. Fornari, H. Maaß, H. B. Vasili, P. Gargiani, M. Valvidares, A. Barla, J. Buck, M. Hoesch, F. Diekmann, S. Rohlf, M. Kalläne, K. Rossnagel, C. Gould, K. Brunner, S. Blügel, V. Hinkov, L. W. Molenkamp, F. Reinert,
Non-local effect of impurity states on the exchange coupling mechanism in magnetic topological insulators,
Npj quantum materials **5**, 87 (2020).

[465] M. Redies, F. R. Lux, J.-P. Hanke, P. M. Buhl, S. Blügel, Y. Mokrousov,
Mixed topology ring states for Hall effect and orbital magnetism in skyrmions of Weyl semimetals,
Phys. Rev. B **102**, 184407 (2020).

[466] M. Winkelmann, E. Di Napoli, D. Wortmann, S. Blügel,
Kerker mixing scheme for self-consistent muffin-tin based all-electron electronic structure calculations,

Phys. Rev. B **102**, 195138 (2020).

[467] L.-C. Zhang, D. Go, J.-P. Hanke, P. M. Buhl, S. Grytsiuk, S. Blügel, F. R. Lux, Y. Mokrousov,
Imprinting and driving electronic orbital magnetism using magnons,
Communications Physics **3**, 227 (2020).

[468] F. Freimuth, S. Blügel, Y. Mokrousov,
Dynamical and current-induced Dzyaloshinskii-Moriya interaction: Role for damping, gyromagnetism, and current-induced torques in noncollinear magnets,
Phys. Rev. B **102**, 245411 (2020).

[469] F. J. Dos Santos, N. Biniskos, S. Raymond, K. Schmalzl, M. dos Santos Dias, P. Steffens, J. Persson, S. Blügel, S. Lounis, T. Brückel,
Spin waves in the collinear antiferromagnetic phase of Mn 5 Si 3,
Phys. Rev. B **103**, 024407 (2021).

[470] E. Mendive-Tapia, M. dos Santos Dias, S. Grytsiuk, J. B. Staunton, S. Blügel, S. Lounis,
Short period magnetization texture of B20-MnGe explained by thermally fluctuating local moments,
Phys. Rev. B **103**, 024410 (2021).

[471] P. Rüßmann, P. Mavropoulos, S. Blügel,
Ab Initio Theory of Fourier-Transformed Quasiparticle Interference Maps and Application to the Topological Insulator Bi2Te3,
Physica status solidi B **258**, 2000031 (2021).

[472] E. Mlynczak, I. Aguilera, P. Gospodaric, T. Heider, M. Jugovac, G. Zamborlini, C. Tusche, S. Suga, V. Feyer, S. Blügel, L. Plucinski, C. M. Schneider,
Spin-polarized quantized electronic structure of Fe(001) with symmetry breaking due to the magnetization direction,
Phys. Rev. B **103**, 035134 (2021).

[473] F. Freimuth, S. Blügel, Y. Mokrousov,
Charge and spin photocurrents in the Rashba model,
Phys. Rev. B **103**, 075428 (2021).

[474] P. Rüssmann, F. Bertoldo, S. Blügel,
The AiiDA-KKR plugin and its application to high-throughput impurity embedding into a topological insulator,
npj computational materials **7**, 13 (2021).

[475] K. Samanta, M. Ležaić, S. Blügel, Y. Mokrousov,
Tailoring the anomalous Hall effect of SrRuO 3 thin films by strain: A first principles study,
Journal of Applied Physics **129**, 093904 (2021).

[476] D. Go, D. Jo, T. Gao, K. Ando, S. Blügel, H.-W. Lee, Y. Mokrousov,
Orbital Rashba effect in a surface-oxidized Cu film,
Phys. Rev. B **103**, L121113 (2021).

[477] J. Bouaziz, H. Ishida, S. Lounis, S. Blügel,

Transverse Transport in Two-Dimensional Relativistic Systems with Nontrivial Spin Textures,
Phys. Rev. Lett. **126**, 147203 (2021).

[478] G.Chen, M. Robertson, M. Hoffmann, C. Ophus, A. L. Fernandes Cauduro, R. Lo Conte, H. Ding, R. Wiesendanger, S. Blügel, A. K. Schmid, K. Liu,
Observation of Hydrogen-Induced Dzyaloshinskii-Moriya Interaction and Reversible Switching of Magnetic Chirality,
Physical review X **11**, 021015 (2021).

[479] M. dos Santos Dias, S. Brinker, A. Lászlóffy, B. Nyári, S. Blügel, L. Szunyogh, S. Lounis,
Proper and improper chiral magnetic interactions,
Phys. Rev. B **103**, L140408 (2021).

[480] F. Freimuth, S. Blügel, Y. Mokrousov,
Laser-induced torques in metallic antiferromagnets,
Phys. Rev. B **103**, 174429 (2021).

[481] F. Freimuth, S. Blügel, Y. Mokrousov,
Spin-orbit torques in strained PtMnSb from first principles,
Phys. Rev. B **103**, 224414 (2021).

[482] Y. Yekta, H. Hadipour, E. Sasioglu, C. Friedrich, S. A. Jafari, S. Blügel, I. Mertig,
Strength of effective Coulomb interaction in two-dimensional transition-metal halides M X 2 and M X 3 (M = Ti , V, Cr, Mn, Fe, Co, Ni; X = Cl , Br, I),
Physical review materials **5**, 034001 (2021).

[482] J. Kipp, K. Samanta, F. R. Lux, M. Merte, D. Go, J.-P. Hanke, M. Redies, F. Freimuth, S. Blügel, M. Ležaić, Y. Mokrousov,
The chiral Hall effect in canted ferromagnets and antiferromagnets,
Communications Physics **4**, 99 (2021).

[483] C. Friedrich, S. Blügel, A. Schindlmayr,
Erratum: Efficient implementation of the G W approximation within the all-electron FLAPW method [Phys. Rev. B 81 , 125102 (2010)],
Phys. Rev. B **104**, 039901 (2021).

[484] F.Zheng, F. N. Rybakov, N. Kiselev, D. Song, A. Kovács, H. Du, S. Blügel, R. E. Dunin-Borkowski,
Magnetic skyrmion braids,
Nature Communications **12**, 5316 (2021).

[485] F. Freimuth, S. Blügel, Y. Mokrousov,
Effect of magnons on the temperature dependence and anisotropy of spin-orbit torque,
Phys. Rev. B **104**, 094434 (2021).

[486] I. Aguilera, H.-J. Kim, C. Friedrich, G. Bihlmayer, S.Blügel,
Z 2 topology of bismuth,
Physical review materials 5, L091201 (2021).

[487] F. Zhu, L. Zhang, X. Wang, F. J. Dos Santos, J. Song, T. Mueller, K. Schmalzl, W. F. Schmidt, A. Ivanov, J. T. Park, J. Xu, J. Ma, S. Lounis, S. Blügel, Y. Mokrousov,

Y. Su, T. Brückel,
Topological magnon insulators in two-dimensional van der Waals ferromagnets CrSiTe3 and CrGeTe3 : Toward intrinsic gap-tunability,
Science advances **7**, eabi7532 (2021).

[488] D. Nabok, S. Blügel, C. Friedrich,
Electron–plasmon and electron–magnon scattering in ferromagnets from first principles by combining GW and GT self-energies,
npj computational materials **7**, 178 (2021).

[489] V. Kuchkin, K. Chichay, B. Barton-Singer, F. N. Rybakov, S. Blügel, B. J. Schroers, N. S. Kiselev,
Geometry and symmetry in skyrmion dynamics,
Phys. Rev. B **104**, 165116 (2021).

[490] P. M.Sheverdyaeva, F. Offi, S. Gardonio, L. Novinec, M. I. Trioni, D. Ceresoli, S. Iacobucci, A. Ruocco, G. Stefani, L. Petaccia, S. Gorovikov, E. Cappelluti, P. Moras, G. Bihlmayer, S. Blügel, C. Carbone,
Topological properties and self-energy effects in elemental Yb,
Phys. Rev. B **104**, 195138 (2021).

[491] K. Rushchanskii, S. Blügel, M. Ležaić,
Ordering of Oxygen Vacancies and Related Ferroelectric Properties in HfO 2 – δ,
Phys. Rev. Lett. **127**, 087602 (2021).

[492] M. Merte, M. Freimuth, T. Adamantopoulos, D. Go, T. G. Saunderson, M. Kläui, L. Plucinski, O. Gomonay, S. Blügel, Y. Mokrousov,
Photocurrents of charge and spin in monolayer Fe 3 GeTe 2,
Phys. Rev. B **104**, L220405 (2021).

