

PUBLICATION LIST of Guang-Yu Guo (2021/12)

(郭光宇教授學術著作目錄)

郭光宇教授已發表了290多篇期刊論文, 含頂尖科技期刊「科學」(Science) (1篇: H17)、物理學頂尖期刊「自然物理」(Nature Physics) (1篇: D14)、「物理評論通訊」(Physical Review Letters) (18篇: A1, C1, C3, C4, C5, C9, C10, C15, 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: F42)、奈米科學頂尖期刊「奈米通訊」(Nano Letters) (1篇: E8)及高影響因子自然期刊「自然通訊」(Nature Commun.) (4篇: A45, D9, F8, F49)等頂尖期刊論文共20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SCI 論文引用9400多次, H-指數 (H-index) 高達49 (參見Web of Science) [若依谷歌學者(Google Scholars), 郭教授的論文已被引用12000多次, H-指數為57]。

近6年來(2016年1月後), 郭教授繼續研究尖端材料(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, 又發表了約70篇期刊論文, 包括物理學頂尖期刊美國物理學會的「物理評論通訊」(**Physical Review Letters**) (影響因子:9.2) (3篇)與「物理評論X」(**Physical Review X**) (影響因子:15.8) (2篇)及高影響因子期刊自然期刊公司的「自然物理」(**Nature Physics**) (影響因子:20.0) (1篇)與「自然通訊」(**Nature Communications**) (影響因子:14.9) (4篇), 這些論文已被引用了900多次。下面依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 more than 290 refereed papers, including 1 <Science> paper [H17], 1 <Nature Physics> paper [D14], 18 <Physical Review Letters> papers [A1, C1, C3, C4, C5, C9, C10, C15, D1, D10, F1, F4, F5, F23, F37, J3, K13, L14] and 2 <Physical Review X> papers [D12, F39], 1 <Journal of American Chemical Society> paper [F42], 1 <Nano Letters> paper [E8], and 4 <Nature Communications> papers [A45, D9, F8, F49]. Except the <Science> paper [H17] and two of the <Physical Review Letters> papers [J3, K13], all these highly prestigious and high impact factor 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 9,400 times, and his H-index is 49 (see Web of Science) [Total citations of his papers would be more than 12,000 times and his H-index would be 57, according to Google Scholars].

In the past 6 years (since Jan., 2016), 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). During this period, he has again published 70 papers in international journals including high-impact factor journals **Nature Physics** (Impact Factor: 20.0) (1 paper) and **Nature Communications** (Impact Factor: 14.9) (4 papers) as well as very prestigious physics journal **Physical Review Letters** (Impact Factor: 9.2) (3 papers) and **Physics Review X** (Impact Factor: 14.9) (2 papers). These 70 papers have already been cited over 900 times. All his papers are listed below according to research topics.

A. Nano-meter Materials and Mesoscopic Systems

Carbon, BN and SiC nanotubes and nanostructures

- A1 (citations: 105) L. Liu, **G.Y. Guo**, C.S. Jayanthi and S.Y. Wu,
Colossal paramagnetic moments in metallic carbon nanotubes,
Phys. Rev. Lett. **88**, 217206 (2002).
- A2 (228) **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 (45) **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 (18) 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 (142) **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 (68) **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. 075416, 2005)
Phys. Rev. B **77**, 049901 (2008).
- A8 (10) **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 (45) **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 (141) I.J. Wu and **G.Y. Guo***
Optical properties of SiC nanotubes: An *ab initio* study, *Phys. Rev. B* **76**, 035343 (2007).
- A11 (50) 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 (107) 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)

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

- A13 X.-F. Jiang and **G. Y. Guo**

Spin gap in doped dimerized chain near half-filling, *Physica B* **334**, 451 (2003).

A14 (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).

A15 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.

A16 (27) X.-F. Jiang and **G.Y. Guo**

Electronic structure and exchange interactions in BaVS₃, *Phys. Rev. B* **70**, 035110 (2004).

A17 (8) 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)

A18 (111) J.C. Tung and **G.Y. Guo***

Systematic *ab initio* study of the magnetic and electronic properties of all 3d transition metal linear and zigzag nanowires,

Phys. Rev. B **76**, 094413 (2007)

A19 (11) 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)

A20 (10) 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)

A21 (36) J. C. Tung and **G. Y. Guo***

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

A22 (13) 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).

A23 (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)

A24 (24) 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)

A25 (12) 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

A26 (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).

