PUBLICATION LIST of Guang-Yu Guo (2023/9)

(郭光宇教授學術著作目錄)

郭光宇教授已發表了約320篇期刊論文,含頂尖科技期刊「科學」(Science)(1篇：H17)、「美國科學院院刊」(PNAS)(1篇：F42)與「自然通訊」(Nature Commun.)(5篇：A46, D9, E23, F8, F51)、物理學頂尖期刊「自然物理」(Nature Physics)(1篇：D15)、「物理評論通訊」(Physical Review Letters)(19篇：A1, C1, C3, C4, C5, C9, C10, C15, C31, D1, D10, F1, F4, F5, F23, F37, J3, K13, L14)與「物理評論X」(Physical Review X)(2篇：D12, F39)、化學頂尖期刊「美國化學學會期刊」(J. Amer. Chem. Soc.)(1篇：F44)、及奈米科學頂尖期刊「奈米通訊」(Nano Letters)(1篇：E8)與「美國化學學會奈米」(ACS Nano)(1篇：A58)等頂尖期刊論文共30多篇。除了那篇「科學」論文[H17]和2篇「物理評論通訊」論文[J3,K13]外，這些頂尖期刊論文都是郭教授於1998年夏加入臺大物理系後發表的。郭教授的論文已被引用14,000多次，H-指數(H-index)高達61［參見谷歌學者 (Google Scholars)：https://scholar.google.com/citations?user=XyumTigAAAAJ&hl=zh-TW ］。

近5年來，郭教授持續積極研究尖端材料(如新興的二維材料，神奇的拓樸材料，金屬氧化物與其異質結構、鐵基超導體及光學超穎材料)新穎物理性質，又發表了50多篇期刊論文，包括頂尖科技期刊「美國科學院院刊」(1篇)與「自然通訊」(2篇)、物理學頂尖期刊「自然物理」(1篇)與「物理評論通訊」(2篇)與「物理評論X」(2篇)、奈米科學頂尖期刊「美國化學學會奈米」(1篇)。下面依研究議題/領域列出郭教授全部已發表的期刊論文。

Prof. Guang-Yu Guo has authored and co-authored about 320 refereed papers, including very prestigious science journal papers: 1 <Science> paper [H17], 1 <PNAS> paper [F42], and 5 <Nature Communications>[A46, D9, E23, F8, F51] ; top physics journal papers: 1 <Nature Physics> paper [D15], 19 <Physical Review Letters> papers [A1, C1, C3, C4, C5, C9, C10, C15, C31, D1, D10, F1, F4, F5, F23, F37, J3, K13, L14] and 2 <Physical Review X> papers [D12, F39]; top chemistry journal papers: 1 <Journal of American Chemical Society> paper [F44]; and top nano science journal papers: 1 <Nano Letters> paper [E8], 1 <ACS Nano> paper [A58] (total 31 papers in highly prestigious journals). Except the <Science> paper [H17] and two of the <Physical Review Letters> papers [J3, K13], all these highly prestigious journal papers were published after he joined the Department of Physics, National Taiwan University in the summer of 1998. His papers have been cited more than 14,000 times, and H-index is 61 (see Google Scholars: https://scholar.google.com/citations?user=XyumTigAAAAJ&hl=zh-TW).

In the past 5 years, Prof. Guo has continued vigorously investigating the novel properties of advanced materials (such as emerging two-dimensional materials, magical topological materials, intriguing metal oxides and their heterostructures, iron-based superconductors and optical metamaterials). In the past 5 years, he published another 50 papers in academic journals including very prestigious journals PNAS (1 paper), Nature Physics (1 paper), Nature Commun. (2 papers), Physical Review Letters (2 papers), Physics Review X (2 papers) and ACS Nano (1 paper).

All his papers are listed below according to research topics/fields.

A. Nanometer Materials and Mesoscopic Systems

Carbon, BN and SiC nanotubes and nanostructures

A1 (citations: 180) L. Liu, **G.Y. Guo**, C.S. Jayanthi and S.Y. Wu,
Colossal paramagnetic moments in metallic carbon nanotori,
Phys. Rev. Lett. 88, 217206 (2002).

A2 (319) **G.Y. Guo***, K.C. Chu, D.S. Wang, C.-G. Duan,
Linear and nonlinear optical properties of carbon nanotubes from first-principles calculations,
Phys. Rev. B **69**, 205416 (2004).

A3 (53) **G.Y. Guo***, K.C. Chu, D.S. Wang, C.-G. Duan,
Static polarizability of carbon nanotubes: *Ab initio* independent-particle calculations,
Comput. Mater. Sci. **30**, 269 (2004).

A4 (25) Y.Y. Chou, **G.Y. Guo**, L. Liu, C.S. Jayanthi and S.Y. Wu,
Electric conductance of single-wall carbon nanotube-contacted carbon nanotorus: Effects of transparency and equivalence of contacts, J. Appl. Phys. **96**, 2249 (2004).

A5 (193) **G.Y. Guo*** and J.C. Lin
Systematic ab initio calculation of the optical properties of BN nanotubes
Phys. Rev. B **71**, 165402 (2005).

A6 (86) **G.Y. Guo** and J.C. Lin
Second harmonic generation and linear electro-optical coefficients of BN nanotubes
Phys. Rev. B **72**, 75416 (2005).

A7 (19) **G.Y. Guo** and J.C. Lin
Second harmonic generation and linear electro-optical coefficients of BN nanotubes (vol. 72, art. no. 02375416, 2005), Phys. Rev. B **77**, 049901 (2008).

A8 (18) **G.Y. Guo**, L. Liu, K.C. Chu, C.S. Jayanthi and S.Y. Wu,
Electro-mechanical responses of single-walled carbon nanotubes: Interplay between the strain-induced energy gap opening and the pinning of the Fermi level
J. Appl. Phys. **98**, 044311 (2005).

A9 (61) **G.Y. Guo***, S. Ishibashi, T. Tamura and K. Terakura
Static dielectric response and Born effective charge of BN nanotubes from ab initio finite electric calculations, Phys. Rev. B **75**, 245403 (2007).

A10 (186) I.J. Wu and **G.Y. Guo***
Optical properties of SiC nanotubes: An *ab initio* study, Phys. Rev. B **76**, 035343 (2007).

A11 (74) I.J. Wu and **G.Y. Guo***
Second-harmonic generation and linear electro-optical coefficients of SiC polytypes and nanotubes, Phys. Rev. B **78**, 035447 (2008).

A12 (148) H. C. Hsueh*, **G. Y. Guo*** and S. G. Louie
Excitonic effects in the optical properties of a SiC sheet and nanotubes
Physical Review B **84**, 085404 (2011)

A13 Y.-S. Huang, Y.-H. Chan and **G. Y. Guo***
Large shift current via in-gap and charge-neutral exciton excitations in a monolayer and nanotubes of BN, Physical Review B **108**, 075413 (2023)

Atomic chains, one-dimensional (1D) and quasi-1D systems

A14 (2) X.-F. Jiang and **G. Y. Guo**
Spin gap in doped dimerized chain near half-filling, Physica B **334**, 451 (2003).

A15 (1) X.-F. Jiang and **G.Y. Guo**
Quantum self-consistent approach to the charge gap of the quasi-one-dimensional organic conductors, Solid State Commun. **129**, 443 (2004).

A16 X.-F. Jiang, **G.Y. Guo** and D.Y. Xing,
An approach to temperature dependence of the magnetic excitation in the spin-Peierls chain with frustration, J. Phys. Soc. Japan **73** (2004) 1561.

A17 (35) X.-F. Jiang and **G.Y. Guo**
Electronic structure and exchange interactions in $BaVS_3$, Phys. Rev. B **70**, 035110 (2004).

A18 (10) S. J. Luo, **G. Y. Guo** and A. Laref

A first-principles study of electronic and magnetic properties of a quasi-one-dimensional organic ferromagnet, Europhys. Lett. **77**, 37006 (2007)

A19 (155) J.C. Tung and **G.Y. Guo***

Systematic *ab initio* study of the magnetic and electronic properties of all 3*d* transition metal linear and zigzag nanowires, Phys. Rev. B **76**, 094413 (2007)

A20 (13) Z.Z. Zhu, J.C. Zheng and **G. Y. Guo**

Possible ferromagnetism in s- and sp-electron element nanowires

Chem. Phys. Lett. **472**, 99 (2009)

A21 (17) S. J. Luo, **G. Y. Guo** and A. Laref

Magnetism of 3d-transition metal (Fe, Co and Ni) nanowires on w-BN (001)

J. Phys. Chem. C **113**, 14615 (2009)

A22 (44) J. C. Tung and **G. Y. Guo***

Magnetic moment and magnetic anisotropy of linear and zigzag 4*d* and 5*d* transition metal nanowires: First-principles calculations, Phys. Rev. B **81**, 094422 (2010).

A23 (27) J. C. Tung and **G. Y. Guo***

An *ab initio* study of the magnetic and electronic properties of Fe, Co, and Ni nanowires on Cu(001) surface, Comp. Phys. Commun. **182**, 84 (2011).

A24 (4) J. C. Tung, Y. K. Wang and **G. Y. Guo**[*],

Magnetic anisotropy and spin-spiral wave in V, Cr and Mn chains on Cu(001) surface: First principles calculations, Journal of Physics D: Applied Physics **44**, 205003 (2011)

A25 (37) J. C. Tung and **G. Y. Guo**[*],

Ab initio studies of spin-spiral waves and exchange interactions in 3d transition metal atomic chains, Physical Review B **83**, 144403 (2011)

A26 (27) M. Cheng, S. Wu, Z.-Z. Zhu* and **G. Y. Guo***, Large second-harmonic generation and linear electro-optic effect in trigonal selenium and tellurium,

Phys. Rev. B **100**, 035202 (2019).

Molecules, nanoparticles, quantum dots and quantum rings

A27 (23) D. M.-T. Kuo, **G.Y. Guo** and Y.-C. Chang

Tunneling current through a quantum dot array, Appl. Phys. Lett. **79**, 3851 (2001).

A28 (37) J. C. Lin and **G. Y. Guo***

Current-spin density functional theory of electronic and magnetic properties of quantum dots and quantum rings, Phys. Rev. B **65**, 35304 (2002).

A29 (1) J. C. Lin and **G. Y. Guo***

Spin-density-functional studies of quantum dots and quantum rings

J. Magn. Magn. Mater. **239**, 240 (2002).

A30 (5) **G.Y. Guo**, Y.K. Wang and Y.Y. Chen,

Ab initio studies of the electronic structure and magnetic properties of bulk and nano-particle $CeCo_2$, J. Magn. Magn. Mater. **272**, E1193-1194 (2004).

A31 (13) J.-H. Li, J.-D. Chai*, **G. Y. Guo**, M. Hayashi*,

The quantified NTO analysis for the electronic excitations of molecular many-body systems

Chemical Physics Letter **514**, 362-367 (2011).

A32 (10) J.-H. Li, J.-D. Chai*, **G. Y. Guo**, M. Hayashi*
Significant role of the DNA backbone in mediating the transition origin of electronic excitations of B-DNA - implication from long range corrected TDDFT and quantified NTO analysis
Physical Chemistry Chemical Physics **14**, 9092-9103 (2012)

A33 (49) J.-H. Li, M. Hayashi, **G. Y. Guo***,
Plasmonic excitations in quantum-sized sodium nanoparticles studied by time-dependent density functional calculations, Phys. Rev. B **88**, 155437 (2013).