[493] D. Popova-Gorelova, A. Bringer, S. Blügel,
Heisenberg representation of nonthermal ultrafast laser excitation of magnetic precessions,
Phys. Rev. B **104**, 224418 (2021).

[494] F. Freimuth, S. Blügel, Y. Mokrousov,
Theory of unidirectional magnetoresistance and nonlinear Hall effect,
Journal of Physics/Condensed matter **34**, 055301 (2022).

[495] M. dos Santos Dias, S. Brinker, A. Lászlóffy, B. Nyári, S. Blügel, L. Szunyogh, S. Lounis,
Reply to “Comment on ‘Proper and improper chiral magnetic interactions,
Phys. Rev. B **105**, 026402 (2022).

[496] C. C. Silva, D. Dombrowski, N. Atodiresei, W. Jolie, F. Farwick zum Hagen, J. Cai, P. T. P. Ryan, P. K. Thakur, V. Caciuc, S. Blügel, D. A. Duncan, T. Michely, T.-L. Lee, C. Busse,
Spatial variation of geometry, binding, and electronic properties in the moiré superstructure of MoS 2 on Au(111),
2D Materials **9**, 025003 (2022).

[497] W. Legrand, Y. Sassi, F. Ajejas, S. Collin, L. Bocher, H. Jia, M. Hoffmann, B. Zimmermann, S. Blügel, N. Reyren, V. Cros, A. Thiaville,

Spatial extent of the Dzyaloshinskii-Moriya interaction at metallic interfaces,
Physical review materials **6**, 024408 (2022).

[498] H.-H. Yang, N. Bansal, P. Rüßmann, M. Hoffmann, L. Zhang, D. Go, Q. Li, A.-A. Haghighirad, K. Sen, S. Blügel, M. Le Tacon, Y. Mokrousov, W. Wulfhekel,
Magnetic domain walls of the van der Waals material Fe 3 GeTe 2,
2D Materials **9**, 025022 (2022).

[499] S. Ghosh, F. Freimuth, O. Gomonay, S. Blügel, Y. Mokrousov,
Driving spin chirality by electron dynamics in laser-excited antiferromagnets,
Communications Physics **5**, 69 (2022).

[500] N. Biniskos, F. J. dos Santos, K. Schmalzl, S. Raymond, M. dos Santos Dias, J. Perßon, N. Marzari, S. Blügel, S. Lounis, T. Brückel,
Complex magnetic structure and spin waves of the noncollinear antiferromagnet Mn5Si3,
Phys. Rev. B **105**, 104404 (2022).

[501] I. Lima Fernandes, S. Blügel, S. Lounis,
Spin-orbit enabled all-electrical readout of chiral spin-textures,
Nature Communications **13**, 1576 (2022).

[502] E. Młyńczak, I. Aguilera, P. Gospodarič, T. Heider, M. Jugovac, G. Zamborlini, J.-P. Hanke, C. Friedrich, Y. Mokrousov, C. Tusche, S. Suga, V. Feyer, S. Blügel, L. Plucinski, C. M. Schneider,
Fe(001) angle-resolved photoemission and intrinsic anomalous Hall conductivity in Fe seen by different ab initio approaches: LDA and GGA versus GW,
Phys. Rev. B **105**, 115135 (2022).

[503] P. Rüssmann, S. Blügel,
Density functional Bogoliubov-de Gennes analysis of superconducting Nb and Nb(110) surfaces,
Phys. Rev. B **105**, 125143 (2022).

[504] M. Redies, G. Michalicek, J. Bouaziz, C. Terboven, M. Müller, S. Blügel, D. Wortmann,
Fast All-Electron Hybrid Functionals and Their Application to Rare-Earth Iron Garnets,
Frontiers in Materials **9**, 851458 (2022).

[505] J. Bouaziz, E. Mendive-Tapia, S. Blügel, J. B. Staunton,
Fermi-Surface Origin of Skyrmion Lattices in Centrosymmetric Rare-Earth Intermetallics,
Phys. Rev. Lett. **128**, 157206 (2022).

[506] D. Nabok, M. Tas, S. Kusaka, E. Durgun, C. Friedrich, G. Bihlmayer, S. Blügel, T. Hirahara, I. Aguilera,
Bulk and surface electronic structure of Bi 4 Te 3 from G W calculations and photoemission experiments,
Physical review materials **6**, 034204 (2022).

[507] M. Sajedi, M. Krivenkov, D. Marchenko, J. Sánchez-Barriga, A. Kaithalikunnel Chandran, A. Varykhalov, E. D. L. Rienks, I. Aguilera, S. Blügel, O. Rader,
Is There a Polaron Signature in Angle-Resolved Photoemission of CsPbBr3?,
Phys. Rev. Lett. **128**, 176405 (2022).

[508] A. Savchenko, F. Zheng, N. Kiselev, L. Yang, F. N. Rybakov, S. Blügel, R. E. Dunin-Borkowski,
Diversity of states in a chiral magnet nanocylinder,
APL materials **10**, 061110 (2022).

[509] J. Goikoetxea, C. Friedrich, G. Bihlmayer, S. Blügel, A. Arnau, M. Blanco-Rey,
Multiplet effects in the electronic correlation of one-dimensional magnetic transition metal oxides on metals,
Phys. Rev. B **106**, 035130 (2022).

[510] A. Savchenko, V. Kuchkin, F. N. Rybakov, S. Blügel, N. S. Kiselev,
Chiral standing spin waves in skyrmion lattice,
APL materials **10**, 071111 (2022).

[511] F. Zheng, N. Kiselev, L. Yang, V. M. Kuchkin, F. N. Rybakov, S. Blügel, R. E. Dunin-Borkowski,
Skyrmion–antiskyrmion pair creation and annihilation in a cubic chiral magnet,
Nature physics **18**, 863–868 (2022).

[512] F. Freimuth, S. Blügel, Y. Mokrousov
Construction of the spectral function from noncommuting spectral moment matrices
Phys. Rev. B **106,** 045135 (2022).

[513] Y.-J. Chen, J.-P. Hanke, M. Hoffmann, G. Bihlmayer, Y. Mokrousov, S. Blügel, C. M. Schneider, C. Tusche,
Spanning Fermi arcs in a two-dimensional magnet,
Nature Communications **13**, 5309 (2022).

[514] J. Carbone, D. Go, Y. Mokrousov, G. Bihlmayer, S. Blügel,
Engineering spin-orbit effects and Berry curvature by deposition of a monolayer of Eu on WSe 2,
Phys. Rev. B **106**, 064401 (2022).

[515] C. Friedrich, S. Blügel, D. Nabok,
Quasiparticle Self-Consistent GW Study of Simple Metals,
Nanomaterials, **12,** 3660 (2022).

[516] M. Schmitt, T. Denneulin, A. Kovács, T. G. Saunderson, P. Rüßmann, A. Shahee, T. Scholz, A. H. Tavabi, M. Gradhand, P. Mavropoulos, B. V. Lotsch, R. E. Dunin-Borkowski, Y. Mokrousov, S. Blügel, M. Kläui,
Skyrmionics spin structures in layered Fe5GeTe2 up to room temperature,
Communications Physic, **5**, 254 (2022).

[517] M. Tas, E. Şaşıoğlu, S. Blügel, I. Mertig, 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. B **6**, 114401 (2022).

[518] T. G. Saunderson, D. Go, S. Blügel, M. Kläui, Y. Mokrousov,
Hidden interplay of current-induced spin and orbital torques in bulk Fe3GeTe2,
Phys. Rev. Research **4**, L042022 (2022).

[519] A. Jacobsson, G. Johansson, O. I. Gorbatov, M. Ležaić, B. Sanyal, S. Blügel, C. Etz,
Efficient parameterisation of non-collinear energy landscapes in itinerant magnets,
Scientific Reports **12**, 18987(2022).

[520] F.N. Rybakov, N. S. Kiselev, A. B. Borisov, L. Döring, C. Melcher, S. Blügel,
Magnetic hopfions in solids,
APL Materials **10**, 111113 (2022).

[521] Y. Mokrousov, M. Merte, F. Freimuth, D. Go, T. Adamantopoulos, F. R. Lux, L. Plucinski, O. Gormonay, S. Blügel,
Photocurrents, inverse Faraday effect, and photospin Hall effect in Mn2Au,
APL Materials **11**, 071106 (2023).

[522] A. Aldarawsheh, I. L. Fernandes, S. Brinker, M. Sallermann, M. Abusaa, S. Blügel, S. Lounis,
Emergence of zero-field non-synthetic single and interchained antiferromagnetic skyrmions in thin films,
Nature Communications **13**, 7369 (2022).