A27 (4) 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).

A28 J. C. Lin and **G. Y. Guo***

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

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

A29 (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

CeCo₂, J. Magn. Magn. Mater. **272**, E1193-1194 (2004).

A30 (9) 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).

A31 (7) 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)

A32 (33) 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

A33 (28) Y.-F. Hsu, and **G. Y. Guo***

Anomalous integer quantum Hall effect in AA-stacked bilayer graphene,

Phys. Rev. B **82**, 165404 (2010)

A34 (25) Y. F. Hsu and **G. Y. Guo***,

Tunneling conductance of grapheme ferromagnet-insulator-superconductor junctions,

Phys. Rev. B **81**, 045412 (2010).

A35 (35) 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)

A36 (9) 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).

A37 (55) 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).

A38 (70) C.-Y. Wang and **G.Y. Guo***,

Nonlinear Optical Properties of Transition-Metal Dichalcogenide MX₂ (M = Mo, W; X = S, Se) Monolayers and Trilayers from First-Principles Calculations,

J. Phys. Chem. C **119**, 13268 (2015)

A39 (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).

- A40 (10) 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).
- A41 (22) C.-S. Tan, Y.-J. Lu, C.-C. Chen, P.-H. Liu, S. J. Gwo, **G. Y. Guo*** and L.-J. Chen*, Magnetic MoS₂ interface monolayer on CdS nanowire by cation exchange, *J. Phys. Chem. C* **120**, 23055 (2016)
- A42 (26) 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)
- A43 (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).
- A44 (7) 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).
- A45 (30) 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).
- A46 (11) 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).
- A47 (23) 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).
- A48 (65) Y. Fang, S. Wu, Z.-Z. Zhu and **G. Y. Guo***, Large magneto-optical effects and magnetic anisotropy energy in two-dimensional Cr₂Ge₂Te₆, *Phys. Rev. B* **98**, 125416 (2018).
- A49 (13) 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).
- A50 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).
- A51 (33) V. K. Gudelli and **G. Y. Guo***, Magnetism and Magneto-optical Effects in Bulk and Few-layer CrI₃: A Theoretical GGA + U Study, *New J. Phys.* **21**, 053012 (2019).
- A52 (2) A. A. Pervishko, D. Yudin, V. K. Gudelli, A. Delin, O. Eriksson and **G.-Y. Guo**, Localized surface electromagnetic waves in CrI₃-based magnetophotonic structures *Optics Express* **28**, 29155-29165 (2020)
- A53 (2) V. K. Gudelli and **G.-Y. Guo***, Antiferromagnetism-induced second-order nonlinear optical responses of centrosymmetric bilayer CrI₃, *Chin. J. Phys.* **68**, 896-907 (2020)
- A54 (1) 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)

- A55 V. K. Gudelli and **G.-Y. Guo***, Large bulk photovoltaic effect and second-harmonic generation in few-layer pentagonal semiconductors PdS₂ and PdSe₂, *New J. Phys.* **23**, 093028 (2021).
- A56 M.-J. Jiang and **G.-Y. Guo***, Large magneto-optical effect and magnetic anisotropy energy in two-dimensional metallic ferromagnet Fe₃GeTe₂, *Phys. Rev. B* (2021, submitted).

B. Layered Transition Metal Dichalcogenides

- B1 (78) **G. Y. Guo**, and W. Y. Liang,
The Electronic Structures of Platinum Dichalcogenides: PtS₂, PtSe₂ and PtTe₂
J. Phys. C: Solid State Phys. **19**, 995 (1986).
- B2 (24) **G. Y. Guo** and W. Y. Liang,
Study of the Electronic Structures of Ni-Group Metal Ditellurides-NiTe₂, PdTe₂ and PtTe₂ 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 (53) **G. Y. Guo** and W. Y. Liang,
Electronic Structures of Intercalation Complexes of the Layered Compound 2H-TaS₂,
J. Phys. C: Solid State Phys. **20**, 4315 (1987).
- B5 (4) D. Sebilliau, **G.Y. Guo** and W.M. Temmerman,
A Band Model for the Electronic and Magnetic Structure of NaCrS₂,
J. Phys.: Condensed Matter **1**, 5653 (1989).
- B6 (112) 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 NbSe₂
J. Phys.: Condens. Matter **6**, 4479 (1994).