Graphene and two-dimensional (2D) materials

A34 (48) Y.-F. Hsu, and **G. Y. Guo***
Anomalous integer quantum Hall effect in AA-stacked bilayer graphene,
Phys. Rev. B **82**, 165404 (2010)

A35 (35) Y. F. Hsu and **G. Y. Guo***,
Tunneling conductance of grapheme ferromagnet-insulator-superconductor junctions,
Phys. Rev. B **81**, 045412 (2010).

A36 (48) T.-W. Chen*, Z.-R. Xiao, D.-W. Chiou, and **G. Y. Guo***,
High Chern number quantum anomalous Hall phases in graphene ribbons with Haldane orbital coupling, Physical. Review B **84**, 165453 (2011)

A37 (14) P.-W. Lo, **G. Y. Guo***, F. B. Anders, Gate-tunable Kondo resistivity and dephasing rate in graphene studied by numerical renormalization group calculations,
Phys. Rev. B **89**, 195424 (2014).

A38 (83) S. C. Liou, C.-S. Shie, C. H. Chen, R. Breitwieser, W. W. Pai, **G. Y. Guo*** and M.-W. Chu*, π-plasmon dispersion in free-standing graphene momentum-resolved electron-loss spectroscopy, Phys. Rev. B **91**, 045418 (2015).

A39 (96) C.-Y. Wang and **G.Y. Guo***,
Nonlinear Optical Properties of Transition-Metal Dichalcogenide MX_2 (M = Mo, W; X = S, Se) Monolayers and Trilayers from First-Principles Calculations,
J. Phys. Chem. C **119**, 13268 (2015)

A40 (1) T.-P. Wu, X.-Q. Wang, **G. Y. Guo**, F. B. Anders and C.-H. Chung*
Quantum criticality of the two-channel pseudogap Anderson model: Universal scaling in linear and non-linear conductance, J. Phys.: Condens. Matter **28**, 175003 (2016).

A41 (13) T.-C. Wang, Z.-Q. Huang, C.-H. Hsu, F.-C. Chuang*, W.-S. Su*, and **G. Y. Guo***,
Tunable magnetic states on zigzag edge of hydrogenated and halogenated group-IV nanoribbons, Scientific Rep. **6**, 39083 (2016).

A42 (25) C.-S. Tan, Y.-J. Lu, C.-C. Chen, P.-H. Liu, S. J. Gwo, **G. Y. Guo*** and L.-J. Chen*,
Magnetic MoS_2 interface monolayer on CdS nanowire by cation exchange,
J. Phys. Chem. C **120**, 23055 (2016)

A43 (56) W.-X. Feng, **G. Y. Guo*** and Y. G. Yao*, Tunable magneto-optical effects in hole-doped group-IIIA metal-monochalcogenide monolayers, **2D Materials** **4**, 015017 (2017)

A44 (5) H.-C. Hsu, M.-J. Jhang, T.-W. Chen and **G. Y. Guo**, Topological phase transitions in an inverted InAs/GaSb quantum well driven by tilted magnetic fields,

Phys. Rev. B **95**, 195408 (2017).

A45 (13) H.-C. Hsu, I. Kleftogiannis, **G. Y. Guo** and V. A, Gopar, Conductance fluctuations in disordered 2D topological insulator wires: From quantum spin-Hall to ordinary phases, J. Phys. Soc. Jpn. **87**, 034701 (2018).

A46 (49) Y.-H. Jiang, P.-W. Lo, D. May, G.-H. Li. **G. Y. Guo**, F. Anders, T. Taniguchi, K. Watanabe, J.-H. Mao, E. Y. Andrei, Inducing Kondo screening of vacancy magnetic moments in graphene with gating and local curvature, **Nature Commun.** **9**, 2349 (2018).

A47 (16) D. May, P.-W. Lo, K. Deltenre, A. Henke, J. Mao, Y. Jiang, G. Li, E. Y. Andrei, **G. Y. Guo**, and F. B. Anders, Modeling of gate controlled Kondo effect at carbon point-defects in graphene, Phys. Rev. B **97**, 155419 (2018).

A48 (32) C. M. Ke, Y. P. Wu*, **G.-Y. Guo***,W. Lin, Z. M. Wu, C. J. Zhou and J. Y. Kang, Tuning the electronic, optical and magnetic properties of monolayer GaSe with a vertical electric field, Phys. Rev. Applied **9**, 044029 (2018).

A49 (122) Y. Fang, S. Wu, Z.-Z. Zhu and **G. Y. Guo***, Large magneto-optical effects and magnetic anisotropy energy in two-dimensional $Cr_2Ge_2Te_6$, Phys. Rev. B **98**, 125416 (2018).

A50 (19) C.-C. Su, C.-S. Li, T.-C. Wang, S.-Y. Guan, R. Sankar, F. Chou, C.-S. Chang, W.-L. Lee, **G.-Y. Guo*** and T.-M. Chuang*, Surface termination dependent quasiparticle scattering interference and magneto-transport study on ZrSiS, New J. Phys. **20**, 103025 (2018).

A51 (1) C. M. Ke, Y. Wu*, **G. Y. Guo***, Z. Wu and J. Kang, Electrically controllable magnetic properties of Fe-doped GaSe monolayer, J. Phys. D: Appl. Phys. **52**, 175001 (2019).

A52 (65) V. K. Gudelli and **G. Y. Guo***, Magnetism and Magneto-optical Effects in Bulk and Few-layer CrI_3: A Theoretical GGA + U Study, New J. Phys. **21**, 053012 (2019).

A53 (9) A. A. Pervishko, D. Yudin, V. K. Gudelli, A. Delin, O. Eriksson and **G.-Y. Guo**, Localized surface electromagnetic waves in CrI_3-based magnetophotonic structures Optics Express **28**, 29155-29165 (2020)

A54 (6) V. K. Gudelli and **G.-Y. Guo***, Antiferromagnetism-induced secondorder nonlinear optical responses of centrosymmetric bilayer CrI_3, Chin. J. Phys. **68**, 896-907 (2020)

A55 (9) M. Cheng, Z.-Z. Zhu and **G.-Y. Guo***, Strong bulk photovoltaic effect and second-harmonic generation in two-dimensional selenium and tellurium, Phys. Rev. B **103**, 245415 (2021)

A56 (7) V. K. Gudelli and **G.-Y. Guo***, Large bulk photovoltaic effect and second-harmonic generation in few-layer pentagonal semiconductors PdS_2 and $PdSe_2$, New J. Phys. **23**, 093028 (2021).

A57 (11) M.-J. Jiang and **G.-Y. Guo***, Large magneto-optical effect and magnetic anisotropy energy in two-dimensional metallic ferromagnet Fe_3GeTe_2, Phys. Rev. B **105**, 014437 (2022).

A58 (10) R. Ghosh, M. Singh, L. W. Chang, H.-I Lin, Y. S. Chen, J. Muthu, B. Papnai, Y. S. Kang, Y.-M. Liao, K. P. Bera, **G.-Y. Guo**, Y.-P. Hsieh, M. Hofmann, and Y.-F. Chen, Enhancing the Photoelectrochemical Hydrogen Evolution Reaction through Nanoscrolling of Two-Dimensional Material Heterojunctions, **ACS Nano** **16**, 5743 (2022)

A59 P. Yang, W. Feng, G.-B. Liu, **G.-Y. Guo**, and Y. Yao, Giant magneto-optical Schäfer-Hubert

effect in the two-dimensional van der Waals antiferromagnets MPS_3 (M=Mn, Fe, Ni), Phys. Rev. B **107**, 214437 (2023)

B. Layered Transition Metal Dichalcogenides

B1 (130) **G. Y. Guo**, and W. Y. Liang,
The Electronic Structures of Platinum Dichalcogenides: PtS_2, $PtSe_2$ and $PtTe_2$
J. Phys. C: Solid State Phys. **19**, 995 (1986).

B2 (28) **G. Y. Guo** and W. Y. Liang,
Study of the Electronic Structures of Ni-Group Metal Ditellurides-$NiTe_2$, $PdTe_2$ and $PtTe_2$ by the Self-consistent LMTO-ASA Method, J. Phys. C: Solid State Phys. **19**, 5365 (1986).

B3 **G. Y. Guo**, W. Y. Liang and A. D. Yoffe,
The LMTO-ASA Method and Band Structures of Layered-Structure Transition Metal Chalcogenides, in *Intercalation in Layered Materials*,
edited by M. S. Dresselhaus (Plenum, New York, 1986).

B4 (79) **G. Y. Guo** and W. Y. Liang,
Electronic Structures of Intercalation Complexes of the Layered Compound 2H-TaS_2,
J. Phys. C: Solid State Phys. **20**, 4315 (1987).

B5 (7) D. Sebilleau, **G.Y. Guo** and W.M. Temmerman,
A Band Model for the Electronic and Magnetic Structure of $NaCrS_2$,
J. Phys.: Condensed Matter **1**, 5653 (1989).

B6 (149) R. Corcoran, P. Meeson, P.A. Probst, M. Springford, H. Harima,
B.L. Gyorffy, **G.Y. Guo** and Y. Onuki,
Quantum Oscillations in the Mixed State of the Type II Superconductor $NbSe_2$
J. Phys.: Condens. Matter **6**, 4479 (1994).

C. Spin Hall and Nernst Effect as well as Anomalous Hall and Nernst Effect

C1 (170) **G. Y. Guo**, Y. Yao and Qian Niu
Ab initio calculation of intrinsic spin Hall Effect in semiconductors,
Phys. Rev. Lett. 94, 226601 (2005).

C2 (59) T. W. Chen, C. M. Huang and **G. Y. Guo**
Conserved spin and orbital angular momentum Hall current in a two-dimensional electron system with Rashba and Dresselhaus spin-orbit coupling, Phys. Rev. B **73**, 235309 (2006).

C3 (41) H. J. Chang, T. W. Chen, J.W. Chen, W.C. Hong, W.C. Tsai, Y. F. Chen and **G. Y. Guo**
Current and strain-induced spin polarization in InGaN/GaN superlattices
Phys. Rev. Lett. 98, 136403 (2007); **98**, 239902 (2007).

C4 (459) **G. Y. Guo**, S. Murakami, T. W. Chen and N. Nagaosa
Intrinsic spin Hall effect in platinum: First-principles calculations
Phys. Rev. Lett. 100, 096401 (2008).

C5 (114) **G. Y. Guo**, S. Maekawa and N. Nagaosa
Enhanced spin Hall effect by resonant skew scattering in the orbital-dependent Kondo effect
Phys. Rev. Lett. 102, 036401 (2009).

C6 (25) T.-W. Chen and **G. Y. Guo**

Torque and conventional spin-Hall currents in two-dimensional spin-orbit coupled systems: Universal relation and hyper-selection rule, Phys. Rev. B **79**, 125301 (2009)

C7 (51) **G. Y. Guo**

Ab initio calculation of intrinsic spin Hall conductivity of Pd and Au

J. Appl. Phys. **105**, 125301 (2009)

C8 (5) T.-W. Chen*****, H.-C. Hsu and **G. Y. Guo***

Transverse force generated by an electric field and transverse charge imbalance in spin-orbit coupled systems, Phys. Rev. B **80**, 165302 (2009)

C9 (40) B. Gu, J. Y. Gan, N. Bulut, T. Ziman, **G. Y. Guo**, N. Nagaosa, and S. Maekawa,

Quantum renormalization of the spin Hall effect, **Phys. Rev. Lett. 105**, 086401 (2010).