[523] Y. H. Lin, C. J. Chen, N. Kumar, T. Y. Yeh, T. H. Lin, S. Blügel, G. Bihlmayer, P. J. Hsu,
Fabrication and Imaging Monatomic Ni Kagome Lattice on Superconducting Pb(111),
Nano Letters **22**, 8475 - 8481 (2022).

[524] M. Bui, S. Rost, M. Auge, J. S. Tu, L. Zhou, I. Aguilera, S. Blügel, M. Ghorbani-Asl, A. V. Krasheninnikov, A. Hashemi, H. P. Komsa, L. Jin, L. Kibkalo, E. N. O'Connell, Q. M. Ramasse, U. Bangert, H. C. Hofsäss, D. Grützmacher, B. Kardynal,
Low-energy Se ion implantation in MoS2 monolayers,
npj 2D materials and applications **6**, 42 (2022).

[525] M. Bui, S. Rost, M. Auge, L. Zhou, C. Friedrich, S. Blügel, S. Kretschmer, A. V. Krasheninnikov, K. Watanabe, T. Taniguchi, H. C. Hofsäss, D. Grützmacher, B. Kardynal,
Optical Properties of MoSe 2 Monolayer Implanted with Ultra-Low-Energy Cr Ions,
ACS applied materials & interfaces **15**, 35321 - 35331 (2023).

[526] S. Ghosh, S. Blügel, Y. Mokrousov,
Ultrafast optical generation of antiferromagnetic meron-antimeron pairs with conservation of topological charge,
Physical Rev. Research **5**, L022077 (2023).

[527] M. Sallermann, H. Jónsson, S. Blügel
Stability of hopfions in bulk magnets with competing exchange interactions
Phys. Rev. B **107,** 104404 (2023).

[528] S. Rost, S. Blügel, C. Friedrich,
Efficient calculation of k-integrated electron energy loss spectra: Application to monolayers of MoS 2, hBN, and graphene,
Phys. Rev. B. **107** (**8**), 085132 (2023).

[529] A. Aldarawsheh, M. Sallermann, M. Abusaa, S. Lounis,
A spin model for intrinsic antiferromagnetic skyrmions on a triangular lattice,
Front. Phys. **11**, 1175317 (2023).

[530] V. M. Kuchkin, N. S. Kiselev, F. N. Rybakov, I. S. Lobanov, S. Blügel, V. M. Uzdin,
Heliknoton in a film of cubic chiral magnet,
Front. Phys. **11,** 1201018 (2023).

[531] G. D. A. Wood, D. D. Khalyavin, D. A. Mayoh, J. Bouaziz, A. E. Hall, S. J. R. Holt, F. Orlandi, P. Manuel, S. Blügel, J. B. Staunton, O. A. Petrenko, M. R. Lees, G. Balakrishnan,
Double-Q ground state with topological charge stripes in the centrosymmetric skyrmion candidate GdRu2Si2
Phys. Rev. B**107**, L180402 (2023).

[532] D. Go, M. Sallermann, F. R. Lux, S. Blügel, O. Gomonay, Y. Mokrousov,
Noncollinear Spin Current for Switching of Chiral Magnetic Textures,
Phys. Rev. 129, 097204 (2023).

[533] M. Jugovac, I. Cojocariu. J. Sánchez-Barriga, P. Gargiani, M. Valvidares, V. Feyer, S. Blügel, G. Bihlmayer, P. Perna,
Inducing Single Spin-Polarized Flat Bands in Monolayer Graphene,
Advanced materials **35**, 2301441 (2023).

[534] M. Dos Santos Dias, N. Biniskos, F. J. dos Santos, K. Schmalzl, J. Perßon, F. Bourdarot, N. Marzari, S. Blügel, T. Brückel, S. Lounis,
Topological magnons driven by the Dzyaloshinskii-Moriya interaction in the centrosymmetric ferromagnet Mn5Ge3,
Nature Communications **14**, 7321 (2023).

[535] F. Zheng, N. S. Kiselev, F. N. Rybakov, L. Yang, W. Shi, S. Blügel, R. E. Dunin Borkowski,
Hopfion rings in a cubic chiral magnet,
Nature **623**, 718 - 723 (2023).

[536] J. P. Carbone, J. Bouaziz, G. Bihlmayer, S. Blügel,
Magnetic properties of 4 f adatoms on graphene: Density functional theory investigations,
Phys. Rev. B **108**, 174431 (2023).

[537] D. Go, D. Jo, K. W. Kim, S. Lee, M. G. Kang, B. G. Park, S. Blügel, H. W. Lee, Y. Mokrousov,
Long-Range Orbital Torque by Momentum-Space Hotspots,
Phys. Rev **130**, 246701 (2023).

[538] K. Z. Rushchanskii, M. Lezaic, S. Blügel,
Doped HfO x Nanoclusters: Polar and Resistive Switching in the Smallest Functional Units,
Phys status solidi A ,2300404 (2023).

[539] X. Wei, A. R. Jalil, P. Rüßmann, Y. Ando, D. Grützmacher, S. Blügel, J. Mayer,
Atomic Diffusion-Induced Polarization and Superconductivity in Topological Insulator-Based Heterostructures,
ACS nano **XXX,** acsnano.3c08601 (2023).

[540] N. Biniskos, F. J. Dos Santos, M. dos Santos Dias, S. Raymond, K. Schmalzl, P. Steffens, J. Perßon, N. Marzari, S. Blügel, S. Lounis, T. Brückel,
An overview of the spin dynamics of antiferromagnetic Mn5Si3,
APL materials **11,** 081103 (2023).

[541] C. R. Gerhorst, A. Neukirchen, D. A. Klüppelberg, G. Bihlmayer, M. Betzinger, G. Michalicek, D. Wortmann, S. Blügel,
*Phonons from density-functional perturbation theory using the all-electron full-potential linearized augmented plane-wave method FLEUR *,*
Electronic structure **6**, 017001 (2024).

[542] E. Bosoni, L. Beal, M. Bercx, P. Blaha, S. Blügel, J. Bröder, M. Callsen, S. Cottenier, A. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, M. Fornari, A. Garcia, et al.,
How to verify the precision of density-functional-theory implementations via reproducible and universal workflows,
Nat Rev Phys **6**, 45–58 (2024).

[543] M. Zeer, D. Go, P. Schmitz, T. G. Saunderson, H. Wang, J. Ghabboun, S. Blügel, W. Wulfhekel, Y. Mokrousov,
Promoting p -based Hall effects by p − d − f hybridization in Gd-based dichalcogenides,
Physical review research **6**, 013095 (2024).

[544] T. Adamantopoulos, M. Merte, D. Go, F. Freimuth, S. Blügel, Y. Mokrousov,
Orbital Rashba Effect as a Platform for Robust Orbital Photocurrents,
Phys. Rev. Lett. **132**, 076901 (2024).

[545] Y. J. Chen, T. H. Chuang, J. P. Hanke, Y. Mokrousov, S. Blügel, C. M. Schneider, C. Tusche,
Magnons in a two-dimensional Weyl magnet,
Applied physics letters **124**, 093105 (2024).

[546] H. Miao, J. Bouaziz, G. Fabbris, W. R. Meier, F. Z. Yang, H. X. Li, C. Nelson, E. Vescovo, S. Zhang, A. D. Christianson, H. N. Lee, Y. Zhang, C. D. Batista, S. Blügel,
Spontaneous Chirality Flipping in an Orthogonal Spin-Charge Ordered Topological Magnet,
Physical review / X **14**, 011053 (2024).

[547] K. Janßen, P. Rüßmann, S. Liberda, M. Schleenvoigt, X. Hao, A. R. Jalil, F. Lentz, S. Trellenkamp, B. Bennemann, E. Zimmermann, G. Mussler, P. Schüffelgen, C. M. Schneider, S. Blügel, D. Grützmacher, L. Plucinski, T. Schäpers,
Characterization of single in situ prepared interfaces composed of niobium and a selectively grown (Bi 1 − x Sb x) 2 Te 3 topological insulator nanoribbon,
Physical review materials **8**, 034205 (2024).

[548] H. R. Ramezani, E. Şaşıoğlu, H. Hadipour, H. R. Soleimani, C. Friedrich, S. Blügel, I. Mertig,
Nonconventional screening of Coulomb interaction in two-dimensional semiconductors and metals: A comprehensive constrained random phase approximation study of M X 2 (M = Mo , W , Nb , Ta ; X = S , Se , Te ,
Phys. Rev. B **109**, 125108 (2024).