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

- C1 (105) **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 (41) 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 (30) 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 InGa_N/Ga_N superlattices
Phys. Rev. Lett. **98**, 136403 (2007); **98**, 239902 (2007).
- C4 (246) **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 (73) **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 (15) 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 (41) **G. Y. Guo**

Ab initio calculation of intrinsic spin Hall conductivity of Pd and Au
J. Appl. Phys. **105**, 125301 (2009)

C8 (4) 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 (30) 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 (65) 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 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 (5) 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 (39) H.-R. Fuh and **G. Y. Guo***

Intrinsic anomalous Hall effect in nickel: A GGA + U study,
Physical Review B **84**, 144427 (2011)

C14 (13) 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 (81) 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 $L1_0\text{FePd}_{1-x}\text{Pt}_x$ alloy
films, **Phys. Rev. Lett.** **109**, 066402 (2012).

C16 (40) 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 (27) 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 (46) **G. Y. Guo***, Q. Niu, N. Nagaosa,

Anomalous Nernst and Hall effects in magnetized platinum and palladium,
Phys. Rev. B **89**, 214406 (2014)

C19 (18) X. Zhou, L. Ma, Z. Shi, **G. Y. Guo***, J. Hu, R. Q. Wu and M. Zhou,

Tuning magnetotransport in PdPt/Y₃Fe₅O₁₂: Effects of magnetic proximity and spin-orbit coupling, *Appl. Phys. Lett.* **105**, 012408 (2014).

C20 (19) H.-L. Huang, J.-C. Tung and **G. Y. Guo***

Anomalous Hall effect and current spin polarization in Co₂FeX (X = Al, Ga, In, Si, Ge, and Sn) Heusler compounds: A systematic ab initio study, *Phys. Rev. B* **91**, 134409 (2015)

C21 (22) 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 (44) **G. Y. Guo*** and T.-C. Wang, Large anomalous Nernst and spin Nernst effects in noncollinear antiferromagnets Mn₃X (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 Mn₃X (X=Sn, Ge, Ga) (vol. 96, 224415, 2017),

Phys. Rev. B **100**, 169907 (2019).

C24 (17) 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 (4) 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 (23) 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 Mn₃XN with X = Ga, Zn, Ag or Ni

Phys. Rev. B **99**, 104428 (2019).

C27 (5) 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 (2) Z. Shi, S. J. Xu, L. Ma, S. M. Zhou and **G.-Y. Guo***, Anomalous Nernst Effect in Epitaxial L₁₀ FePd_{1-x}Pt_x Alloy Films: Berry Curvature and Thermal Spin Current,

Phys. Rev. Applied **13**, 054044 (2020).

C29 (2) 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).

D. Topological Insulators and Topological Semimetals

D1 (34) 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}RhO₂, *Phys. Rev. Lett.* **116**, 256601 (2016).

D2 (13) 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 Cd₃As₂

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

D3 (9) 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 (7) H.-S. Lu and **G. Y. Guo***, Strain and onsite-correlation tunable quantum anomalous Hall phases in ferromagnetic (111) LaXO₃ bilayers (X=Pd, Pt), *Phys. Rev. B* **99**, 104405 (2019).
- D5 (5) H.-S. Lu and **G. Y. Guo***, Anomalous ferromagnetism and magneto-optical Kerr effect in semiconducting double perovskite Ba₂NiOsO₆ and its (111) (Ba₂NiOsO₆)/(BaTiO₃)₁₀ superlattice, *Phys. Rev. B* **100**, 054443 (2019).
- D6 (12) 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 (16) 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 (11) 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 (15) 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 (35) 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 (2) R. Sankar, I. P. Muthuselvan, 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 (30) 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 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 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).
- D14 J. Ahn, **G.-Y. Guo**, N. Nagaosa and A. Vishwanath, Riemannian Geometry of Resonant Optical Responses, **Nature Physics** (2021, <https://doi.org/10.1038/s41567-021-01465-z>).
- D15 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).

E. Photonic Crystals, Nanoplasmonics and Metamaterials

- E1 (13) T. I. Weng and **G. Y. Guo**
Band structure of honeycomb photonic crystal slabs, *J. Appl. Phys.* **99**, 93102 (2006).