C10 (102) B. Gu, I. Sugai, T. Ziman, **G. Y. Guo**, N. Nagaosa, T. Seki, K. Takanashi and S. Maekawa,

Surface-assisted spin Hall effect in Au films with Pt impurity,

Phys. Rev. Lett. 105, 216401 (2010)

C11 (5) B. Gu, J.-Y. Gan, N. Bulut, **G. Y. Guo**, N. Nagaosa, and S. Maekawa,

Orbital-dependent Kondo effect for Fe in Au: Combined approach of density functional theory and quantum Monte Carlo method, J. Phys. Conf. Ser. **200**, 062007 (2010)

C12 (8) B. Gu, T. Ziman, **G. Y. Guo**, N. Nagaosa, and S. Maekawa,

Giant spin Hall effect of Au films with Pt impurities: Surface-assisted skew scattering

J. Appl. Phys. **109**, 07C502 (2011)

C13 (52) H.-R. Fuh and **G. Y. Guo***

Intrinsic anomalous Hall effect in nickel: A GGA + U study,

Physical Review B **84**, 144427 (2011)

C14 (21) J.-C. Tung, H.-R. Fuh and **G. Y. Guo***

Anomalous and spin Hall effects in hcp cobalt from GGA + U calculations

Physical Review B **86**, 024435 (2012)

C15 (102) P. He, L. Ma, Z. Shi, **G. Y. Guo***, J.-C. Zheng, Y. Xin and S. M. Zhou*

Chemical composition tuning of the anomalous Hall effect in isoelectronic $L1_0$ $FePd_{1-x}Pt_x$ alloy films, **Phys. Rev. Lett. 109**, 066402 (2012).

C16 (85) J.-C. Tung and G. Y. Guo*

High spin polarization of anomalous Hall current in Co-based Heusler alloys

New J. Phys. **15**, 033014 (2013).

C17 (38) Y. Q. Zhang, N. Y. Sun, R. Shan, J. W. Zhang, S. M. Zhou, Z. Shi and **G. Y. Guo**

Anomalous Hall effect in epitaxial permalloy thin films

J. Appl. Phys. **114**, 163714 (2013).

C18 (71) **G. Y. Guo***, Q. Niu, N. Nagaosa,

Anomalous Nernst and Hall effects in magnetized platinum and palladium,

Phys. Rev. B **89**, 214406 (2014)

C19 (33) X. Zhou, L. Ma, Z. Shi, **G. Y. Guo***, J. Hu, R. Q. Wu and M. Zhou,

Tuning magnetotransport in $PdPt/Y_3Fe_5O_{12}$: Effects of magnetic proximity and spin-orbit coupling, Appl. Phys. Lett. **105**, 012408 (2014).

C20 (42) H.-L. Huang, J.-C. Tung and **G. Y. Guo***
Anomalous Hall effect and current spin polarization in Co_2FeX (X = Al, Ga, In, Si, Ge, and Sn) Heusler compounds: A systematic ab initio study, Phys. Rev. B **91**, 134409 (2015)

C21 (26) L. Ma, H.-A. Zhou, L. Wang, X.-L. Fan*, W.-J. Fan, D.-S. Xue, K. Xia, Z. Wang, R.-Q. Wu, **G. Y. Guo**, L. Sun, X. Wang, X.-M. Cheng and S.-M. Zhou*,
Spin orbit coupling controlled spin pumping and spin Hall magnetoresistance effects,
Adv. Electron. Mater. **2**, 1600112 (2016).

C22 (84) **G. Y. Guo*** and T.-C. Wang, Large anomalous Nernst and spin Nernst effects in noncollinear antiferromagnets Mn_3X (X=Sn, Ge, Ga), Phys. Rev. B **96**, 224415 (2017).

C23 (3) **G. Y. Guo*** and T.-C. Wang, Large anomalous Nernst and spin Nernst effects in noncollinear antiferromagnets Mn_3X (X=Sn, Ge, Ga) (vol. 96, 224415, 2017),
Phys. Rev. B **100**, 169907 (2019).

C24 (31) D. Qu, S. Y. Huang, **G. Y. Guo** and C. L. Chien, Inverse spin Hall effect in Au_xTa_{1-x} alloy films, Phys. Rev. B **97**, 024402 (2018).

C25 (9) P. C. Chen, Y. M. Du, B. Y. Yang, P. H. Lin, **G. Y. Guo**, M. Pakala, and C. H. Lai*, Large enhancement of spin-orbit torques in Pd/CoFeB: The role of boron,
Phys. Rev. Mater. **2**, 064408 (2018).

C26 (67) X.-D. Zhou, J.-P. Hanke, W.-X. Feng, F. Li, **G. Y. Guo**, Y.-G. Yao, S. Blügel and Y. Mokrousov, Spin-order dependent anomalous Hall effect and magneto-optical effect in the noncollinear antiferromagnets Mn_3XN with X = Ga, Zn, Ag or Ni
Phys. Rev. B **99**, 104428 (2019).

C27 (20) H. Chen, T.-C. Wang, D. Xiao, **G. Y. Guo**, Q. Niu, A. H. MacDonald,
Manipulating anomalous Hall antiferromagnets with magnetic fields,
Phys. Rev. B **101**, 104418 (2020).

C28 (11) Z. Shi, S. J. Xu, L. Ma, S. M. Zhou and **G.-Y. Guo***, Anomalous Nernst Effect in Epitaxial $L1_0$ $FePd_{1-x}Pt_x$ Alloy Films: Berry Curvature and Thermal Spin Current,
Phys. Rev. Applied **13**, 054044 (2020).

C29 (20) X. Zhou, W.-X. Feng, X. Yang, **G.-Y. Guo** and Y. Yao, Crystal Chirality Magneto-Optical Effects in Collinear Antiferromagnets, Phys. Rev. B **104**, 024401 (2021).

C30 (4) **G. Y. Guo**, Anisotropic spin Hall and spin Nernst effects in bismuth semimetal,
J. Magn. Magn. Mater. **563**, 169949 (2022).

C31 (5) C. Xiao, W. Wu, H. Wang, Y.-X. Huang, X. Feng, H. Liu, **G.-Y. Guo**, Q. Niu, S. A. Yang, Time-Reversal-Even Nonlinear Current Induced Spin Polarization,
Phys. Rev. Lett. 130, 166302 (2023).

D. Topological Insulators and Topological Semimetals

D1 (55) J. Zhou, Q.-F. Liang, H. Weng, Y. B. Chen, S.-H. Yao, Y.-F. Chen*, J. Dong and **G. Y. Guo***, Predicted quantum topological Hall effect and noncoplanar antiferromagnetism in $K_{0.5}RhO_2$, **Phys. Rev. Lett. 116**, 256601 (2016).

D2 (18) S.-T. Guo, R. Sankar, Y.-Y. Chien, T.-R. Chang, H.-T. Jeng, **G. Y. Guo**, F. C. Chou and W.-L. Lee*, Large transverse current in topological Dirac semimetal Cd_3As_2

Scientific Reports **6**, 2748 (2016).

D3 (13) H. K. Chandra and **G. Y. Guo***
Quantum anomalous Hall phase and half-metallic phase in ferromagnetic (111) bilayers of 4d and 5d transition metal perovskites, Phys. Rev. B **95**, 104408 (2017).

D4 (8) H.-S. Lu and **G. Y. Guo***, Strain and onsite-correlation tunable quantum anomalous Hall phases in ferromagnetic (111) $LaXO_3$ bilayers (X=Pd, Pt), Phys. Rev. B **99**, 104405 (2019).

D5 (12) H.-S. Lu and **G. Y. Guo***, Anomalous ferromagnetism and magneto-optical Kerr effect insemiconducting double perovskite Ba_2NiOsO_6 and its (111) $(Ba_2NiOsO_6)/(BaTiO_3)_{10}$ superlattice, Phys. Rev. B **100**, 054443 (2019).

D6 (27) R. Sankar, I. P. Muthuselvan, K. R. Babu, G. S. Murugan, K. Rajagopal, T. C. Wu, C. Y. Wen, W. L. Lee, **G.-Y. Guo** and F. C. Chou, Crystal growth and magnetic properties of topological nodal-line semimetal GdSbTe with antiferromagnetic spin ordering, Inorganic Chem. **58**, 11730 (2019).

D7 (38) K. R. Babu and **G. Y. Guo***, Electron-phonon coupling, superconductivity and nontrivial band topology in NbN polytypes, Phys. Rev. B **99**, 104508 (2019).

D8 (29) Y. Yen and **G. Y. Guo***, Tunable large spin Hall and spin Nernst effects in the Dirac semimetals ZrXY (X=Si, Ge; Y=S, Se, Te), Phys. Rev. B **101**, 064430 (2020)

D9 (56) W.-X. Feng, X. Zhou, J.-P. Hanke, **G. Y. Guo**, S. Blügel, Y. Mokrousov, Y. Yao*, Topological Magneto-Optical Effect and its Quantization in Noncoplanar Antiferromagnets, **Nature Commun. 11**, 118 (2020).

D10 (110) H. X. Wang, Z. K. Lin, B. Jiang, **G.-Y. Guo** and J. H. Jiang, Higher-Order Weyl Semimetals, **Phys. Rev. Lett. 125**, 146401 (2020).

D11 (13) R. Sankar, I. P. Muthuselvam, K. Rajagopal, K. R. Babu, G. S. Murugan, K. S. Bayikadi, K. Moovendaran, C. T. Wu, **G. Y. Guo** Anisotropic Magnetic Properties of Nonsymmorphic Semimetallic Single Crystal NdSbTe, Crystal Growth and Design **20**, 6585 (2020).

D12 (138) J. Ahn, **G.-Y. Guo*** and N. Nagaosa, Low-Frequency Divergence and Quantum Geometry of the Bulk Photovoltaic Effect in Topological Semimetals, **Phys. Rev. X 10**, 041041 (2020)

D13 (5) B. B. Prasad and **G.-Y. Guo***, Tunable spin Hall and spin Nernst effects in Dirac line-node semimetals XCuYAs (X = Zr, Hf; Y = Si, Ge), Phys. Rev. Mater. **4**, 124205 (2020).

D14 (6) Y. Yen, C.-L. Chiu, P.-H. Lin, R. Sankar, T.-M. Chuang and **G.-Y. Guo***, Dirac Nodal Line and Rashba Spin-split Surface States in Nonsymmorphic ZrGeTe, New J. Phys. **23**, 103019 (2021).

D15 (81) J. Ahn, **G.-Y. Guo**, N. Nagaosa and A. Vishwanath, Riemannian Geometry of Resonant Optical Responses, **Nature Physics 18**, 290 (2022).

D16 H.-S. Lu and **G.-Y. Guo***, High temperature ideal Weyl semimetal phase and quantum anomalous Hall phase in ferromagnetic BaEuNiOsO6 and its (111) (BaEuNiOsO6)/(BaTiO3)10 superlattice, Phys. Rev. B **104**, 184417 (2021).

D17 (4) T.-Y. Hsieh, B. B. Prasad and **G. Y. Guo***, Helicity-tunable spin Hall and spin Nernst effects

in unconventional chiral fermion semimetals XY (X=Co, Rh; Y=Si, Ge),
Phys. Rev. B **106**, 165102 (2022).

D18 (1) M.-C. Jiang, **G.-Y. Guo**, M. Hirayama, T. Yu, T. Nomoto, R. Arita, Efficient hydrogen evolution reaction due to topological polarization, Phys. Rev. B **106**, 165120 (2022).

