

Curriculum Vitae

NAME: CAO, CHAO

DATE OF BIRTH: 1981/07/12

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CURRENT ADDRESS (BUSINESS):

Department of Physics, Center for Correlated Matter

Zhejiang University

Hangzhou, Zhejiang 310058

P. R. China

TOTAL CITATION: >2300 (WEB OF SCIENCE)

H-INDEX: 27 (WEB OF SCIENCE)

<https://scholar.google.com/citations?user=TVlt1jcAAAAJ&hl=en>

EMPLOYMENT

Professor

Dec. 2021 - today

Department of Physics and Center for Correlated Matter, Zhejiang University

Professor

Mar. 2010 - Dec. 2021

Department of Physics, Hangzhou Normal University

Post Doctoral Researcher

Jan. 2009 - Feb. 2010

Department of Physics, University of Florida

Supervisor: Hai-Ping Cheng (cheng@qtp.ufl.edu)

EDUCATION

University of Florida, Department of Physics

Gainesville, FL 32611, U. S. A.

Aug. 2003 - Dec. 2008, Ph. D.

Supervisor: Hai-Ping Cheng (cheng@qtp.ufl.edu)

Fudan University, Department of Physics

Shanghai, Shanghai 200433, P. R. China

Sep. 1999 - Jun. 2003, Bachelor

RESEARCH INTERESTS

First-principles modelling of i) strongly correlated systems and unconventional superconductors, ii) frustrated magnetic systems and iii) nano-scale transport devices.

HONORS AND AWARDS

2013 Zhejiang Provincial Talents Program

2009 APS Nicholas Metropolis Award for Outstanding Doctoral Thesis Work in Computational Physics

2008 Chinese Government Award for Outstanding Self-Financed Students Abroad

PUBLICATIONS

Top 10 cited Publications

1. **Chao Cao***, P. J. Hirschfeld and Hai-Ping Cheng, Proximity of antiferromagnetism and superconductivity in $\text{LaFeAsO}_{1-x}\text{F}_x$: Effective Hamiltonian from ab initio studies, *Physical Review B* **77**, 220506 (2008) (Google Citation > 300)
2. **Chao Cao***, Min Wu, J. Z. Jiang and Hai-Ping Cheng, Transition metal adatom and dimer adsorbed on graphene: Induced magnetization and electronic structures, *Physical Review B* **81** 205424 (2010) (Google Citation > 280)
3. Min Wu, **Chao Cao** and J.-Z. Jiang*, Light non-metallic atom (B, N, O and F)-doped graphene: a first-principles study, *Nanotechnology* **21**, 505202 (2010) (Google Citation > 210)
4. Min Wu, **Chao Cao** and J.-Z. Jiang*, Electronic structure of substitutionally Mn-doped graphene, *New Journal of Physics* **12**, 063020 (2010) (Google Citation >100)
5. **Chao Cao*** and Jianhui Dai, Block Spin Ground State and Three-Dimensionality of $(\text{K, Tl})_y\text{Fe}_{1.6}\text{Se}_2$, *Physical Review Letters* **107**, 056401 (2011) (Google Citation >90)
6. A. F. Kemper, **Chao Cao**, P. J. Hirschfeld*, and Hai-Ping Cheng, Effects of cobalt doping and three-dimensionality in BaFe_2As_2 , *Physical Review B* **80**, 104511 (2009) (Google Citation >80)
7. H. Jiang, G.-H. Cao and **Chao Cao***, Electronic structure of quasi-one-dimensional superconductor $\text{K}_2\text{Cr}_3\text{As}_3$ from first-principles calculations, *Scientific Reports* **5**, 16054 (2015) (Google Citation >70)
8. Y.-K. Li, Lin Li, J.-L. Wang, T.-T. Wang, X.-F. Xu, C.-Y. Xi, Chao Cao and J.-H. Dai, Resistivity plateau and negative magnetoresistance in the topological semimetal TaSb_2 , *Physical Review B* **94**, 121115 (2016) (Google Citation >70)
9. **Chao Cao*** and Jianhui Dai, Electronic Structure of KFe_2Se_2 from First-Principles Calculations, *Chinese Physics Letters* **28**, 057402 (2011) (Google Citation >60)
10. Yan Wang, **Chao Cao** and Hai-Ping Cheng*, Metal-terminated graphene nanoribbons, *Physical Review B* **82**, 205429 (2010) (Google Citation >60)

Full Publication List (Reverse Time Ordered)