- E2 (7) 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 (12) 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 (13) V. Klimov and **G. Y. Guo**
Bright and dark plasmon modes in three nanocylinder cluster
J. Phys. Chem. C **114**, 22398 (2010).
- E5 (80) 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 (41) 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 (21) V. Klimov*, S. L. Sun, **G. Y. Guo***,
Coherent perfect nanoabsorbers based on negative refraction, *Optics Express* **20**, 13071 (2012)
- E8 (913) 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 (7) **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 (44) 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 (17) 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 (20) 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 (4) 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 (18) 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 (6) 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 (4) V. V. Klimov, D. V. Guzатов, 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 (50) 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 (1) 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 (9) 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 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).

F. Transition Metal Oxides

Charge, orbital and spin orderings

F1 (84) 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 $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$ studied by soft x-ray linear dichroism

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

F2 (43) 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 ($\text{M} = \text{Fe}, \text{Co}$), J. Magn. Mater. **282**, 287 (2004).

F4 (233) H.-T. Jeng*, **G.Y. Guo***, D. J. Huang

Charge-orbital ordering and Verwey transition in magnetite, **Phys. Rev. Lett.** **93**, 156403 (2004).

F5 (88) 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 (74) 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 (48) 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 (102) H.T. Jeng and **G.Y. Guo**, First-principles investigations of the electronic structures and the magnetocrystalline anisotropy in strained magnetite Fe₃O₄, 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 CrO₂, 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 CrO₂,
J. Appl. Phys. **92**, 1419 (2002).
- F12 (23) H.T. Jeng and **G.Y. Guo**
First-principles investigations of the magnetocrystalline anisotropy in strained Co-substituted magnetite (CoFe₂O₄), J. Magn. Magn. Mater **240**, 88 (2002).
- F13 (20) H.T. Jeng and **G.Y. Guo**
First-principles investigations of the magnetocrystalline anisotropy in strained Ni-substituted magnetite (NiFe₂O₄), J. Magn. Magn. Mater. **240**, 436 (2002).
- F14 (31) 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 CrO₂, Phys. Rev. B **66**, 174440 (2002).
- F15 (27) 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)FeMoO₆ (0 ≤ x ≤ 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 Sr₂FeMO₆ (M= Mo, W),
Int. J. Mod. Phys. B **17**, 3500 (2003).
- F17 (175) H.T. Jeng and **G.Y. Guo**
First-principles investigations of orbital magnetic moments and electronic structures of the double perovskites Sr₂FeMoO₆, Sr₂FeReO₆ and Sr₂CrWO₆, Phys. Rev. B. **67**, 94438 (2003).
- F18 (21) 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 CrO₂, Phys. Rev. B **67**, 214419 (2003).
- F19 (4) Y. K. Wang, **G.Y. Guo** and H.-T. Jeng,
An *ab initio* studies of the magnetocrystalline anisotropy and magnetoelastic coupling of half-metallic CrO₂, J. Magn. Magn. Mater. **282**, 139 (2004).
- F20 (22) 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 Sr₂CrMO₆ (M = Mo, W): B' 4d-5d 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 CrO₂ and Fe₃O₄ studied by MCD in soft x-ray

absorption, J. Electr. Spec. Rel. Pheno. **137-40**, 633 (2004).

- F22 (17) 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 LaSrMnO₄ studied by soft x-ray linear dichroism, J. Electr. Spec. Rel. Pheno. **137**, 641 (2004).
- F23 (149) 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 Fe₃O₄, **Phys. Rev. Lett.** **93**, 077204 (2004).
- F24 (18) 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 CrO₂ studied by magnetic circular dichroism in resonant photoemission, Phys. Rev. B **71**, 52407 (2005).
- F25 (34) 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 Sr₂FeMoO₆ (M=Mo,W): B' 4d-5d system, Solid State Commun. **133**, 265 (2005).
- F26 (58) Y. K. Wang and **G. Y. Guo**
Robust half-metallic antiferromagnets LaAVOsO₆ and LaAMoYO₆ (A=Ca,Sr,Ba; Y=Re,Tc) from first-principles calculations, Phys. Rev. B **73**, 064424 (2006).
- F27 (11) 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 (30) Y. K. Wang, P. H. Lee and **G. Y. Guo**,
Half-metallic antiferromagnetic nature of La₂VTcO₆ and La₂VCuO₆ from ab initio calculations, Physical Review B **80**, 224418 (2009).
- Ferroelectric, Magnetic and Multiferroic Oxides**
- F29 (18) C. H. Lin, C.M. Huang, and **G. Y. Guo**
Systematic *ab initio* study of the phase diagram of epitaxially strained SrTiO₃
J. Appl. Phys. **100**, 084104 (2006)
- F30 (50) 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/BiFeO₃/La_{2/3}Sr_{1/3}MnO₃ junctions, J. Appl. Phys. **104**, 053904 (2008)
- F32 (21) S. Ju and **G. Y. Guo**
Colossal nonlinear optical magnetoelectric effects in multiferroic Bi₂FeCrO₆
Appl. Phys. Lett. **92**, 202504 (2008).
- F33 (12) S. Ju and **G.Y. Guo**
First-principles study of crystal, electronic structure and second-harmonic generation in a polar double perovskite Bi₂ZnTiO₆, J. Chem. Phys. **129**, 194704 (2008).
- F34 (11) 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 LiCu₂O₂
Phys. Rev. B **78**, 214105 (2008)