D19 K. R. Babu and **G. Y. Guo***, Structure and composition tunable superconductivity, band topology and elastic response of hard binary niobium nitrides Nb_2N, Nb_4N_3 and Nb_4N_5, Phys. Rev. B **108**, 064505 (2023).

D20 (3) H.-C. Hsu, J.-S. You, J. Ahn and **G.-Y. Guo***,
Nonlinear photoconductivities and quantum geometry of chiral multifold fermions
Phys. Rev. B **107**, 155434 (2023).

E. Photonic Crystals, Nanoplasmonics and Metamaterials

E1 (25) T. I. Weng and **G. Y. Guo**
Band structure of honeycomb photonic crystal slabs, J. Appl. Phys. **99**, 93102 (2006).

E2 (9) K.-M. Lin and **G. Y. Guo**
Uncoupled modes and all-angle negative refraction in walled honeycomb photonic crystals
J. Opt. Soc. Am. B **25**, C75 (2008).

E3 (22) H. Y. Chung, **G. Y. Guo**, H.-P. Chiang, D. P. Tsai, P. T. Leung, Accurate description of the optical response of a multilayered spherical system in the long wavelength approximation, Physical Review B **82**, 165440 (2010)

E4 (18) V. Klimov and **G. Y. Guo**
Bright and dark plasmon modes in three nanocylinder cluster
J. Phys. Chem. C **114**, 22398 (2010).

E5 (110) W. T. Chen, C. J. Chen, P. C. Wu, S. Sun, L. Zhou, **G. Y. Guo**, C. T. Hsiao, K.-Y. Yang, N. I. Zheludev and D. P. Tsai, Optical magnetic response in three-dimensional metamaterial of upright plasmonic meta-molecules, Optics Express **19**, 12837 (2011)

E6 (59) C. C. Chen, C. T. Hsiao, S. L. Sun, K. Y. Yang, P. C. Wu, W. T. Chen, Y. H. Tang, Y. F. Chau, E. Plum, **G. Y. Guo**, N. I. Zheludev and D. P. Tsai,
Fabrication of three dimensional split ring resonators by stress-driven assembly method
Optics Express **20**, 9415 (2012)

E7 (37) V. Klimov*, S. L. Sun, **G. Y. Guo***,
Coherent perfect nanoabsorbers based on negative refraction, Optics Express **20** , 13071 (2012)

E8 (1324) S. L. Sun, K.-Y. Yang, C.-M. Wang, T.-K. Juan, W. T. Chen, C. Y. Liao, Q. He, S. Xiao, W.-T. Kung, **G. Y. Guo**, L. Zhou and D. P. Tsai,
High-efficiency broadband anomalous reflection by gradient meta-surfaces
Nano Letters **12**, 6223 (2012)

E9 (9) **G. Y. Guo***, V. Klimov*, S. Sun, and W.-J. Zheng,
Metamaterial slab-based super-absorbers and perfect nanodetectors for single dipole sources,
Optics Express **21**, 11338 (2013).

E10 (64) S. Sun, H.-T. Chen, W.-J. Zheng, and **G.Y. Guo***,
Dispersion relation, propagation length and mode conversion of surface Plasmon polaritons

in silver double-nanowire systems, Optics Express **21**, 14591 (2013)

E11 (29) V. Klimov*, **G. Y. Guo***, M. Pikhota,
Plasmon Resonances in Metal Nanoparticles with Sharp Edges and Vertices: A Material Independent Approach, J. Phys. Chem. C **118**, 13052 – 13058 (2014)

E12 (4) R.-C. Shiu, Y.-C. Lan and **G. Y. Guo***
Optical multiple bistability in metal-insulator-metal plasmonic waveguides side-coupled with twin racetrack resonators, J. Opt. Soc. Amer. B **31**, 2581-2586 (2014)

E13 (22) V. V. Klimov*, I. V. Zabkov, A. A. Pavlov, R.-C. Shiu, H.-C. Chan and **G. Y. Guo***,
Manipulation of polarization and spatial properties of light beams with chiral metafilms
Optics Express **24**, 6172 (2016).

E14 (8) V. D. Guzatov, V. V. Klimov*, H.-C. Chan and **G. Y. Guo***
Tuning spontaneous radiation of chiral molecules by asymmetric chiral nanoparticles,
Optics Express **25**, 6036 (2017)

E15 (31) H. C. Chan and **G. Y. Guo***, Tuning topological phase transitions in hexagonal photonic lattices made of triangular rods, Phys. Rev. B **97**, 045422 (2017).

E16 (11) H.-C. Chan, S. Sun and **G. Y. Guo***,
Near-infrared left-handed metamaterials by arrays of upright split-ring pairs
J. Phys. D: Appl. Phys. **51**, 265103 (2018).

E17 (5) V. V. Klimov, D. V. Guzatov, I. V. Zabkov, H.-C. Chan and **G. Y. Guo***, Size and host-medium effects on topologically protected surface states in bi-anisotropic 3D optical waveguides, Phys. Rev. B **98**, 075433 (2018).

E18 (127) H.-X. Wang, **G.-Y. Guo** and J.-H. Jiang, Band topology in classical waves: Wilson-loop approach to topological numbers and fragile topology, New J. Phys. **21**, 093029 (2019).

E19 (16) H.-X. Wang, H. Chen, J.-H. Jiang and **G.-Y. Guo***, Tunable edge states in reconfigurable photonic crystals, J. Appl. Phys. **126**, 193105 (2019).

E20 (17) R.-C. Shiu, H.-C. Chan, H.-X. Wang and **G.-Y. Guo***, Photonic Chern insulators made of gyromagnetic hyperbolic metamaterials, Phys. Rev. Mater. **4**, 065202 (2020).

E21 (1) H.-X. Wang, C. Liang, Y. Poo, P.-G. Luan and **G.-Y. Guo**, The topological edge modes and Tamm modes in Su-Schrieffer-Heeger LC-resonator circuits,
J. Phys. D: Appl. Phys. **54**, 435301 (2021).

E22 (3) H.-X. Wang, Y. Chen, **G.-Y. Guo**, H.-Y. Kee, and J.-H. Jiang, Possible realization of optical Dirac points in woodpile photonic crystals, Optics Exp. **30**, 17204 (2022).

E23 (3) Y. Wang, H.-X. Wang, L. Liang, L. Fan, Z.-K. Lin, F. Li, X. Zhang, P.-G. Luan, Y. Poo, J.-H. Jiang, **G.-Y. Guo**, Hybrid topological photonic crystals,
Nature Commun. **14**, 4457 (2023).

F. Transition Metal Oxides

Charge, orbital and spin ordering

F1 (112) D.J. Huang, W.B. Wu, **G.Y. Guo**, H.-J. Lin, T.Y. Hou, C.F. Chang, C.T. Chen, A. Fujimori, T. Kimura, H.B. Huang, A. Tanaka and T. Jo,
Orbital ordering in $La_{0.5}Sr_{1.5}MnO_4$ studied by soft x-ray linear dichroism

Phys. Rev. Lett. **92**, 87202 (2004).

F2 (66) X.-F. Jiang and **G.Y. Guo**

Electronic structure, magnetism and optical properties of $FeSiO_4$ fayalite at ambient and high pressures: An GGA+U study, Phys. Rev. B **69**, 155108 (2004).

F3 (5) X.-F. Jiang and **G.Y. Guo**

First-principles study of the electronic structure and magnetism in fayalites: M_2SiO_4 (M = Fe, Co), J. Magn. Magn. Mater. **282**, 287 (2004).

F4 (304) H.-T. Jeng*, **G.Y. Guo***, D. J. Huang

Charge-orbital ordering and Verwey transition in magnetite,

Phys. Rev. Lett. **93**, 156403 (2004).

F5 (123) D.J. Huang, H.-J. Lin, J. Okamoto, K.S. Chao, H.-T. Jeng, **G.Y. Guo**, C.-H. Hsu, C.-M. Huang, D.C. Ling, W.B. Wu, C.S. Yang and C.T. Chen,

Charge-orbital ordering and Verwey transition in magnetite measured by resonant soft x-ray scattering, **Phys. Rev. Lett.** 96, 096401 (2006).

F6 S. Ju, T.Y. Cai, **G.Y. Guo** and Z.Y. Li

Percolation transition and colossal magnetoresistive effects in a complex network

Appl. Phys. Lett. **89**, 082506 (2006).

F7 (102) H.-T. Jeng*, **G.Y. Guo***, D. J. Huang

Charge-orbital ordering in low-temperature structures of magnetite: GGA+U investigations

Phys. Rev. B **74**, 195115 (2006)

F8 (62) H. Y. Huang, Z. Y. Chen, R.-P. Wang, F. M. F. de Groot, W. B. Wu, J. Okamoto, A. Chainani, A. Singh, Z.-Y. Li, J.-S. Zhou, H.-T. Jeng, **G. Y. Guo**, J.-G. Park, L. H. Tjeng, C. T. Chen and D. J. Huang *, Jahn-Teller distortion driven magnetic polarons in magnetite,

Nature Commun. **8**, 15929 (2017).

Half-metallic oxides

F9 (168) H.T. Jeng and **G.Y. Guo**, First-principles investigations of the electronic structures and the magnetocrystalline anisotropy in strained magnetite Fe_3O_4, Phys. Rev. B **65**, 094429 (2002).

F10 H.T. Jeng and **G.Y. Guo**, First-principles calculation of the orbital magnetic moment of O and Cr in half-metallic CrO_2, Mat. Res. Soc. Symp. Proc. 718, D4.14.6 (MRS, Pittsburgh, 2002).

F11 (23) H.-T. Jeng and **G.Y. Guo**,

First-principles investigations of the orbital magnetic moments in CrO_2,

J. Appl. Phys. **92**, 1419 (2002).

F12 (40) H.T. Jeng and **G.Y. Guo**

First-principles investigations of the magnetocrystalline anisotropy in strained Co-substituted magnetite ($CoFe_2O_4$), J. Magn. Magn. Mater **239**, 88 (2002).

F13 (25) H.T. Jeng and **G.Y. Guo**

First-principles investigations of the magnetocrystalline anisotropy in strained Ni-substituted magnetite ($NiFe_2O_4$), J. Magn. Magn. Mater. **240**, 436 (2002).

F14 (57) D.J. Huang, H.-T. Jeng, C.F. Chang, **G.Y. Guo**, J. Chen, W.P. Wu, S.C. Chung, S.G. Shyu, C.C. Wu, H.J. Lin and C.T. Chen,

Orbital magnetic moments of oxygen and chromium in CrO_2, Phys. Rev. B **66**, 174440 (2002).

F15 (28) T.-S. Chan, R.-S. Liu, **G. Y. Guo**, S.-F. Hu, J.-G. Lin, J.-M. Chen and J. P. Attfield, Chemical tuning of structure, magnetization and conductivity of the self-doped double perovskite $(Sr_{2-x}Ca_x)FeMoO_6$ ($0 \leq x \leq 2.0$) System, Chem. Mater. **15**, 425 (2003).

F16 T.-S. Chan, R.S. Liu, **G.Y. Guo**, and C.Y. Huang
Synthesis and characterization of double perovskites Sr_2FeMO_6 (M= Mo, W), Int. J. Mod. Phys. B **17**, 3500 (2003).

F17 (234) H.T. Jeng and **G.Y. Guo**
First-principles investigations of orbital magnetic moments and electronic structures of the double perovskites Sr_2FeMoO_6, Sr_2FeReO_6 and Sr_2CrWO_6, Phys. Rev. B. **67**, 94438 (2003).