[549] J. Bouaziz, G. Bihlmayer, C. E. Patrick, J. B. Staunton, S. Blügel,
Origin of incommensurate magnetic order in the R AlSi magnetic Weyl semimetals (R = Pr , Nd , Sm),
Physical review / B **109**, L201108 (2024).

[550] R. Chen, D. Go, S. Blügel, W. Zhao, Y. Mokrousov,
Dzyaloshinskii-Moriya interaction from unquenched orbital angular momentum,
Phys. Rev. B **109**, 144417 (2024).

[551] B. Muñiz Cano, A. Gudín, J. Sánchez-Barriga, O. Clark, A. Anadón, J. M. Díez, P. Olleros-Rodríguez, F. Ajejas, I. Arnay, M. Jugovac J. Rault, P. Le Fèvre, F. Bertran, D. Mazhjoo, G. Bihlmayer, O. Rader, S. Blügel, R. Miranda, J. Camarero, M. A. Valbuena, P. Perna,
Rashba-like Spin Textures in Graphene Promoted by Ferromagnet-Mediated Electronic Hybridization with a Heavy Metal,
ACS nano **18**, 15716 – 15728 (2024).

[552] J. Kipp, F. R. Lux, T. Pürling, A. Morrison, S. Blügel, D. Pinna, Y. Mokrousov,
Machine learning inspired models for Hall effects in non-collinear magnets,
IOP Publishing **5**, 025060 (2024).

[553] L. Yang, A. S. Savchenko, F. Zheng, N. S. Kiselev, F. N. Rybakov, X. Han, S. Blügel, R. E. Dunin-Borkowski,
Embedded Skyrmion Bags in Thin Films of Chiral Magnets
Advanced materials, 2403274 (2024).

[554] M. Jugovac, I. Cojocariu, V. Feyer, S. Blügel, G. Bihlmayer, P. Perna,
Spin-dependent electronic phenomena in heavily-doped monolayer graphene,
Carbon **230**, 119666 - (2024).

[555] R. Mozumder, J. Wasmer, D. Antognini Silva, S. Blügel, P. Rüssmann,
High-throughput magnetic co-doping and design of exchange interactions in topological insulators,
Physical review materials **8**, 104201 (2024).

[556] P. Härtl, M. Vogt, M. Leisegang, G. Bihlmayer, S. Blügel, M. Bode,
Spin Spiral State at a Ferromagnetic Gd Vacuum Interface,
Physical review letters **133**, 186701 (2024).

[557] A. R. Jalil, T. W. Schmitt, P. Rüßmann, X.-K. Wei, B. Frohn, M. Schleenvoigt, W. Wittl, X. Hou, A. Schmidt, K. Underwood, G. Bihlmayer, M. Luysberg, J. Mayer, S. Blügel, D. Grützmacher, P. Schüffelgen,
Engineering Epitaxial Interfaces for Topological Insulator — Superconductor Hybrid Devices with Al Electrodes,
Advanced quantum technologies **0**, 2400343 (2024).

[558] V. Blum, R. Asahi, J. Autschbach, C. Bannwarth, G. Bihlmayer, S. Blügel, L. A. Burns, T. D. Crawford, W. Dawson, W. A. de Jong, C. Draxl, C. Filippi, L. Genovese, P. Giannozzi, N. Govind, S. Hammes-Schiffer, J. R. Hammond, B. Hourahine, A. Jain, Y. Kanai, P. R. C. ; Kent, A. H. Larsen, S. Lehtola, X. Li, R. Lindh, et al.
Roadmap on methods and software for electronic structure based simulations in chemistry and materials,
Electronic structure **6**, 042501 (2024).

[559] J. A. M. Paddison, J. Bouaziz, A. F. May, Q. Zhang, S. Calder, D. Abernathy, J. B. Staunton, S. Blügel, A. D. Christianson,
Spin dynamics of the centrosymmetric skyrmion material GdRu2Si2
Cell reports / Physical science **5** (11), 102280 - (2024).

[560] J. P. Carbone, G. Bihlmayer, S. Blügel,
Magnetic anisotropy of 4f atoms on a WSe2 monolayer: a DFT + U study,
npj computational materials **11**(1), 12 (2025).

[561] T. Knispel, V. Tseplyaev, G. Bihlmayer, S. Blügel, T. Michely, and J. Fischer,
Atomic-scale Dzyaloshinskii-Moriya-modified Yoshimori spirals in an Fe double layer on Ir(110),
Physical Review B **111**, L020405 (2025).

[562] E. Şaşıoğlu, M. Tas, S. Ghosh, W. Beida, B. Sanyal, S. Blügel, I. Mertig, I. Galanakis,
Spin gapped metals: A novel class of materials for multifunctional spintronic devices,
Journal of magnetism and magnetic materials **615**, 172792 - (2025).

[563] W. Beida, E. Şaşıoğlu, M. Tas, C. Friedrich, S. Blügel, I. Mertig, I. Galanakis,
Correlation effects in two-dimensional M X 2 and M A 2 Z 4 (M = Nb , Ta ; X = S , Se , Te ; A = Si , Ge ; Z = N , P) cold metals: Implications for device applications,
Phys. Rev. Materials **9**, 014006 (2025).

II. Confernce contributions with scientific quality assurance

[1] P. H. Dederichs, S. Blügel, R. Zeller, and A. Oswald,
Ground State of Constrained Systems,
in: Proceedings of the 15th Int. Symposium on Electronic Structure of Metals and Alloys (Johnsbach, GDR, 1985).

[2] S. Blügel, M. Weinert, and P. H. Dederichs,
Ab-Initio Calculations of 3d-Metal Monolayers on Pd(001),
in: Proceedings of the 18th Int. Symposium on Electronic Structure of Metals and Alloys (Gaußig, GDR, 1988).

[3] S. Blügel, M. Weinert, and P. H. Dederichs,
Magnetic Overlayers on Pd(001),
Physica Scripta T **25**, 301 (1989).

[4] S. Takizawa, S. Blügel, K. Terakura, and T. Oguchi,
Pressure Induced Phase Transition of CuPt Alloy: A Theoretical Study,
in: Proceedings of the 21th Int. Symposium on Electronic Structure of Solids (Gaussig, FRG, 1991).

[5] T. Asada and S. Blügel,
"Prediction of magnetic structures of ultra-thin Fe films on Cu(100): Successful understanding of experimental findings",
J. Magn. Magn. Mater. **177-181**, 1233, (1998).

[6] R. Abt and S. Blügel,
"First-principles investigation of the formation of Mn/Ag(100) surface alloy",
Phil. Mag. B **78**, 659 (1998).

[7] I. Turek, J. Kudrnovský, S. Blügel,
"Surface magnetism of disordered alloys",
Acta Physica Slovaca **48,** No. 6, 1-4 (1999).

[8] T. Asada, S. Blügel, G. Bihlmayer, S. Handschuh, and R. Abt,
"First-principles investigation of the stability of 3d monolayer/Fe(001) against bilayer formation",
(44th Magnetism and Magnetic Materials Conference) (1999),
J. Appl. Phys. **87**, 5935 (2000).

[9] P. Kurz, G. Bihlmayer, and S. Blügel,
"Non-Collinear Magnetism of Cr und Mn Monolayers on Cu(111)",
(44th Magnetism and Magnetic Materials Conference) (1999),
J. Appl. Phys. **87**, 6101 (2000).

[10] K. Schroeder, A. Antons, R. Berger, S. Blügel,
"Ad-atom Kinetics on Surfactant-covered Si(111), Ab initio Calculations",
Phase Trans. **75**, 91-99 (2002).

[11] Ph. Kurz, G. Bihlmayer, K. Hirai, and S. Blügel,
"Itinerant magnets on a triangular Cu(111) lattice",
Phase Trans. **75**, 101-112 (2002).

[12] I. Turek, J. Kudrnovský, V. Drchal, P. Bruno, and S. Blügel,
Ab initio theory of exchange interactions in itinerant magnets,
Physica Status Solidi B **236**, 318-324 (2003).

[13] M. Morgenstern, D. Haude, J. Klijn, Chr. Meyer, L. Sacharow, S. Heinze, S. Blügel, and R. Wiesendanger,
Comparing the Local Density of States of Three and Two Dimensional Electron Systems by Low-Temperature Scanning Tunneling Spectroscopy,
Physica E **16**, 121 (2003).

[14] I. Turek, S. Blügel, G. Bihlmayer, and P. Weinberger,
Exchange interation at surfaces of Fe, Co, and Gd,
Czech. J. Phys. **53**, 81, (2003).