F35 (45) S. Ju*, T.Y. Cai, and **G.Y. Guo***

Electronic structure, linear, and nonlinear optical responses in magnetoelectric multiferroic material BiFeO₃, *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 (32) 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 (15) T.-Y. Cai, S.-C. Liu, S. Ju*, C.-Y. Liu and **G. Y. Guo***, Double perovskite ScFe_{1-x}CrO₃ (0.17 < x < 0.83): Multiferroic semiconductors for highly efficient ferroelectric photovoltaics and spintronics, *Phys. Rev. Applied* **8**, 034034 (2017).

F39 (6) 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 (11) 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)

Phosphors and light-emitting materials

F42 (313) C. C. Lin, Z. R. Xiao, **G.-Y. Guo**, T.-S. Chan, R.-S. Liu,

Versatile phosphate phosphors ABPO₄ in white light-emitting diodes: Collocated characteristic analysis and theoretical calculations, **J. Am. Chem. Soc.** **132**, 3020 (2010)

Low-dimensional magnetic oxides

F43 (5) G. N. Rao, V. N. Singh, R. Sankar, I. P. Muthuselvam, **G. Y. Guo*** and F. C. Chou*
Antiferromagnetism of Ni₂NbBO₆ with S = 1 dimer quasi-one-dimensional armchair chains
Phys. Rev. **91**, 014423 (2015)

F44 (10) I. P. Muthuselvam, R. Sankar, V. N. Singh, G. N. Rao, **G.-Y. Guo***, and F. C. Chou*
Magnetic orderings of Li₂Cu(WO₄)₂ with tungstate-bridged quasi-1D spin-1/2 chains
Inorg. Chem. **54**, 4303 (2015)

F45 (10) 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 Li₂Ni(WO₄)₂,
Phys. Rev. B **92**, 014413 (2015).

F46 (12) 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 Ba₂CuTeO₆,
Phys. Rev. B **93**, 104401 (2016).

F47 (16) 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 Na₂Ni₂TeO₆

with a Ni honeycomb lattice, Phys. Rev. B **95**, 104408 (2017)

F48 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

F49 (50) 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 LaAlO₃ and SrTiO₃, **Nature Commun.** **7**, 12773 (2016).

F50 (5) 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 SrTiO₃/LaAlO₃/SrTiO₃, Phys. Rev. Mater. **3**, 075003 (2019).

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

G1 (25) **G.Y. Guo**, W.M. Temmerman and G.M. Stocks

On the Metal-Semiconductor Transition and Antiferromagnetism in La₂CuO₄
J. Phys. C: Solid State Phys. **21**, L103 (1988).

G2 (24) **G.Y. Guo** and W.M. Temmerman

Electronic Structures and Magnetism in La₂NiO₄, 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 T_c Superconductors
Physica C **153-155**, 1215 (1988).

G4 (29) W.M. Temmerman, Z. Szotek and **G.Y. Guo**

A Local Spin-Density Study of Antiferromagnetism in La₂CuO₄ and YBa₂Cu₃O₆
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 T_c Superconductors
Phys. Scripta T **25**, 78 (1989).

G6 (18) **G.Y. Guo** and W.M. Temmerman

Electronic and Magnetic Properties of La₂NiO₄: 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 T_c Superconductors
in *Proc. of the International Symposium on the Electronic Structure of High T_c Superconductors* (Pergamon, Oxford, 1989).

G8 (10) **G.Y. Guo**, Z. Szotek and W.M. Temmerman,

Effects of Doping and Structure on the Electronic Properties of Nd₂CuO₄
Physica C **162-164** (1989) 1351.