F18 (38) D. J. Huang, J. Chen, C.F. Chang, W.P. Wu, S.C. Chung, A. Tanaka, **G.Y. Guo**, H.J. Lin, S.G. Shyu, C.C. Wu, L.H. Tjeng and C.T. Chen, Anomalous spin polarization and dualistic electronic nature of CrO_2, Phys. Rev. B **67**, 214419 (2003).

F19 (6) Y. K. Wang, **G.Y. Guo** and H.-T. Jeng,
An *ab initio* studies of the magnetocrystalline anisotropy and magnetoelastic coupling of half-metallic CrO_2, J. Magn. Magn. Mater. **282**, 139 (2004).

F20 (27) T.S. Chan, R.S. Liu, **G.Y. Guo**, S.F. Hu, J.G. Lin, J.F. Lee, L.Y. Jang, C.R. Chang, C.Y. Huang, Structural, electrical and magnetic characterization of the double perovskites Sr_2CrMO_6 (M = Mo, W): B' 4*d*-5*d* system, Solid State Commun. **131**, 531 (2004).

F21 (13) D.J. Huang, C.F. Chang, J. Chen, H.J. Lin, S.C. Chung, H.T. Jeng, **G.Y. Guo**, W.B. Wu, S.G. Shyu, and C.T. Chen, Orbital moments of CrO_2 and Fe_3O_4 studied by MCD in soft x-ray absorption, J. Electr. Spec. Rel. Pheno. **137-40**, 633 (2004).

F22 (26) W.B. Wu, D.J. Huang, **G.Y. Guo**, T.Y. Hou, H.J. Lin, C.F. Chang, C.T. Chen, A. Fujimori, T.Kimura, A. Tanaka, T. Jo, Orbital polarization of $LaSrMnO_4$ studied by soft x-ray linear dichroism, J. Electr. Spec. Rel. Pheno. **137**, 641 (2004).

F23 (210) D. J. Huang, H.-T. Jeng, C.F. Chang, **G.Y. Guo**, H.-J. Lin and C.-T. Chen, Spin and orbital magnetic moments of Fe_3O_4, **Phys. Rev. Lett. 93**, 077204 (2004).

F24 (28) C. F. Chang, D.J. Huang, A. Tanaka, **G.Y. Guo**, S.C. Chung, S.-T. Kao, S.G. Shyu and C.-T. Chen, Electronic structure of CrO_2 studied by magnetic circular dichroism in resonant photoemission, Phys. Rev. B **71**, 52407 (2005).

F25 (48) T.S. Chan, R.S. Liu, **G.Y. Guo**, S.F. Hu, J.G. Lin, J.M. Chen, C.R. Chang, Effects of B'-site transition metal on the properties of double perovskites Sr_2FeMoO_6 (M=Mo,W): B' 4d-5d system, Solid State Commun. **133**, 265 (2005).

F26 (74) Y. K. Wang and **G. Y. Guo**
Robust half-metallic antiferromagnets La*A*VOsO_6 and La*A*Mo*Y*O_6 (*A*=Ca,Sr,Ba; *Y*=Re,Tc) from first-principles calculations, Phys. Rev. B **73**, 064424 (2006).

F27 (13) R. S. Liu, T. S. Chan, S. Mylswamy, **G. Y. Guo**, J. M. Chen, and J. P. Attfield
Band overlap via chemical pressure control in double perovskite (Sr Ca)FeMoO (0<x<2.0) with TMR effect, Current Appl. Phys. **8**, 110 (2008)

F28 (41) Y. K. Wang, P. H. Lee and **G. Y. Guo**,
Half-metallic antiferromagnetic nature of La_2VTcO_6 and La_2VCuO_6 from ab initio calculations, Physical Review B **80**, 224418 (2009).

Ferroelectric, multiferroic and nonlinear optical oxides

F29 (30) C. H. Lin, C.M. Huang, and **G. Y. Guo**
Systematic *ab initio* study of the phase diagram of epitaxially strained $SrTiO_3$
J. Appl. Phys. **100**, 084104 (2006)

F30 (61) S. Ju, T.Y. Cai, **G.Y. Guo**, Z.Y. Li
Electrically controllable spin filtering and switching in multiferroic tunneling junctions
Phys. Rev. B **75**, 064419 (2007)

F31 (8) S. Ju, T.Y. Cai, **G.Y. Guo**, Z.Y. Li
Theory of tunneling magnetoresistance and tunneling electroresistance in $Co/BiFeO_3/La_{2/3}Sr_{1/3}MnO_3$ junctions, J. Appl. Phys. **104**, 053904 (2008)

F32 (32) S. Ju and **G. Y. Guo**
Colossal nonlinear optical magnetoelectric effects in multiferroic Bi_2FeCrO_6
Appl. Phys. Lett. **92**, 202504 (2008).

F33 (16) S. Ju and **G.Y. Guo**
First-principles study of crystal, electronic structure and second-harmonic generation in a polar double perovskite Bi_2ZnTiO_6, J. Chem. Phys. **129**, 194704 (2008).

F34 (17) C.L. Chen, K.W. Yeh, D.J. Huang, F.C. Hsu, Y.C. Lee, S.W. Huang, S. Ju*, T.Y. Cai, **G.Y. Guo**, H.J. Lin, S.M. Rao, and M.K. Wu
Orbital polarization of the unoccupied states in multiferroic $LiCu_2O_2$
Phys. Rev. B **78**, 214105 (2008)

F35 (54) S. Ju*, T.Y. Cai, and **G.Y. Guo***
Electronic structure, linear, and nonlinear optical responses in magnetoelectric multiferroic material $BiFeO_3$, J. Chem. Phys. **130**, 214708 (2009)

F36 (3) S. Ju, T. Y. Cai, C. I. Wei, and **G. Y. Guo**,
Second-harmonic generation with magnetic-field controllability, Optics Letters **34**, 3860 (2009).

F37 (38) M. H. Lee, C.-P. Chang, F.-T. Huang, **G. Y. Guo**, B. Gao, C. H. Chen, S.-W. Cheong and M. W. Chu*, Hidden antipolar order parameter and entangled Neel-type charged domain walls in hybrid improper ferroelectrics,
Phys. Rev. Lett. **119**, 157601 (2017).

F38 (29) T.-Y. Cai, S.-C. Liu, S. Ju*, C.-Y. Liu and **G. Y. Guo***, Double perovskite $ScFe_{1-x}CrO_3$ ($0.17 < x < 0.83$): Multiferroic semiconductors for highly efficient ferroelectric photovoltaics and spintronics, Phys. Rev. Applied **8**, 034034 (2017).

F39 (18) Y. M. Sheu*, Y. M. Chang, C. P. Chang, Y. H. Li, K. R. Babu, **G.Y. Guo**, T. Kurumaji, and Y. Tokura, Picosecond creation of switchable optomagnets from a polar antiferromagnet with giant photoinduced Kerr rotations, **Phys. Rev. X** **9**, 031028 (2019) .

F40 (25) W. Song, **G.-Y. Guo**, S. Huang, L. Yang and L. Yang, First-principles studies of second-order nonlinear optical properties of organic-inorganic hybrid halide perovskites,
Phys. Rev. Applied **13**, 014052 (2020).

F41 M.-W. Chu, **G. Y. Guo**, W. T. Chen, M. H. Lee, S. H. Lee, Y.-C. Lai, C. H. Du and C. H. Chen, Probing charge orders and hidden topology at atomic scale by cryogenic scanning transmission electron microscopy and spectroscopy, Phys. Rev. B **103**, 115130 (2021)

F42 (6) Y. Okamura, T. Morimoto, N. Ogawa, Y. Kaneko, **G.-Y. Guo**, M. Nakamura, M. Kawasaki, N. Nagaosa, Y. Tokura, Y. Takahashi, Photovoltaic effect by soft phonon excitation, **Proc. Natl. Academ. Sci. USA (PNAS) 119**, e2122313119 (2022).

F43 (2) S. Toyoda, J.-C. Liao, **G.-Y. Guo**, Y. Tokunaga, T. Arima, and N. Ogawa, Magnetic-field switching of second-harmonic generation in noncentrosymmetric magnet $Eu_2MnSi_2O_7$, Phys. Rev. Mater. B **7**, 024403 (2023)

Phosphors and light-emitting materials

F44 (369) C. C. Lin, Z. R. Xiao, **G.-Y. Guo**, T.-S. Chan, R.-S. Liu, Versatile phosphate phosphors $ABPO_4$ in white light-emitting diodes: Collocated characteristic analysis and theoretical calculations, **J. Am. Chem. Soc. 132**, 3020 (2010)

Low-dimensional magnetic oxides

F45 (7) G. N. Rao, V. N. Singh, R. Sankar, I. P. Muthuselvam, **G. Y. Guo*** and F. C. Chou* Antiferromagnetism of Ni_2NbBO_6 with S = 1 dimer quasi-one-dimensional armchair chains Phys. Rev. **91**, 014423 (2015)

F46 (14) I. P. Muthuselvam, R. Sankar, V. N. Singh, G. N. Rao, **G.-Y. Guo***, and F. C. Chou* Magnetic orderings of $Li_2Cu(WO_4)_2$ with tungstate-bridged quasi-1D spin-1/2 chains Inorg. Chem. **54**, 4303 (2015)

F47 (12) S. K. Karna, C. W. Wang, R. Sankar, M. Avdeev, A. Singh, I. P. Muthuselvam, V. N. Singh, **G.-Y. Guo**, and F. C. Chou* Antiferromagnetic spin structure and negative thermal expansion of $Li_2Ni(WO_4)_{(2)}$, Phys. Rev. B **92**, 014413 (2015).

F48 (17) G. N. Rao, R. Sankar, A. Singh, I. P. Muthuselvam, W. T. Chen, V. N. Singh, **G. Y. Guo*** and F. C. Chou*, Tellurium-bridged two-leg spin ladder in Ba_2CuTeO_6, Phys. Rev. B **93**, 104401 (2016).

F49 (39) S. K. Karna, Y. Zhao, R. Sankar, M. Avdeev, P. C. Tseng, W. Wang, G. J. Shu, K. Matan, **G. Y. Guo** and F. C. Chou, Sodium layer chiral distribution and spin structure of $Na_2Ni_2TeO_6$ with a Ni honeycomb lattice, Phys. Rev. B **95**, 104408 (2017)

F50 (1) M.-W. Chu, **G. Y. Guo**, W. T. Chen, M. H. Lee, S. H. Lee, Y.-C. Lai, C. H. Du and C. H. Chen, Probing charge orders and hidden topology at atomic scale by cryogenic scanning transmission electron microscopy and spectroscopy, Phys. Rev. B **103**, 115130 (2021)

Oxide interfaces

F51 (73) P.-W. Lee, V. N. Singh, **G. Y. Guo***, H.-J. Liu, J.-C. Lin, Y.-H. Chu, C. H. Chen and M. W. Chu*, Hidden lattice instabilities as origin of the conductive interface between insulating $LaAlO_3$ and $SrTiO_3$, **Nature Commun. 7**, 12773 (2016).

F52 (8) C.-P. Su, A. Kr. Singh, T.-C. Wu, M.-C. Chen, Y.-C. Lai, W.-L. Lee, **G. Y. Guo** and M.-W. Chu*, Impact of strain-field interference on the coexistence of electron and hole gases in $SrTiO_3/LaAlO_3/SrTiO_3$, Phys. Rev. Mater. **3**, 075003 (2019).