[15] A. V. Postnikov, J. Kortus, and S. Blügel,
Ab initio Simulations of Fe-based Ferric Wheels,
Molecular Physics Reports **38**, 56 (2003).

[16] A. V. Postnikov, S. G. Chiuzbăian, M. Neumann, and S. Blügel,

Electron Sprectroscopy and density functional study of "ferric wheel" molecules,
J. Phys. Chem. Solid. **65**, 813 (2004).

[17] S. di Napoli, G. Bihlmayer, S. Blügel, M. Alouani, H. Dreyssé, A. M. Llois,
Band contribution to the electronic transport in noncollinear magnetic materials: application to $LaMn_2Ge_2$,
Physica B.: Condensed Matter **354**, 154-157 (2004).

[18] V. Caciuc, H. Hölscher, S. Blügel, and H. Fuchs,
Hysteretic behaviour of the tip-sample interaction on InAs(110) surface: An ab initio study,
Nanotechnology **16**, 59 (2005).

[19] A. V. Postnikov, A. V. Galakhov, and S. Blügel,
Magnetic interactions in a Cu-containing heterospin polymer,
Phase Trans. **78**, 689 (2005).

[20] A. V. Postnikov, G. Bihlmayer and S. Blügel,
Exchange parameters in Fe-based molecular magnets,
Comput. Mater. Sci. **36**, 91 (2006).

[21] Y. Mokrousov, N. Atodiresei, G. Bihlmayer and S. Blügel,
Magnetism in Molecular Vanadium-Benzene Sandwiches,
AIP Conf. Proc. **786**, 444 (2007).

[22] P. M. Kowalski, G. Beridze, Y. Li, Y. Ji, C. Friedrich, E. Şaşioğlu and S. Blügel,
Feasible and Reliable AB Initio Approach to Computation of Materials Relevant for Nuclear Waste Management,
in: Additive Manufacturing and Strategic Technologies in Advanced Ceramics / Shimamura, Kiyoshi (Editor); Hoboken, NJ, USA: John Wiley & Sons, Inc., 2016; ISBN 9781119236009,
Ceramic Transactions Series **258**, 205-217 (2016).

III. Review article with and without scientific quality assurance

[1] S. Blügel,
First Principles Calculations of the Electronic Structures of Magnetic Overlayers on Transition Metal Surfaces,
Jül. Report 2197 (1988).

[2] H. Akai, M. Akai, S. Blügel, B. Drittler, H. Ebert, K. Terakura, R. Zeller, and P. H. Dederichs,
Theory of Hypefine Interactions in Metals,
Prog. Theo. Phys. (Suppl) **101**, 11 (1990).

[3] T. Asada, G. Bihlmayer, S. Handschuh, S. Heinze, Ph. Kurz, and S. Blügel,
First-principles theory of ultra-thin magnetic films,
J. Phys.: Condens. Matter **11**, 9347 (1999).

[4] Ph. Kurz, G. Bihlmayer, F. Föster, S. Blügel, and L. Nordström

FLAPW goes Non-collinear,
http://www.psi-k.org/newsletters/News_38/newsletter_38.pdf

[5] S. Heinze und S. Blügel,
Magnetische Ordnung wird sichtbar,
Physik in unserer Zeit **32** (4), 154 (2001).

[6] M. Heide, G. Bihlmayer, P. Mavropoulos, A. Bringer, S. Blügel,
Spin-Orbit Driven Physics on Metal Surfaces,
http://psi-k.dl.ac.uk/newsletters/News 78/Highlight 78.pdf

[7] C. Friedrich, M. Betzinger, M. Schlipf, S. Blügel, A. Schindlmayr,
Hybrid functionals and GW approximation in the FLAPW method,
http://psi-k.dl.ac.uk/newsletters/News 108/Highlight 108.pdf

[8] C. Carbone, S. Gardonio, P. Moras, S. Lounis, M. Heide, G. Bihlmayer, N. Atodiresei, P. H. Dederichs, S. Blügel, S. Vlaic, A. Lehnert, S. Ouazi, S. Rusponi, H. Brune, J. Honolka, A. Enders, K. Kern, S. Stepanow, C. Krull, T. Balashov, A. Mugarza, P. Gambardella,
Self-assembled nanoscale magnetic networks on surfaces: fundamental interactions and functional properties,
Advanced Functional Materials **21**, 1212 (2011).

[9] Y. Mokrousov, H. Zhang, F. Freimuth, B. Zimmermann, N. H Long, J. Weischenberg, I. Souza, P. Mavropoulos, S. Blügel,
Anisotropy of spin relaxation and transverse transport in metals,
J. Phys.: Condens. Matter **25**, 163201 (2013).
and
http://www.psi-k.org/newsletters/News 111/Highlight 111.pdf

[10] V. Caciuc, M. C. Lennartz, N. Atodiresei, S. Tsukamoto, S. Karthäuser, S. Blügel,
Systematic chemical functionalization of hybrid molecule-surface interfaces,
Physica Status Solidi B **250**, 2267 (2013).

IV. Book chapters

[1] P. H. Dederichs, H. Akai, S. Blügel, and R. Zeller,
"Electronic Structure and Magnetic Properties of Impurities in Metals",
in: NATO-Advanced Study Institute on "Alloy Phase Stability", (ed., M. Nijhoff),
Maleme, Crete (1987).

[2] S. Blügel,
"Ground State Results of Ferromagnetic Monolayers",
in: Structure and Properties of Surfaces and Interfaces, (eds., A. Gonis and G. M. Stocks),
Plenum, New York and London (1991).

[3] K. Kobayashi, K. Terakura, and S. Blügel,
"Optimum Adsorbtion Sites and Electronic Structure of Alkali Adsorbed Si(001) Surfaces",

in: Proc. 13th Taniguchi Symposium on Molecular Dynamics Simulations, (ed., F. Yonezawa),
Springer, Berlin (1992).

[4] M. Weinert and S. Blügel,
"First-Principles Calculations of Magnetic Interfaces and Multilayers",
in: Magnetic Multilayers (eds., L. H. Bennett and R. E. Watson),
World Scientific, Singapore (1993).

[5] R. Berger, S. Blügel, A. Antons, W. Kromen, K. Schroeder,
"A Parallelized ab initio Molecular Dynamics Code for the Investigation of Atomistic Growth Processes",
in: Proceedings of the NIC (Neumann Institute for Computing) Workshop "Molecular Dynamics on parallel Computers", (eds., R. Esser, P. Grassberger, J. Grotendorst, M. Lewerenz),
World Scientic, London, p. 185 (1999).

[6] G. Bihlmayer, R. Abt, S. Blügel, and T. Asada,
"Influence of magnetism for the alloy formation of ultrathin films",
in: International Symposium on Structure and Dynamics of Heterogeneous Systems, (eds., P. Entel and S. E. Wolf),
World Scientific, p. 179 (2000).

[7] K. Schroeder, A. Antons, R. Berger, W. Kromen, and S. Blügel,
"Surface Diffusion and Models for the Kinetics of Epitaxial Growth",
in: International Symposium on Structure and Dynamics of Heterogeneous Systems, (eds., P. Entel and S. E.Wolf),
World Scientific, p. 71 (2000).

[8] S. Blügel,
„Der Schatz im Quantensee: Metalle und Kristalle",
in: …und er würfelt doch! Die Erforschung des ganz Großen, des ganz Kleinen und der ganz Vielen, (eds., H. Müller-Krumbhaar und H.-F. Wagner),
Wiley-VCH, Berlin (2001).

[9] B. Hillebrands, S. Blügel,
„Magnetismus",
in: Bergmann Schaefer, Lehrbuch der Experimentalphysik, Band 6, Festkörper, 2. Auflage,
Walter de Gruyter, Berlin, New York (2005).

[10] Y. Mokrousov, N. Atodiresei, G. Bihlmayer, S. Blügel,
"Magnetism in Molecular Vanadium-Benzene Sandwiches",
in: Electronic Properties of Novel Nanostructures: XIX International Winterschool/Euroconference on Electronic Properties of Novel Materials, (ed., H. Kuzmany),
American Institute of Physics conference proceedings **786,** p. 444 (2005), ISBN 0-7354-0275-2.

[11] S. Blügel and G. Bihlmayer,
"Full-Potential Linearized Augmented Planewave Method",
in: NIC Winterschool 2006: Computational Nanoscience: Do It Yourself!, (eds., J.

Grotendorst, S. Blügel, D. Marx), John von Neumann Institute for Computing, Jülich, NIC Series **31**, p. 85-129 (2006), ISBN 3-00-017350-1.