G9 (30) W.M. Temmerman, P.A. Sterne, **G.Y. Guo** and Z. Szotek,

Electronic Structure Calculations of High T_c Materials, Molecular Simulation **4**, 153 (1989).

G10 (182) **G.Y. Guo** and W.M. Temmerman

Suppression of Superconductivity in PrBa₂Cu₃O₇: 4*f* and Conduction-band Hybridization Effect,

Phys. Rev. B **41**, 6372 (1990).

G11 (16) 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 (3) S. Sen and **G.-Y. Guo***, Pressure induced Lifshitz transition in ThFeAsN ,
Phys. Rev. Mater. **4**, 104802 (2020).

G14 (2) S. Sen and **G.-Y. Guo***, Electronic structure, lattice dynamics, and magnetic properties
of ThXAsN ($X = \text{Fe, Co, Ni}$) superconductors, Phys. Rev. B **102**, 224505 (2020).

H. Magnetic Transition metals, Thin Films, Superlattices, Surfaces and Interfaces

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 (10) **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 (28) **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 (55) **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 (4) 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 (124) **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 (6) H.H. Wang and **G.Y. Guo**
Gradient-corrected density functional calculation of structural and magnetic properties of bcc,
fcc and hcp Cr, J. Magn. Magn. Mater. **209**, 98 (2000).

H8 (1) **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 (31) 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 (4) 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 magnetostrictions

- H12 (69) **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 (46) **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 (23) **G. Y. Guo**, W. M. Temmerman and H. Ebert
An *ab initio* Study of Magnetic Anisotropy of $\text{Fe}_n/\text{Cu}(\text{Ag})_m$ 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, Dordrecht, 1994).
- H16 (7) 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 (102) 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 (21) **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 (16) **G. Y. Guo**
Magnetocrystalline Anisotropy Oscillations Predicted in Fe/Au (001) Superlattices,
J. Phys.: Condens. Matter **11**, 4329 (1999).
- H20 (18) **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 Anisotropy and Magnetism in L10 FeCu Alloy
J. Magn. Magn. Mater. **209**, 214 (2000).
- H23 (25) 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 **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 (14) 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 L1₀ FePdPt films,
Appl. Phys. Lett. **104**, 192402 (2014).

H26 (8) 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 (34) **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 (5) **G. Y. Guo** and H. Ebert

First-principles Study of the Magnetic Hyperfine Field in Fe Multilayers
Hyperfine Interactions **97/98**, 11 (1996).

Magneto-optical Kerr effect

H30 (50) **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 (107) **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 (23) **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 (58) W.-X. Feng, **G. Y. Guo***, J. Zhou, Y. Yao and Q. Niu

Large Magneto-Optical Kerr Effect in Noncollinear Antiferromagnets Mn₃X (X =Rh, Ir, Pt)
Phys. Rev. B **92**, 144426 (2015)

X-ray magnetic dichroism

H36 (116) **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 (2) 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 (59) 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 (13) 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 (4) 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 (8) P.-C. Wei, T.-S. Huang, S. W. Lin, **G. Y. Guo**, Y. Y. Chen,
Thermoelectric properties optimization of Fe₂VGa 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 (20) S. P. Collins, D. Laundry and **G. Y. Guo**
Spin and Orbital Magnetic x-ray Diffraction in HoFe₂, J. Phys.: Condens. Matter **5**, L637 (1993)

Interpretation of x-ray magnetic dichroism

- I2 (32) **G.Y. Guo**
Interpretation of x-ray circular dichroism: multiple-scattering theory approach
Phys. Rev. B **57**, 10295 (1998).
- I3 (45) **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 (42) **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 (15) 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 (47) 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 (88) 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, Dordrecht, 1994).

I10 (14) 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 Rare Earth Compounds

J1 (5) **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 (9) 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 (6) 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 (145) **G.Y. Guo**, G.A. Botton and Y. Nishino

Electronic Structure of Possible 3d 'Heavy-fermion' Compounds Fe_2VAI ,

J. Phys.: Condens. Matter **10**, L119-L126 (1998).

J7 (6) 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 antiferromagnetic semimetal,