F53 I. C. Lin, M. H. Lee, P. C. Wu, S. C. Lin, J. W. Chen, C.-C. Li, **G. Y. Guo**, Y.-H. Chu, R. Sankar and M.-W. Chu, Atomic-scale observation of spontaneous hole doping and concomitant lattice instabilities in strained nickelate films, New J. Phys. **24**, 023011 (2022)

G. Cu-based and Fe-based Superconductors and Related Materials

G1 (6) **G.Y. Guo**, W.M. Temmerman and G.M. Stocks
On the Metal-Semiconductor Transition and Antiferromagnetism in La_2CuO_4
J. Phys. C: Solid State Phys. **21**, L103 (1988).

G2 (24) **G.Y. Guo** and W.M. Temmerman
Electronic Structures and Magnetism in La_2NiO_4, J. Phys. C: Solid State Phys. **21**, L803 (1988).

G3 (1) G.M. Stocks, W.M. Temmerman, Z. Szotek, **G.Y. Guo**, and P.J. Durham
Ground State Properties and Electronic Structure of High Tc Superconductors
Physica C **153-155**, 1215 (1988).

G4 (47) W.M. Temmerman, Z. Szotek and **G.Y. Guo**
A Local Spin-Density Study of Antiferromagnetism in La_2CuO_4 and $YBa_2Cu_3O_6$
J. Phys. C: Solid State Phys. **21**, L867 (1988).

G5 W.M. Temmerman, **G.Y. Guo**, Z. Szotek and G.M. Stocks,
Local Spin Density Calculations for the High Tc Superconductors
Phys. Scripta T **25**, 78 (1989).

G6 (27) **G.Y. Guo** and W.M. Temmerman
Electronic and Magnetic Properties of La_2NiO_4: The Importance of La-O Planes
Phys. Rev. B **40**, 285 (1989).

G7 W. M. Temmerman, **G. Y. Guo**, Z. Szotek, P.J. Durham and G.M. Stocks
On the Validity of the Band Model for High Tc Superconductors
in *Proc. of the International Symposium on the Electronic Structure of High Tc Superconductors* (Pergamon, Oxford, 1989).

G8 (12) **G.Y. Guo**, Z. Szotek and W.M. Temmerman,
Effects of Doping and Structure on the Electronic Properties of Nd_2CuO_4
Physica C **162-164** (1989) 1351.

G9 (41) W.M. Temmerman, P.A. Sterne, **G.Y. Guo** and Z. Szotek,
Electronic Structure Calculations of High Tc Materials, Molecular Simulation **4**, 153 (1989).

G10 (215) **G.Y. Guo** and W.M. Temmerman
Suppression of Superconductivity in $PrBa_2Cu_3O_7$: 4*f* and Conduction-band Hybridization Effect,
Phys. Rev. B **41**, 6372 (1990).

G11 (20) Z. Szotek, **G.Y. Guo**, and W.M. Temmerman,
Effects of Structure and Doping on the Electronic Properties of La_2CuO_4 and Nd_2CuO_4
Physica C **175**, 1 (1991).

G12 (1) W.M. Temmerman, H. Winter, Z. Szotek, and **G.Y. Guo**,
On the Failure of the LSD to Describe the Antiferromagnetic Ground-state of La_2CuO_4
Physica B **172**, 279 (1991).

G13 (14) S. Sen and **G.-Y. Guo***, Pressure induced Lifshitz transition in ThFeAsN,
Phys. Rev. Mater. **4**, 104802 (2020).

G14 (10) S. Sen and **G.-Y. Guo***, Electronic structure, lattice dynamics, and magnetic properties of ThXAsN (X = Fe, Co, Ni) superconductors: A first-principles study,

Phys. Rev. B **102**, 224505 (2020).

H. Magnetic Transition Metal Systems

Bulk transition metals

H1 (2) **G.Y. Guo**, J.E. Inglesfield, M. Arnott and W.M. Temmerman
A Study of Magnetic Overlayers of Fe on Cu (001),
J. Phys.: Condensed Matter **1**, SB243 (1989).

H2 (15) **G.Y. Guo**, H. Ebert, W.M. Temmerman, K. Schwarz and P. Blaha
Relativistic Effects on the Structural and Magnetic Properties of Iron
Solid State Commun. **79**, 121 (1991).

H3 (30) **G.Y. Guo**, Giant orbital magnetic moments of Fe and Co in alkali metals Cs, Rb and K
Phys. Rev. B **62**, R14609 (2000).

H4 (80) **G. Y. Guo** and H. H. Wang
Calculated elastic constants and electronic and magnetic properties of bcc, fcc and hcp Cr crystals and films, Phys. Rev. B **62**, 5136 (2000).

H5 (8) F. Schedin, L. Hewitt, P. Morrall, V.N. Petrov, G. Thornton and **G.Y. Guo**
Observation of an exchange-split alloy surface state, Phys. Rev. B **61,** 9032 (2000).

H6 (171) **G. Y. Guo** and H. H. Wang
Gradient-corrected density functional calculation of elastic constants of Fe, Co and Ni in bcc, fcc and hcp structures, Chinese J. Phys.**38**, 949 (2000).

H7 (12) H.H. Wang and **G.Y. Guo**
Gradient-corrrected density functional calculation of structural and magnetic properties of bcc, fcc and hcp Cr, J. Magn. Magn. Mater. **209**, 98 (2000).

H8 (2) **G. Y. Guo**, On the origin of the giant magnetic moments of Fe and Co in Cs films
J. Magn. Magn. Mater.**240**, 334 (2002).

H9 **G.Y. Guo**
First-principles studies of the magnetic properties of hcp Cr/Cu (111) and Cr/Ru (0001) superlattices, Mat. Res. Soc. Symp. Proc. **721**, E7.7.1 (MRS, Pittsburgh, 2002).

H10 (46) H.C. Hsueh, J. Crain, **G.Y. Guo**, H.Y. Chen, C.C. Lee, K.P. Chang, and H.L. Shih,
Magnetism and mechanical stability of α-Iron, Phys. Rev. B **66**, 52420 (2002).

H11 (7) T. J. Zhang and **G. Y. Guo**
Density functional theory calculation of electronic and magnetic properties of hexagonal V/Ru thin films and superlattices, Phys. Rev. B **71**, 214442 (2005).

Magnetic anisotropy energy and magnetostriction

H12 (95) **G. Y. Guo**, W. M. Temmerman, and H. Ebert
First-Principles Determination of the Magnetisation Direction of Fe Monolayer in Noble Metals, J. Phys.: Condensed Matter **3**, 8205 (1991).

H13 (62) **G. Y. Guo**, W. M. Temmerman and H. Ebert
A Relativistic Spin-Polarised Band Theoretical Study of Magnetic Properties of Nickel and Iron, Physica B **172**, 61 (1991).

H14 (31) **G. Y. Guo**, W. M. Temmerman and H. Ebert

An *ab initio* Study of Magnetic Anisotropy of Fe*n*/Cu(Ag)*m* Multilayers
J. Mag. Mag. Materials **104**, 1772 (1992).

H15 **G. Y. Guo**, H. Ebert, W.M. Temmerman and P. J. Durham
Magnetic x-ray Dichroism and Anisotropy Energy in Fe and Co Multilayers
in *Metallic Alloys: Experimental and Theoretical Perspectives*
edited by J.S. Faulkner and R.G. Jordan (Kluwer Academic, Dordercht, 1994).

H16 (12) H. A. Durr, **G.Y. Guo**, B.T. Thole and G. van der Laan
Magnetocrystalline Anisotropy of Ultrathin Fe Films on Ni (110),
J. Phys.: Condens. Matter **8**, L111 (1996).

H17 (140) H.A. Durr, **G.Y. Guo**, G. van der Laan, J. Lee, G. Lauhoff and J.A.C. Bland,
Element-specific Magnetic Anisotropy Measurements with Transversal Magnetic
Circular x-ray Dichroism, **Science** **277**, 213 (1997).

H18 (26) **G. Y. Guo**
Strain, Interdiffusion, Magnetism and Double Spin-orientation Transitions
in Cu/Ni/Cu Sandwiches, J. Magn. Magn. Mater. **176**, 97-110 (1998).

H19 (18) **G. Y. Guo**
Magnetocrystalline Anisotropy Oscillations Predicted in Fe/Au (001) Superlattices,
J. Phys.: Condens. Matter **11**, 4329 (1999).

H20 (20) **G. Y. Guo**, D. J. Roberts and G. A. Gehring
First-principles Investigations of the Magnetocrystalline Anisotropy in Strained fcc Co,
Phys. Rev. B **59**,14466 (1999)

H21 (13) **G.Y. Guo**
Orientation-dependence of the Magnetoelastic Coupling Constants in Strained fcc Co and Ni:
An *Ab Initio* Study, J. Magn. Magn. Mater. **209**, 33 (2000).

H22 B. K. Wang, **G. Y. Guo** and C.-R. Chang
First-principles Studies of the Magnetic Anistropy and Magnetism in L10 FeCu Alloy
J. Magn. Magn. Mater. **209**, 214 (2000).

H23 (38) M. Faehnle, M. Komelj, R. Q. Wu and **G. Y. Guo**,
Magnetoelasticity of Fe: Possible failure of ab initio electron theory with the local-spin-density approximation and with the generalized gradient approximation,
Phys. Rev. B **65**, 144436 (2002)

H24 (1) **G.Y. Guo**, Y.L. Wang and C.T. Chen
On the orbital magnetic moments and anisotropy energies of ordered $Fe_{0.5}Pd_{0.5}$ alloys,
J. Magn. Magn. Mater. **239**, 66 (2002).

H25 (22) X. Ma, P. He, L. Ma, **G. Y. Guo***, H. B. Zhao*, S. M. Zhou, G. Luepke*,
Spin-orbit interaction tuning of perpendicular magnetic anisotropy in $L1_0$ FePdPt films,
Appl. Phys. Lett. **104**, 192402 (2014).

H26 (11) C.-H. Chang, K.-P. Dou, **G.-Y. Guo**, C.-C. Kaun, Quantum-well induced engineering of magnetocrystalline anisotropy in ferromagnetic films, NPG Asia Mater. **9**, e424 (2017)

Magnetic hyperfine field

H27 (47) **G. Y. Guo** and H. Ebert

First-principles Study of the Magnetic Hyperfine Field in Fe and Co Multilayers
Phys. Rev. B **53**, 2492 (1996).

H28 **G. Y. Guo** and H. Ebert
An *ab initio* Investigation of the Hyperfine Field Anisotropy Fe and Co Multilayers
J. Magn. Magn. Mater. **156**, 289 (1996).

H29 (14) **G. Y. Guo** and H. Ebert
First-principles Study of the Magnetic Hyperfine Field in Fe Multilayers
Hyperfine Interactions **97/98**, 11 (1996).

Magnetooptical Kerr effect

H30 (76) **G.Y. Guo** and H. Ebert
Theoretical Investigation of the Orientation Dependence of the Magneto-optical Kerr Effect in Co, Phys. Rev. B (Rapid Comm.) **50**, 10377 (1994).

H31 (150) **G.Y. Guo** and H. Ebert
Band-theoretical Investigation of the Magneto-optical Kerr Effect in Fe and Co Multilayers, Phys. Rev. B **51**, 12633 (1995).

H32 (6) H. Ebert, **G.Y. Guo** and G. Schutz,
Magneto-optical Properties of Transition Metal Systems in the Visible and X-ray Regime
IEEE Trans. Magn. **31**, 3301 (1995).