[12] S. Blügel and G. Bihlmayer,
"Magnetism of Low-Dimensional Systems: Theory",
in: Handbook of Magnetism and Advanced Magnetic Materials 1, (eds., H. Kronmüller and S.P.P. Parkin),
John Wiley & Sons, Ltd., Chichester, West Sussex, United Kingdom, p. 598 (2007), ISBN 978-0-470-02217-7.

[13] G. Bihlmayer, M. Heide, Y. Mokrousov, A. Thiess, S. Heinze, S. Blügel,
"Spin-orbit induced phenomena at surfaces: wires and surfaces",
in: John von Neumann Institute for Computing Symposium 2010, Proceedings,
IAS Series **3**, (2010).

[14] C. Busse, P. Lazic, R. Djemour, J. Coraux, T. Gerber, N. Atodiresei, V. Caciuc, R. Brako, A.T. N'Diaye, S. Blügel, J. Zegenhagen, T. Michely,
"Graphene on Ir(111): A weakly bonded system",
(ed., G. Admans
ESRF Highlights, p. 33 (2010), http://www.esrf.eu.

[15] G. Bihlmayer, M. Heide, Y. Mokrousov, A. Thiess, S. Heinze, S. Blügel,
"Anisotropic Magnetic Interactions in Low Dimensions",
in: NIC Symposium 2010, John von Neumann Institute for Computing,
Forschungszentrum Jülich, 2010, (eds., G. Münster, D. Wolf, M. Kremer),
Jülich, Forschungszentrum, Zentralbibliothek, Schriften des Forschungszentrums Jülich,
IAS Series, p. 175-182 (2010), ISBN 978-3-89336-606-4.

[16] P. Lazic, N. Atodiresei, V. Caciuc, S. Blügel,
"Van der Waals Interaction of Molecules on Surfaces from First Principles",
in: NIC Symposium 2010, John von Neumann Institute for Computing,
Forschungszentrum Jülich, 2010, (eds., G. Münster, D. Wolf, M. Kremer),
Jülich, Forschungszentrum, Zentralbibliothek, Schriften des Forschungszentrums Jülich,
IAS Series, p. 227-234 (2010), ISBN 978-3-89336-606-4.

[17] A. Schindlmayr, C. Friedrich, E. Sasioglu, S. Blügel,
"First-principles calculation of electronic excitations in solids with SPEX",
(ed., F. M. Dolg), Oldenbourg Wissenschaftsverlag, München,
Progress in Physical Chemistry **3**, p. 67-78 (2010), ISBN 978-3-48659-827-8.

[18] C. Friedrich, M. Betzinger, M. Schlipf, S. Blügel, A. Schindlmayr,
"Hybrid functionals and GW approximation in the FLAPW method",
Psi-K Newsletters, Highlight **108**, p. 63-107 (2011).

[19] N. Atodiresei, V. Caciuc, P. Lazic, S. Blügel,
"Understanding Molecular Electronics and Spintronics from First Principles Simulations",
in: NIC Symposium 2012, Proceedings, (eds., K. Binder, G. Münster, and M.Kremer),
John von Neumann Institute for Computing, Jülich,
NIC Series **45**, (2012), ISBN 978-3-89336-758-0.

[20] M. Lezaic, P. Mavropoulos, K. Z. Rushchanskii, I. Slipukhina, S. Blügel,
"Computational Studies of Insulating Magnetic Oxides",

in: NIC Symposium 2012, Proceedings, (eds., K. Binder, G. Münster, and M.Kremer), John von Neumann Institute for Computing, Jülich, NIC Series **45**, p. 251-258 (2012), ISBN 978-3-89336-758-0.

[21] R. Zeller, A. Thiess, M. Bolten, P. H. Dederichs, S. Blügel, *„KKRnano: Precise Density Functional Calculations for Thousands of Atoms",* in: NIC Symposium 2012, Proceedings, (eds., K. Binder, G. Münster, and M.Kremer), John von Neumann Institute for Computing, Jülich, NIC Series **45**, p. 267 - 274 (2012), ISBN 978-3-89336-758-0.

[22] Y. Mokrouosov, H. Zhang, F. Freimuth, B. Zimmermann, N. H. Long, J. Weischenberg, I. Souza, P. Mavropoulos, S. Blügel, *„Anisotropy of spin relaxation and transverse transport in metals",* Psi-k Scientific Highlight **111**, (2012).

[23] N. Atodiresei, V. Caciuc, P. Lazic, S. Blügel, *"Chemical and van der Waals interactions at hybrid organic-metal interfaces",* Ab initio (from electronic structure) calculation of complex processes in materials, p. 21-39 (2013).

[24] C. Friedrich, E. Şaşıoğlu, M. C. T. D. Müller, A. Schindlmayr, S. Blügel, *„Spin Excitations in Solids from Many-Body Perturbation Theory",* First Principles Approaches to Spectroscopic Properties of Complex Materials Topics in Current Chemistry **347**, p. 259 - 301 (2014).

[25] M. Callsen, V. Caciuc, N. Kiselev, N. Atodiresei, S. Blügel, *"Magnetic Hardening Induced by Non- Magnetic Organic Molecules",* JARA-FIT 2014, p. 135-136 (2014).

[26] S. Fahrendorf, N. Atodiresei, C. Besson, V. Caciuc, F. Matthes, S. Blügel, P. Kögerler, D. Bürgler, C. M. Schneider, *„Accessing 4f-states in single-molecule spintronics",* JARA-FIT 2014, p. 129-130 (2014).

[27] I. Aguilera, I. Nechaev, C. Friedrich, S. Blügel, E. V. Chulkov, *"Many-Body Effects in the Electronic Structure of Topological Insulators",* Topological Insulators: Fundamentals and Perspectives, ed. Frank Ortmann, Stephan Roche, Sergio O. Valenzuela, Wiley-VCH Weinheim, p. 161-187 (2015).

[28] G. Bihlmayer, Y. M. Koroteev, T. V. Menshchikova, E. V. Culkov, S. Blügel, *"Ab Initio Calculations of Two-Dimensional Topological Insulators",* Topological Insulators: Fundamentals and Perspectives, ed. Frank Ortmann, Stephan Roche, Sergio O. Valenzuela, Wiley-VCH Weinheim, p. 103-130 (2015).

[29] P. Kowalski, G. Beridze, Y. Li, Y. Ji, C. Friedrich, E. Şaşioğlu, S.Blügel, *„Feasible and Reliable AB Initio Approach to Computation of Materials Relevant for Nuclear Waste Management",* Additive Manufacturing and Strategic Technologies in Advanced Ceramics / Shimamura, Kiyoshi (Editor); Hoboken, NJ, USA: John Wiley & Sons, Inc., 2016, ISBN: 9781119236009, Hoboken, NJ, USA: John Wiley & Sons, Inc., Ceramic Transactions Series 258, 205-217 (2016).

[30] U. Alekseeva, G. Michalicek, D. Wortmann, S.Blügel,
„Hybrid Parallelization and Performance Optimization of the FLEUR Code: New Possibilities for All-Electron Density Functional Theory",
Euro-Par 2018: Parallel Processing / Aldinucci, Marco (Editor), 24th International Conference on Parallel and Distributed Computing, Turin, Italy, 27 Aug 2018 - 31 Aug 2018, Springer International Publishing, Lecture Notes in Computer Science 11014, 735-748 (2018).

[31] G. Bihlmayer, P. Buhl, B. Dupe, I. Lima Fernandes, F. Freimuth, J. Gayles, S. Heinze, N. Kiselev, S. Lounis, Y. Mokrousov, S. Blügel,
"Magnetic skyrmions: structure, stability, and transport phenomena",
Psi-k Newsletter - Highlights **139**, p. 40 (2018).

[32] J. Bröder, D. Wortmann, S. Blügel,
"Using the AiiDA-FLEUR package for all-electron ab initio electronic structure data generation and processing in materials science",
In Extreme Data Workshop 2018 Proceedings Jülich: Forschungszentrums Jülich, IAS Series 40, p 43-48 (2019)

[33] C. Friedrich, M. C. T. D. Müller, S. Blügel,
"Spin Excitations in Solid from Many-Body Perturbation Theory",
Handbook of Materials Modeling / Andreoni, Wanda (Editor); Cham: Springer International Publishing, 2019, Chapter 74-2, ISBN: 978-3-319-42913-7, Springer International Publishing, p. 1-39 (2019).