K. High Performance Alloys, Intermetallics Compounds and Superconductors

- K1 (44) B. Ginatempo, **G.Y. Guo**, W.M. Temmerman, J.B. Staunton and P.J. Durham,
Electronic Structure of Ordered and Disordered Alloys: Cu₃Pd, Cu₃Pt, Cu₃Au
Phys. Rev. B **42**, 2761 (1990).
- K3 (7) 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 (3) 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 (25) 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 (88) 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 (4) 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 (7) 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 (2) R.G. Jordan and **G.Y. Guo**
Surface States on the (001) Surface of CuAu I, Phys. Rev. B **55**, 7222 (1997).
- K13 (30) 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 Cu₃Au
Solid State Commun. **105** (1998) 125.
- K15 (10) L.-S. Hsu, **G.Y. Guo**, J.D. Denlinger and J.W. Allen
Experimental and theoretical study of the electronic structure of PtGa₂,

Phys. Rev. B **63**, 155105 (2001).

K16 (20) L.-S. Hsu, **G.Y. Guo**, J.D. Denlinger and J.W. Allen

Experimental and theoretical study of the electronic structure of AuAl₂
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_xB₂C superconductors,
MRS Proceedings **731**, 301 (2002).

K18 (29) **G.Y. Guo**, Y.K. Wang and L.-S. Hsu

First-principles and experimental studies of the electronic structure and magnetism in Ni₃Al,
Ni₃Ga and Ni₃In, J. Magn. Magn. Mater. **239**, 91 (2002).

K19 (2) L.-S. Hsu, **G.Y. Guo**, J.D. Denlinger and J. W. Allen,

Experimental and theoretical studies of the electronic structures of AuAl₂ and PtGa₂,
Surface Review and Letters **9**, 251 (2002).

K20 (21) L.-S. Hsu, Y.K. Wang, **G.Y. Guo**, and C.S. Lue

Experimental and theoretical study of the electronic structures of Fe₃Al, Fe₂VAl, Fe₂VGa,
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 Ni₃Al, Ni₃Ga, Ni₃In and NiGa,
J. Appl. Phys. **92**, 1419 (2002).

K22 (10) **G. Y. Guo**, Y. K. Wang and L.-S. Hsu,

Ab initio studies of structural stability and magnetism in Ni₃In, Phys. Rev. B **66**, 54440 (2002).

K19 (7) L.-S. Hsu, Y.K. Wang and **G.Y. Guo**,

Experimental and theoretical study of the electronic structure of Fe₃Al,
Nuclear Instruments and Methods B **199**, 200 (2003).

K23 (5) 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, Magnetic Semiconductors and Semiconductor Surfaces

L1 (25) **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 **G.Y. Guo**, J. Crain and W.M. Temmerman,

On the New High Pressure Phase of InSb, Japanese J. Appl. Phys. **32**, Suppl. 32-1, 39 (1993)

L4 (32) 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 (13) **G.Y. Guo**, Surface electronic structure and magnetic properties of semiconductor FeSi,
Physica E **10**, 383 (2001).

- L6 (116) 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. Mater. **282**, 275 (2004).
- L7 (7) 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 (8) D. J. Cai, J. Y. Kang and **G. Y. Guo***, Microscopic origin of light emission from
AlyGa $1-y$ /GaN superlattices: Band profile and active site, Phys. Rev. B **80**, 045311 (2009).
- L9 (29) 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 (14) 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 (1) D. J. Cai, and **G. Y. Guo**
Spatial localization of quantized states responsible for sharp optical transition in AlGa N /Ga N
superlattice, J. Appl. Phys. **107**, 103533 (2010).
- L12 (30) 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 principles
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 principles calculations and experimental study on the
spin-polarized band structure of Co-doped PbPdO $_2$, Appl. Phys. Lett. **101**, 222104 (2012).
- L14 (29) 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 $_2$ FeAl/(Ga,Mn)As bilayer,
Phys. Rev. Lett. **111**, 027203 (2013).
- L15 (23) 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 (4) 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 AlGa N quantum wells induced by polarized
orbitals, ACS Photonics **4**, 2197 (2017).
- L17 (9) 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 $_x$ Se phototransistor,
ACS Appl. Mater. Interfaces **11**, 24269 (2019).
- L18 (4) W.-K. Li and **G.-Y. Guo***, A First Principle Study on Magneto-Optical Effects in
Ferromagnetic Semiconductors Y $_3$ Fe $_5$ O $_{12}$ and Bi $_3$ Fe $_5$ O $_{12}$, Phys. Rev. B **103**, 014439 (2021).
- L19 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 (41) 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 (10) 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 (54) 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 (23) 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 (2) 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).