H33 (32) **G.Y. Guo** and H. Ebert,
On the Origins of the Enhanced Magneto-optical Kerr Effect in Ultrathin Fe and Co Multilayers, J. Magn. Magn. Mater. **156**, 173 (1996).

H34 (5) L. Ma, J. Hu, M. Costa, Z. Shi, J. Li, X. G. Xu, Y. Jiang, **G. Y. Guo**, R. Q. Wu, S. M Zhou, Magneto-optical Kerr effect in L10 FePdPt ternary alloys: Experiments and first-principles calculations, J. Appl. Phys. **115**, 183903 (2014).

H35 (101) W.-X. Feng, **G. Y. Guo***, J. Zhou, Y. Yao and Q. Niu
Large Magneto-Optical Kerr Effect in Noncollinear Antiferromagnets Mn_3X (X =Rh, Ir, Pt)
Phys. Rev. B **92**, 144426 (2015)

X-ray magnetic dichroism

H36 (166) **G.Y. Guo**, H. Ebert, W.M. Temmerman and P.J. Durham,
First-principles Calculation of Magnetic x-ray Dichroism in Fe and Co multilayers
Phys. Rev. B **50**, 3861 (1994).

H37 (10) **G.Y. Guo**, H. Ebert, W.M. Temmerman and P.J. Durham,
Band Theoretical Investigation of Circular Magnetic X-ray Dichroism in Fe and Co multilayers, J. Mag. Mag. Mat. **148**, 66 (1995).

H38 (12) T. Boske, W. Clemens, D. Schmitz, J. Kojnok, M. Schafer, V. Cros, **G.Y. Guo** and W. Eberhardt, The Coupling of Cr to Fe Studied by Circular Magnetic X-ray Dichroism
Appl. Phys. A **61**, 119 (1995).

H39 (4) J. Schwitalla, H. Ebert, **G.Y. Guo**, and G. Schutz,
A Fully Relativistic Description of Circular and Linear Magnetic X-ray Dichroism in Magnetic Multilayer Systems, Physica B **208-209**, 757 (1995).

H40 (106) M.M. Schwickert, **G.Y. Guo**, M.A. Tomaz, W.L. O'Brien and G.R. Harp
X-ray Magnetic Linear Dichroism at the L-edge of Metallic Co, Fe, Cr and V
Phys. Rev. B **58**, R4289 (1998)

Tunneling and magnetoresistance

H41 (16) S.S. Liu and **G.Y. Guo**,
Voltage-dependence of Magnetoresistance in Ferromagnetic Tunneling Junctions: A Rigorous Free Electron Model Study, J. Magn. Magn. Mater. **209**, 135 (2000).

H42 (1) S.S. Liu and **G. Y. Guo**,
Spin Current Source and Spin Valve based on Double Barrier Magnetic Tunneling Junctions
Chinese J. Phys. **38**, 1074 (2000).

H43 S. Ju, T.-Y. Cai, **G.-Y. Guo** and Z.-Y. Li
Percolation transition and colossal magnetoresistance effects in a complex network
Appl. Phys. Lett. **89**, 082506 (2006).

H44 (6) Y.-F. Hsu, T.-W. Chiang, **G. Y. Guo***, S. F. Lee*, J.-J. Liang
Effect of Transport-Induced Charge Inhomogeneity on Point-Contact Andreev Reflection Spectra at Ferromagnet-Superconductor Interfaces, J. Phys. Soc. Jpn. **81**, 084701 (2012)

Thermoelectric materials

H45 (15) P.-C. Wei, T.-S. Huang, S. W. Lin, **G. Y. Guo**, Y. Y. Chen,
Thermoelectric properties optimization of Fe_2VGa by tuning electronic density of states via titanium doping, J. Appl. Phys. **118**, 165102 (2015).

I. Photoelectron Spectroscopies Using Synchrotron Radiation

Magnetic x-ray scattering

I1 (34) S. P. Collins, D. Laundy and **G. Y. Guo**
Spin and Orbital Magnetic x-ray Diffraction in $HoFe_2$, J. Phys.: Condens. Matter **5**, L637 (1993)

Interpretation of x-ray magnetic dichroism

I2 (44) **G.Y. Guo**
Interpretation of x-ray circular dichroism: multiple-scattering theory approach
Phys. Rev. B **57**, 10295 (1998).

I3 (74) **G.Y. Guo**
What does the K-edge X-ray Magnetic Circular Dichroism Spectrum Tell Us
J. Phys.: Condensed Matter **8**, L747 (1996).

Magneto-x-ray Kerr effects

I4 (57) **G.Y. Guo**
Spin and Orbital Polarized Multiple Scattering Theory of Magneto-x-ray Effects in Fe, Co and Ni, Phys. Rev. B **55**, 11619 (1997).

I5 **G.Y. Guo**
Spin and Orbital Polarized Multiple Scattering Theory of Magneto-x-ray Effects in Fe
J. de Phys. IV (Colloques) C **2**, 117 (1997).

I6 (24) D. Knabben, F.U. Hillebrecht and **G.Y. Guo**
Transverse Magneto-optic Kerr Effect at the Fe 2p Threshold
J. Magn. Magn. Mater. **190**, 349 (1998).

Dichroic x-ray fluorescence

I7 (57) C.F. Hague, J.-M. Mariot, **G.Y. Guo**, K. Hricovini and G. Krill,
Coster-Kronig Contributions to Magnetic Circular Dichroism in the $L_{2,3}$ X-ray Fluorescence of Iron, Phys. Rev. B (Rapid Comm.) **51**, 1370 (1995).

X-ray absorption and photoemission

I8 (116) B. Poumellec, P.J. Durham and **G.Y. Guo**,
Electronic Structure and X-ray Absorption Spectrum of Rutile TiO_2
J. Phys.: Condensed Matter **3**, 8195 (1991).

I9 (3) P.J. Durham and **G.Y. Guo**, UV and x-ray Photoemission from Metal and Alloys
in *Metallic Alloys: Experimental and Theoretical Perspectives*
edited by J. S. Faulkner and R. G. Jordan (Kluwer Academic, Dordercht, 1994).

I10 (23) H. Ebert and **G.Y. Guo**
A Relativistic Description of Spin- and Angular-resolved Core Level Photoemission Spectroscopy for Magnetic Solids, J. Mag. Mag. Mat. **148**, 174 (1995).

J. Heavy Fermion and Related 4*f* and 5*f* Metal Compounds

J1 (8) **G.Y. Guo**, On the Fermi Surface of $CeAl_2$, Physica B **165-166**, 335 (1990).

J2 (4) M.B. Suvasini, **G.Y. Guo**, W.M. Temmerman and G.A. Gehring
Metamagnetic Transition and Electronic Structure of UPt_3, Physica B **186-188**, 860 (1993).

J3 (15) M.B. Suvasini, **G.Y. Guo**, W.M. Temmerman and G.A. Gehring,
Metamagnetic Transition and Magnetic Properties of UPt_3,
Phys. Rev. Lett. **71**, 2983 (1993).

J4 (9) M.B. Suvasini, **G.Y. Guo**, W.M. Temmerman and G.A. Gehring
Band Theoretical Study of the Fermi Surface of CeB_6, Physica B **206-207**, 37 (1995).

J5 (15) M.B. Suvasini, **G.Y. Guo**, W.M. Temmerman and G.A. Gehring,
The Fermi Surface of CeB_6, J. Phys.: Condensed Matter **8**, 7105 (1996).

J6 (172) **G.Y. Guo**, G.A. Botton and Y. Nishino
Electronic Structure of Possible 3*d* 'Heavy-fermion' Compounds Fe_2VAl,
J. Phys.: Condens. Matter **10**, L119-L126 (1998).

J7 (15) I. P. Muthuselvan, R. Nehru, K. R. Babu, K. Saranya, S. N. Kaul, S. M. Chen, W.-T. Chen, Y. W. Liu, **G. Y. Guo**, F. X. Xiu, R. Sankar, Gd_2Te_3: An antiferrmagnetic semimetal,
J. Phys.: Condens. Matter **31**, 285802 (2019)

K. High Performance Alloys and Intermetallics Compounds

K1 (59) B. Ginatempo, **G.Y. Guo**, W.M. Temmerman, J.B. Staunton and P.J. Durham,
Electronic Structure of Ordered and Disordered Alloys: Cu_3Pd, Cu_3Pt, Cu_3Au
Phys. Rev. B **42**, 2761 (1990).

K3 (14) R.G. Jordan, Y. Liu, S.L. Qiu and X. Xu, P.J. Durham and **G.Y. Guo**
Origin of Long Period Superlattices in Ag-Mg Alloys, Phys. Rev. B **47**, 16521 (1993).

K4 (7) G.A. Botton, **G.Y. Guo** and C.J. Humphreys,
The Bonding Character of Intermetallic alloys by EELS, Inst. Phys. Conf. Ser. **147**, 535 (1995).

K5 (4) S.L. Qiu, R.G. Jordan, A.T. Dorsey, P.J. Durham, **G.Y. Guo** and M.W. Ruckman
Cu Local Density of States in CuAu from Photoemission Measurements,
Phys. Rev. B **51**, 1513 (1995).

K6 (30) J.M. Zhang and **G.Y. Guo**
Electronic Structure and Phase Stability of Three Series of B2 Ti-transition-metal Compounds,
J. Phys.: Condens. Matter **7**, 6001 (1995).

K7 G.A. Botton, **G.Y. Guo**, W.M. Temmerman and C.J. Humphreys,
Electron Energy Loss Spectroscopy as a Tool to Probe the Electronic Structure
of Intermetallic Alloys, in *Proc. 1st International Alloy Conf., Athens 1996*
edited, A. Gonis, A. Meike, P. Turchi (Plenum Press).

K8 G.A. Botton, **G.Y. Guo**, W.M. Temmerman, Z. Szotek,
C.J. Humphreys, Yang Wang, G.M. Stocks, W.A. Shelton and D.M.C. Nicholson,
Electronic Structure Studies of B2-type Transition Metal Aluminides and
Alloys: Experiments and Theory, *Mat. Res. Soc. Sym. Proc.* Vol. **408**, 567
(Materials Research Society, Pittsburgh, 1996).

K9 (115) G.A. Botton, **G.Y. Guo**, W.M. Temmerman and C.J. Humphreys,
Experimental and Theoretical Study of the Electronic Structure of Fe, Co and Ni aluminides
with the B2 structure, Phys. Rev. B **54**, 1682 (1996).

K10 (8) R.G. Jordan, X. Xu, S.L. Qiu, P.J. Durham and **G.Y. Guo**
The Long-period Superlattices in CuAu II, J. Phys.: Condens. Matter **8**, 1503 (1996).

K11 (9) R.G. Jordan, **G.Y. Guo** and L.R. Masliah,
Surface States at the M-point on Cu (100), Solid State Commun. **99**, 73 (1996).

K12 (3) R.G. Jordan and **G.Y. Guo**
Surface States on the (001) Surface of CuAu I, Phys. Rev. B **55**, 7222 (1997).

K13 (43) J.M. Zhang and **G.Y. Guo**, A Microscopic Theory of the Shape Memory Effect in TiNi
Phys. Rev. Lett. **78**, 4789 (1997)

K14 (2) R.G. Jordan and **G.Y. Guo**
Core Level Shifts and Density of States at the (100) Surface of Cu_3Au
Solid State Commun. **105** (1998) 125.