[34] P. Gambardella, S. Blügel,
"Magnetic Surfaces, Thin Films and Nanostructures",
Springer Handbook of Surface Science / M. Rocca, T. Rahman, L. Vattuone, 1st ed. 2020, Cham: Springer International Publishing, 2020, Tokyo: Springer814959, Springer Handbooks (2020).

V. Lecture Notes of the Spring School of the Institute for Solid State Research (IFF)

[1] S. Blügel,
„Elektronische Struktur von Halbleiteroberflächen",
in: Synchrotronstrahlung zur Erforschung kondensierter Materie, Jülich: 23. Ferienkurs des Instituts für Festkörperforschung (IFF), 1992,
Ferienkurse des Forschungszentrums Jülich GmbH, ISBN 3-89336-088-8.

[2] S. Blügel,
„Magnetische Wechselwirkung II - Itineranter Austausch im Jelliummodell",
in: Magnetismus von Festkörpern und Grenzflächen, Jülich: 24. Ferienkurs des Instituts für Festkörperforschung (IFF), 1993,
Ferienkurse des Forschungszentrum Jülich GmbH, ISBN 3-89336-110-3.

[3] S. Blügel,
„Bandmagnetismus II - Oberflächen, Grenzflächen und Hyperfeinfelder",

in: Magnetismus von Festkörpern und Grenzflächen, Jülich: 24. Ferienkurs des Instituts für Festkörperforschung (IFF), 1993,
Ferienkurse des Forschungszentrum Jülich GmbH, ISBN 3-89336-110-3.

[4] S. Blügel,
„Theorie der Rastertunnelmikroskopie“,
in: Physik der Nanostrukturen, Jülich: 29. Ferienkurs des Instituts für Festkörperforschung (IFF), 1998.
Schriften des Forschungszentrums Jülich, Matter and Materials **1**, ISBN 3-89336-217-7.

[5] S. Blügel,
„Theorie der magnetischen Anisotropie und Magnetostriktion“,
in: Magnetische Schichtstrukturen in Forschung und Anwendung, Jülich: 30. Ferienkurs des Instituts für Festkörperforschung (IFF), 1999,
Schriften des Forschungszentrums Jülich, Matter and Materials **2**, ISBN 3-89336-335-5.

[6] S. Blügel,
„Der Quantum-Hall Effekt“,
in: Femtosekunden und Nano-eV, Jülich: 31. Ferienkurs des Instituts für Festkörperforschung (IFF), 2000,
Schriften des Forschungszentrums Jülich, Matter and Materials **3**, ISBN 3-89336-256-8.

[7] P. Mavropoulos, K. Sato, S. Blügel,
“Spintronics: Transport and Materials”,
in: Fundamentals of Nanoelectronics, Jülich: 34. Ferienkurs des Instituts für Festkörperforschung (IFF), 2003,
Schriften des Forschungszentrums Jülich, Matter and Materials **14**, ISBN 3-89336-319-X.

[8] S. Blügel,
“Reduced Dimensions: Magnetic Moment and Magnetic Structure”,
in: Magnetism goes Nano, Jülich: 36. Ferienkurs des Instituts für Festkörperforschung (IFF), 2005,
Schriften des Forschungszentrums Jülich, Matter and Materials **26**, ISBN 3-89336-381-5.

[9] S. Blügel,
“Density Functional Theory in Practice”,
in: Computional Condensed Matter Physics, Jülich: 37. Ferienkurs des Instituts für Festkörperforschung (IFF), 2006,
Schriften des Forschungszentrums Jülich, Matter and Materials **32**, ISBN 3-89336-430-7.

[10] S. Blügel,
“Electronic structure of matter: Reduced dimensions”,
in: Probing the Nanoworld, Jülich: 38. Ferienkurs des Instituts für Festkörperforschung (IFF), 2007.
Schriften des Forschungszentrums Jülich, Matter and Materials **34**, ISBN 3-89336-462-6.

[11] S. Blügel,
“Magnetismus in reduced Dimensions”,
in: Spintronics: From the GMR to Quantum Computing, Jülich: 40. Ferienkurs des Instituts für Festkörperforschung (IFF), 2009,
Schriften des Forschungszentrums Jülich, Matter and Materials **10**, ISBN 3-89336-559-3.

[12] S. Blügel,
"Exchange interactions",
in: 41th IFF Spring School 2010 "Electronic Oxides - Correlation Phenomena, Exotic Phases, and Novel Functionalities", (eds.: S. Blügel, Th. Brückel, R. Waser, C.M. Schneider), Schriften des Forschungszentrum Jülich,
Key Technologies **13**, p. A6.1-A6.28 (2010), ISBN- 978-3-89336-609-5.

[13] S. Blügel,
"Scattering Theory: Born Series",
in: 43rd IFF Spring School 2012 "Scattering Methods for Condensed Matter Research: Towards Novel Applications at Future Sources", (eds.: M. Angst, Th. Brückel, D. Richter, R. Zorn), Schriften des Forschungszentrum Jülich,
Key Technologies **33**, p. A2-A2.29 (2012), ISBN 978-3-89336-759-7.

[14] S. Blügel,
"Complex Magnetism",
in: 45th IFF Spring School 2014 "Computing Solids – Models, ab-initio methods and supercomputing", (eds.: S. Blügel, N. Helbig, V. Meden, D. Wortmann), Schriften des Forschungszentrum Jülich,
Key Technologies **74**, p. C4-C4.50 (2014), ISBN 978-3-89336-609-5.

[15] S. Blügel, G. Bihlmayer,
"Electronic Structure of Matter",
in: 47th IFF Spring School 2016 "Memristive Phenomena – From Fundamental Physics to Neuromorphic Computing", (eds. R. Waser, M. Wuttig), Schriften des Forschungszentrum Jülich,
Schlüsseltechnologien **113**, p. A2-A2.40 (2016), ISBN 978-3-95806-091-3.

[16] S. Blügel,
"Non-collinear magnetism in density functional theory",
in: 48th IFF Spring School 2017 "Topological Matter - Topological Insulators, Skyrmions and Majoranas", (eds. S. Blügel, Y. Mokrousov, T. Schäpers, Y. Ando), Schriften des Forschungszentrums Jülich,
Schlüsseltechnologien **139**, p. C5-C5.45 (2017), ISBN 978-3-95806-202-3.

[17] S. Blügel,
"Scattering theory: Born series and dynamical theory",
In: 50th IFF Spring School 2019 "Scattering! Soft, Functional and Quantum Materials", (ed. M. Angst, T. Brückel, S. Förster, K. Friese, R. Zorn), Schriften des Forschungszentrums Jülich,
Schlüsseltechnologien **190**, p. A2-A2.34 (2019), ISBN 978-3-95806-380-8.

VI. Edited books

[1] S. Blügel, G. Gompper, E. Koch, H. Müller-Krumbhaar, R. Spatschek, R. G. Winkler (eds.),
"Computational Condensed Matter Physics",
37. Ferienkurs des Instituts für Festkörperforschung (IFF), 2006,
Schriften des Forschungszentrums Jülich, Matter and Materials **32**, ISBN 3-89336-430-7.

[2] J. Grotendorst, S. Blügel, D. Marx (eds.),
"*Computational Nanoscience: Do It Yourself*!",
Lecture Notes of Winter School 2006, Forschungszentrum, Verlag, 2006, Schriften des Forschungszentrum Jülich,
NIC Series **31**, p. 522 (2006), ISBN 3-00-017350-1.

[3] J. Grotendorst, N. Attig, S. Blügel, D. Marx (eds.),
"Multiscale Simulation Method in Molecular Sciences",
Lecture Notes of Winter School 2009, Forschungszentrum, Verlag, 2009, Schriften des Forschungszentrum Jülich,
NIC Series **42**, p. 588 (2014), ISBN 978-3-9810843-8-2.

[4] S. Blügel, Th. Brückel, R. Waser, C.M. Schneider (eds.),
"Electronic Oxides - Correlation Phenomena, Exotic Phases, and Novel Functionalities",
Lecture Notes of the 41th IFF Spring School 2010, Forschungszentrum, Verlag, 2010, Schriften des Forschungszentrum Jülich, Reihe Schlüsseltechnologien / Key Technologies **13,** (2010), ISBN 978-3-89336-609-5.

[5] S. Blügel, N. Helbig, V. Meden, D. Wortmann (eds.),
"Computing Solids: Models, ab-initio methods and supercomputing",
Lecture Notes of the 45th IFF Spring School 2014, Forschungszentrum, Verlag, 2014, Schriften des Forschungszentrum Jülich, Reihe Schlüsseltechnologien / Key Technologies **74**, (2014), ISBN 978-3-89336-912-6.