K15 (17) L.-S. Hsu, **G.Y. Guo**, J.D. Denlinger and J.W. Allen
Experimental and theoretical study of the electronic structure of $PtGa_2$,
Phys. Rev. B **63**, 155105 (2001).

K16 (43) L.-S. Hsu, **G.Y. Guo**, J.D. Denlinger and J.W. Allen
Experimental and theoretical study of the electronic structure of $AuAl_2$
J. Phys. Chem. Solids **62**, 1047 (2001).

K17 (3) L.-S. Hsu, Y.K. Wang, **G.Y. Guo**, Y.-J. Huang and M.-D. Lan,
Modeling and photoabsorption study of $YPd_{2-x}Rh_xB_2C$ superconductors,

MRS Proceedings **731**, 301 (2002).

K18 (38) **G.Y. Guo**, Y.K. Wang and L.-S. Hsu
First-principles and experimental studies of the electronic structure and magnetism in Ni_3Al, Ni_3Ga and Ni_3In, J. Magn. Magn. Mater. **239**, 91 (2002).

K19 (3) L.-S. Hsu, **G.Y. Guo**, J.D. Denlinger and J. W. Allen,
Experimental and theoretical studies of the electronic structures of $AuAl_2$ and $PtGa_2$,
Surface Review and Letters **9**, 251 (2002).

K20 (26) L.-S. Hsu, Y.K. Wang, **G.Y. Guo**, and C.S. Lue
Experimental and theoretical study of the electronic structures of Fe_3Al, Fe_2VAl, Fe_2VGa,
Phys. Rev. B **66**, 205203 (2002).

K21 (22) L.-S. Hsu, Y.K. Wang and **G.Y. Guo**,
Experimental and theoretical study of the electronic structures of Ni_3Al, Ni_3Ga, Ni_3In and NiGa,
J. Appl. Phys.**92**, 1419 (2002).

K22 (13) **G. Y. Guo**, Y. K. Wang and L.-S. Hsu,
Ab initio studies of structural stability and magnetism in Ni_3In, Phys. Rev. B **66**, 54440 (2002).

K23 (10) L.-S. Hsu, Y.K. Wang and **G.Y. Guo**,
Experimental and theoretical study of the electronic structure of Fe_3Al,
Nuclear Instruments and Methods B **199**, 200 (2003).

K24 (7) L.-S. Hsu, Y.K. Wang and **G.Y. Guo**,
Experimental and theoretical study of the electronic structures of intermetallic compounds and alloys containing Fe or Ni, J. Alloys and Compounds **375**, 44 (2004).

L. Semiconductors and Magnetic Semiconductors

L1 (36) **G.Y. Guo**, J. Crain, P. Blaha and W. M. Temmerman,
Structural and Electronic Properties of InSb Under Pressure, Phys. Rev. B **47**, 4841 (1993).

L2 **G.Y. Guo**. Surface Electronic Structure of GaAs (110)-Bi (1 ML) in *Proc. of 21st International Conf. on Physics of Semiconductors*, *Beijing, 10-14 August 1992*, edited by P. Jiang and H.-Z. Zheng, (World Scientific, Singapore, 1993)

L3 (6) **G.Y. Guo**, J. Crain and W.M. Temmerman,
On the High Pressure Phase of InSb, Japanese J. Appl. Phys. **32**, Suppl. 32-1, 39 (1993)

L4 (47) H.-C. Hsueh, J.R. Maclean, **G.Y. Guo**, M.-H. Lee, S.J. Clark, G.J. Ackland and J. Crain, Pressure-induced Polymorphism in CuCl: An *ab initio* Study,
Phys. Rev. B **51**, 12216 (1995).

L5 (18) **G.Y. Guo**, Surface electronic structure and magnetic properties of semiconductor FeSi,
Physica E **10**, 383 (2001).

L6 (147) C.-H. Chien, S. H. Chiou, **G. Y. Guo**,Y.-D. Yao,
Electronic structure and magnetic moments of 3d transition metal doped ZnO,
J. Magm. Magm. Mater. **282**, 275 (2004).

L7 (14) Z. R. Xiao, **G. Y. Guo**, P. H. Lee, H. S. Hsu and J. A. C. Huang
Oxygen vacancy induced ferromagnetism in V_2O_{5-x}, J. Phys. Soc. Japan **77**, 023706 (2008).

L8 (10) D. J. Cai, J. Y. Kang and **G. Y. Guo***, Microscopic origin of light emission from AlyGa1-

y/GaN superlattices: Band profile and active site, Phys. Rev. B **80**, 045311 (2009).

L9 (49) Z. R. Xiao and **G. Y. Guo***, Structural, electronic and magnetic properties of V_2O_{5-x}: An ab initio study, J. Chem. Phys. **130**, 214704 (2009).

L10 (29) D. J. Cai and **G. Y. Guo***, Tuning linear and nonlinear optical properties of wurtzite GaN by c-axial stress, J. Phys. D: Appl. Phys. **42**, 185107 (2009).

L11 (4) D. J. Cai, and **G. Y. Guo**
Spatial localization of quantized states responsible for sharp optical transition in AlGaN/GaN superlattice, J. Appl. Phys. **107**, 103533 (2010).

L12 (37) S. W. Chen, S. C. Huang, **G. Y. Guo***, J. M. Lee, S. Chiang, W. C. Chen, Y. C. Liang, K. T. Lu and J. M. Chen*, Gapless band structure of $PbPdO_2$: A combined first princples calculation and experimental study, Appl. Phys. Lett. **99**, 012103 (2011).

L13 (12) S. W. Chen, S. C. Huang, **G. Y. Guo***, S. Chiang, J. M. Lee, S. A. Chen, S. C. Haw, K. T. Lu and J. M. Chen*, A combined first princples calculations and experimental study on the spin-polarized band structure of Co-doped $PbPdO_2$, Appl. Phys. Lett. **101**, 222104 (2012).

L14 (43) S. H. Nie, Y. Y. Chin, W. Q. Liu, J. C. Tung, J. Lu, H. J. Lin, **G. Y. Guo***, K. K. Meng, L. Chen, L. J. Zhu, D. Pan, C. T. Chan, Y. B. Xu, W. S. Yan, and J. H. Zhao*, Ferromagnetic interfacial interaction and the proximity effect in a Co_2FeAl/(Ga,Mn)As bilayer, **Phys. Rev. Lett. 111**, 027203 (2013).

L15 (31) C.-R. Wang, J.C. Tung, R. Sankar, C.-T. Hsieh, Y.-Y. Chien, **G. Y. Guo***, F. C. Chou and W.-L. Lee*, Magnetotransport in copper-doped noncentrosymmetric BiTeI, Phys. Rev. B **88**, 081104(R) (2013)

L16 (11) L. Chen, J. Zheng, W. Lin*, J. Li, K. Li, P. Sun, **G.-Y. Guo** and J. Kang*, Abnormal radiative interband transitions in high-Al-content AlGaN quantum wells induced by polarized orbitals, ACS Photonics **4**, 2197 (2017).

L17 (18) C. R. P. Inbaraj, V. K. Gudelli, R. J. Mathew, R. K. Ulaganathan, R. Sankar, H. Y. Lin, H.-I. Lin, Y.-M. Liao, H.-Y. Cheng, K.-H. Lin, F. C. Chou, Y.-T. Chen, C.-H. Lee, **G.-Y. Guo** and Y.-F. Chen*, Sn-doping enhanced ultrahigh mobility $In_{1-x}Sn_xSe$ phototransistor, ACS Appl. Mater. Interfaces **11**, 24269 (2019).

L18 (14) W.-K. Li and **G.-Y. Guo***, A First Principle Study on Magneto-Optical Effects in Ferromagnetic Semiconductors $Y_3Fe_5O_{12}$ and $Bi_3Fe_5O_{12}$, Phys. Rev. B **103**, 014439 (2021).

L19 (10) M. Sotome, M. Nakamura, T. Morimoto, Y. Zhang, **G.-Y. Guo**, M. Kawasaki, N. Nagaosa, Y. Tokura and N. Ogawa, Terahertz emission spectroscopy of ultrafast exciton shift current in the noncentrosymmetric semiconductor CdS, Phys. Rev. B **103**, L241111 (2021)

M. Computational Methods

M1 W. M. Temmerman, Z. Szotek, H. Winter and **G. Y. Guo**
Computational Methods in Electronic Structure Calculations of Complex Solids in *Supercomputational Science*, edited by S. Wilson and R. G. Evans (Plenum Press, New York, 1990).

M2 S. C. Lovatt, B. L. Gyorffy and **G. Y. Guo**
Solution of the Single-site Aspherical Scattering Problem for the Dirac Equation in *Applications*

of Multiple Scattering Theory to Materials Science, edited by W. H. Butler, P. H. Dederichs, A. Gonis and R.L. Weaver (Materials Research Society, Pittsburgh, 1992).

M3 (2) **G. Y. Guo** and W. M. Temmerman,
A Multi-atom, Self-consistent, Relativistic KKR Electronic Structure Program:
Numerical Aspects and Applications,
in *Applications of Multiple Scattering Theory to Materials Science*, edited by W. H. Butler, P. H. Dederichs, A. Gonis and R.L. Weaver (Materials Research Society, Pittsburgh, 1992).

M4 (45) S. C. Lovatt, B. L. Gyorffy and **G. Y. Guo**
Relativistic Spin-polarized Scattering Theory for Space-filling Potentials,
J. Phys.: Condensed Matter **5**, 8005 (1993)

M5 (20) H. Ebert and **G. Y. Guo**,
Calculation of Magnetic X-ray Dichroism (MXD) Spectra using the Spin Polarized Relativistic Linear Muffin-Tin-Orbital Method of Band Structure, Solid State Comm. **91**, 85 (1994).

M6 (76) H. Ebert, H. Freyer and A. Vernes, and **G. Y. Guo**
Manipulation of the Spin-orbit Coupling using the Dirac Equation for Spin-dependent Potentials, Phys. Rev. B **53**, 7721 (1996).

M7 S. V. Beiden, **G. Y. Guo**, W. M. Temmerman, Z. Szotek, G. A. Gehring,
Yang Wang, G.M. Stocks, D.M.C. Nicholson, W.A. Shelton and H. Ebert,
O(N) Multiple Scattering Method for Relativistic and Spin-polarized Systems
Mater. Res. Soc. Symp. Proc. Vol. **408**, 73 (MRS, Pittsburgh, 1996).

N. Polymers

N1 (29) R.-L. Fu, **G. Y. Guo** and X. Sun,
Effects of the electric field on self-trapping excited states in conjugated polymers,
Phys. Rev. B **62**, 15735 (2000).

N2 (3) R.-L. Fu and **G. Y. Guo**
Effects of electron-electron interactions on the polarization characteristics of electroluminescent polymers, J. Infrared Millim. Wave **19**, 259 (2000).

N3 (1) R.-L. Fu, **G. Y Guo**, W.-M. Zheng and X. Sun
Dynamical study on the self-trapping excitons in conjugated polymers under electric fields, Synthetic Metals **119**, 531 (2001).

N4 (2) M. Mustaqeem, S. Kamal, N. Ahmad, P.-T. Chou, K.-H. Lin, Y.-C. Huang, **G.-Y. Guo**, C. R. P. Inbaraj, W.-K. Li, H.-C. Yao, K.-L. Lu, and Y.-F. Chen,
Chiral metal-organic framework based spin-polarized flexible photodetector with ultrahigh sensitivityspin, **Mater. Today Nano** **21**, 100303 (2023)