VII. Patents

[1] X. Nie, S. Blügel,
Electric field for the change of the magnetization in thin films, patented at the patent office Munich Amtl. Az. 19841034.4, (2000). European Patent Nr. 1099217, permitted for Germany, France and United Kingdom.

[2] E. Sasioglu, S. Blügel,
Magnetische Tunneldiode und magnetischer Tunneltransistor, European Patent Nr. PT 1.2725, (2016), European Patent Nr. 3371836, permitted for Germany, France, Ireland, Japan, Netherlands, Sweden, Switzerland and United Kingdom.

[3] Blügel, S. ; Sasioglu, E.
Magnetische Tunneldiode und magnetischer Tunneltransistor,
Patent No.: PT 1.2725; 16788508.6 (2016).

[4] Bröder, J. ; Wortmann, D.
Verfahren zur Auswertung von Rumpfelektronenspektren,
Patent No.: PT 1.2815; 102018208587.0 (2018).

[5] Gaudin, G. ; Miron, I. M. ; Yang, H. ; Vatajelu, I. ; Pinna, D.
"In materio computing" classification device,
Patent No.: PT 1.2953; 21306379.5 (2021).

[6] Gaudin, G. ; Miron, I. M. ; Yang, H. ; Vatajelu, I. ; Pinna, D.
Improved classification device of the "in materio computing" type,
Patent No.: PT 1.2953; 21306379.5 (2023).

VIII. Dataset Publications

[1] P. Rüssmann, F. Bertoldo. S. Blügel,
The JuDiT database of impurities embedded into a topological insulator,
Materials Cloud Archive, 2020.94 (2020).

[2] J. Broeder, D. Wortmann, S. Blügel,
JuCLS database of core-level shifts from all-electron density functional theory simulations for chemical analysis of X-ray photoelectron spectra,
Materials Cloud Archive, 2020.139 (2020).

[3] P. Rüßmann, S. Blügel,
Density functional Bogoliubov-de Gennes analysis of superconducting Nb and NB(110) surfaces,
Materials Cloud Archive, 2021.163 (2021).

[4] P. Rüßmann, J. Ribas Sobreviela, M. Sallermann, M. Hoffmann, F. Rhiem, S. Blügel,
The AiiDA-Spirit plugin for automated spin-dynamics simulations and multi-scale modelling based on first-principles calculations,
Materials Cloud Archive, 2021.203 (2021).

[5] R. Kovacik, P. Mavropoulos, S. Blügel,
The JuHemd (Jülich-Heusler-magnetic-database) of the Monte Carlo simulated critical temperatures of the magnetic phase transition for experimentally reported Heusler and Heusler-like materials,
Materials Cloud Archive 2022.28 (2022).

[6] P. Rüssmann, S. Bluegel,
Dataset of proximity induced superconductivity in a topological insulator,
Materials Cloud Archive 2022.123 (2022).

[7] R. Hilgers, D. Wortmann, S. Blügel,
ML-ready Curie temperatures and descriptors extracted from the JuHemd database,
Materials Cloud Archive 2022.174 (2022).

[8] E. Bosoni, L. Beal, M. Bercx, P. Blaha, S. Blügel, J. Boeder, M. Callsen, S. Cottenier, A. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, M. Fornari, A. Garcia, et al.,
How to verify the precision of density-functional-theory implementations via reproducible and universal workflows,
Materials Cloud Archive 2023.81 (2023).

[9] P. Rüssmann, X. K. Wei, A. Rehman Jalil, Y. Ando, D. Grützmacher, S. Blügel, J. Mayer,
Pd-doping of Bi_2Te_3 and superconductivity of Pd(Bi,Te)x from density functional theory,
Materials Cloud Archive 2023.99 (2023).

[10] R. Hilgers, D. Wortmann, S. Blügel,
Density of states of full and inverse Heusler magnetic alloys,
Materaials Cloud Archive (2023), DOI: 10.24435/materialscloud:v5-5z

[11] R. Hilgers, D. Wortmann, S. Blügel,
Relaxed thin film structures of one, two, and three magnetic 3d transition metal layers on

FCC noble-metal substrates based on FLAPW PBE calculations,
Materaials Cloud Archive (2023), DOI: 10.24435/materialscloud:dk-wq

[12] R. Hilgers, D. Wortmann, S. Blügel,
Relaxed thin film structures of one, two, and three magnetic 3d transition metal layers on FCC noble-metal substrates based on FLAPW PBE calculations,
Materaials Cloud Archive (2023), DOI: 10.24435/materialscloud:dk-wq

[13] K. Janßen, P. Rüßmann, S. Liberda, M. Schleenvoigt, X. Hou, A. R. Jalil, F. Lentz, S. Trellenkamp, E. Zimmermann, G. Mussler, P. Schüffelgen, C. M. Schneider, S. Blügel, D. Grützmacher, L. Plucinski, T. Schäpers,
Single in-situ interface characterization composed of niobium and a selectively grown (Bi1-xSbx)2Te3 topological insulator nanoribbon,
Materaials Cloud Archive (2023), DOI: 10.24435/materialscloud:gt-0r

[14] P. Rüßmann, M. Bahari, S. Blügel, B. Trauzettel,
Proximity-induced Cooper pairing at low and finite energies in the gold Rashba surface state,
Materaials Cloud Archive (2023), DOI: 10.24435/materialscloud:20-9z

[15] P. Härtl, M. Vogt, G. Bihlmayer, S. Blügel, M. Bode,
Spin Spiral State at a Ferromagnetic Gd Vacuum Interface,
University of Würzburg (2024), DOI:10.58160/exfegur3wv777f1k

IX. Software-Releases

[1] M. Hoffmann, N. Ohs, S. Blügel,
Maple scripts for the calculation of Hubbard matrices and their subsequent downfolding by Loewdin's partitioning,
Zenodo (2019), DOI: 10.5281/zenodo.3609779

[2] P. Rüssmann, D. Antognini Silva, F. Bertoldo, J. Broeder, J. Chico, R. Mozumder, J. Wasmer, S. Blügel,
JuDFTteam/aiida-kkr,
Zenodo (2020), DOI: 10.5281/zenodo.3628251

[3] R. Hilgers, D. Wortmann, S. Blügel,
Data processing for the JuHemd database and ML-training and evaluation scripts,
Zenodo, (2022), DOI: 10.5281/zenodo.7452756

[4] G. P. Müller, M. Sallermann, S. Mavros, F. Rhiem, D. Schürhoff, M. Hoffmann, I. Meyer, C. Disselkamp, M. Redies, P. Buhl, J. R. Stuckert, A. V. Ivanov, N. S. Kiselev, H. Jónsson, S. Blügel,
spirit-code/spirit: New Desktop GUI, update to C++14
Zenodo (2023), DOI: 10.5281/zenodo.7746552

[5] D. Wortmann, G. Michalicek, N. Baadji, M. Betzinger, G. Bihlmayer, J. Broeder, T. Burnus, J. Enkovaara, F. Freimuth, C. Friedrich, C.-R. Gerhorst, S. Grandberg Cauchi, U.

Grytsiuk, A. Hanke, J.-P. Hanke, M. Heide, S. Heinze, R. Hilgers, H. Janssen, D. A. Klüppelberg, R. Kovacik, P. Kurz, M. Lezaic, G. K. H. Madsen, Y. Mokrousov, A. Neukirchen, M. Redies, S. Rost, M. Schlipf, A. Schindlmayr, M. Winkelmann, S. Blügel,
FLEUR,
Zenodo (2023), DOI: 10.5281/zenodo.7778444

[6] M. Hoffmann, N. Ohs, W. Beida, S. Blügel,
Maple scripts for the calculation of Hubbard matrices and their subsequent downfolding by Loewdin's partitioning,
Zenodo (2023), DOI: 10.5281/zenodo.8060563

[7] P. Rüssmann, J. Ribas Sobreviela, M. Sallermann, M. Hoffmann, F. Rhiem, S. Blügel,
JuDFTteam/aiida-spirit: Version 0.2.1,
Zenodo (2023), DOI: 10.5281/ zenodo.8070769

[8] R. Hilgers, D. Wortmann, S. Blügel,
Workflow, data processing, data analysis and predictive ML scripts used for DFT-integrated machine learning methodology in combination with the FLAPW code FLEUR,
Zenodo (2023), DOI: 10.5281/ zenodo.10056614

[9] R. Hilgers, D. Wortmann, S. Blügel,
Code collection for machine learning assisted materials screening in the search for novel half-metallic Heusler alloys,
Zenodo (2023), DOI: 10.5281/zenodo.10075055