1. **Chao Cao**[†] and Jian-Xin Zhu[†], Pressure dependent electronic structure in CeRh_6Ge_4 , *under review*
2. Chenchao Xu, **Chao Cao**[†] and Jian-Xin Zhu[†], Pressure-induced concomitant topological and metal-insulator quantum phase transition in $\text{Ce}_3\text{Pd}_3\text{Bi}_4$, *accepted by npj Quantum Materials*
3. Guo-Xiang Zhi, Chenchao Xu, Si-Qi Wu, Fanlong Ning and **Chao Cao**[†], WannSymm: A symmetry analysis code for Wannier orbitals, *Computer Physics Communications* **271**, 108196 (2022)
4. Zhongzheng Wu, Yuan Fang, *et al.*, Revealing the Heavy Quasiparticles in the Heavy-Fermion Superconductor CeCu_2Si_2 , *Physical Review Letters* **127**, 067002 (2021)
5. Yi Wu, Yongjun Zhang, *et al.*, Anisotropic c - f Hybridization in the Ferromagnetic Quantum Critical Metal CeRh_6Ge_4 , *Physical Review Letters* **126**, 216406 (2021)
6. Yi Wu, Wenhao Zhang, *et al.*, Interfacial electron-phonon coupling and quantum confinement in ultrathin Yb films on graphite, *Physical Review B* **104** L161402 (2021)
7. Q. Zhu, Q. Wang, L. Li, Z. Yang, J. Yang, B. Chen, **Chao Cao**[†], Hangdong Wang[†] and J. Du, Shubnikov-de Haas oscillations and electronic structure in the Dirac semimetal SrAgAs , *Physical Review B* **104**, 144305 (2021)
8. Z. Liu, Chenchao Xu, **Chao Cao**[†], W. Zhu, Z. F. Wang and Jinlong Yang[†], Doping dependence of electronic structure of infinite-layer NdNiO_2 , *Physical Review B* **103**, 045103 (2021)
9. A. Wang, Z. Y. Nie, *et al.*, Nodeless superconductivity in $\text{Lu}_{5-x}\text{Rh}_6\text{Sn}_{18+x}$ with broken time reversal symmetry, *Physical Review B* **103**, 024503 (2021)
10. Yi Wu, Yuan Fang, *et al.*, Bandwidth-control orbital-selective delocalization of $4f$ electrons in epitaxial Ce films, *Nature Communications* **12**, 2520 (2021)

11. Bing-Hua Lei, Shilie Pan, Zhihua Yang*, **Chao Cao**[†], and David J. Singh^{††}, Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions, *Physical Review Letters* **125**, 187402 (2020)
12. H. Yang, W. You, J. Wang, J. Huang, C. Xi, X. Xu, **Chao Cao**[†], *et al.*, Giant anomalous Nernst effect in the magnetic Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$, *Physical Review Materials* **4**, 024202 (2020)
13. **Chao Cao**^{*}, G.-X. Zhi and Jian-Xin Zhu[†], From Trivial Kondo Insulator $\text{Ce}_3\text{Pt}_3\text{Bi}_4$ to Nodal-line Semimetal $\text{Ce}_3\text{Pd}_3\text{Bi}_4$, *Physical Review Letters* **124**, 166403 (2020)
14. Peiran Zhang, Huiqiu Yuan*, and **Chao Cao**[†], Coexistence of nontrivial band topology and superconductivity in noncentrosymmetric compound LaNiSi , LaPtSi , and LaPtGe , *Physical Review B* **101**, 245145 (2020)
15. Chenchao Xu, Ninghua Wu, Guo-Xiang Zhi, Bing-Hua Lei, Xu Duan, Fanlong Ning, **Chao Cao**^{*}, Qijin Chen, Coexistence of nontrivial topological properties and strong ferromagnetic fluctuations in $A_2\text{Cr}_3\text{As}_3$ ($A=\text{Na, K, Rb}$ and Cs), *npj Computational Materials* **6**, 30 (2020)
16. Si-Qi Wu, **Chao Cao**^{*}, and Guang-Han Cao, Lifshitz transition and nontrivial H-doping effect in the Cr-based superconductor $\text{KCr}_3\text{As}_3\text{H}_x$, *Physical Review B* **100**, 155108 (2019)
17. Peng Li, Zhongzheng Wu, Fan Wu, Chunyu Guo, Yi Liu, Haijiang Liu, Zhe Sun, Ming Shi, Fanny Rodolakis, Jessica L. McChesney, **Chao Cao**, Huiqiu Yuan, Frank Steglich, and Yang Liu, Large Fermi surface expansion through anisotropic mixing of conduction and f electrons in the semimetallic Kondo lattice CeBi , *Physical Review B* **100**, 155110 (2019)
18. C. Xu, Q. Chen, and **Chao Cao**^{*}, Electronic structure of Ni-doped $\text{EuRbFe}_4\text{As}_4$: Unique crystal field splitting and multiband RKKY interactions, *Communications Physics* **2**, 16 (2019)
19. Y. Shao, Z. Sun, Y. Wang, C. Xu, R. Sankar, A. J. Breindel, **Chao Cao**, *et al.*, Optical signatures of Dirac nodal lines in NbAs_2 , *Proceedings of National Academy of Sciences* **4**, 1168 (2018)
20. C. Guo, F. Wu, Z. Z. Wu, M. Smidman, **Chao Cao**, *et al.*, Weyl fermions in a canonical heavy-fermion semimetal YbPtBi , *Nature Communications* **9**, 4622 (2018)
21. X. Duan, F. Wu, J. Chen, P. Zhang, Y. Liu, H. Yuan, and **Chao Cao**^{*}, Tunable electronic structure and topological properties of LnPn ($\text{Ln}=\text{Ce, Pr, Gd, Sm, Yb}$; $\text{Pn}=\text{Sb, Bi}$), *Communications Physics* **1**, 71 (2018)
22. P. Li, Z. Z. Wu, F. Wu, **Chao Cao**, *et al.*, Tunable electronic structure and surface states in rare-earth monobismuthides with partially filled f -shell, *Physical review B* **98**, 085103 (2018)
23. B.-H. Lei, Z.-H. Yang, H.-W. Yu, **Chao Cao**, *et al.*, Module-Guided Design Scheme for Deep-Ultraviolet Nonlinear Optical Materials, *Journal of the American Chemical Society* **140**, 10726 (2018)
24. Y. P. Li, C. C. Xu, M. S. Shen, J. H. Wang, X. H. Yang, X. J. Yang, Z. W. Zhu, **Chao Cao**^{*}, and Zhu-An Xu*, Quantum transport in a compensated semimetal W_2As_3 with nontrivial Z(2) indices, *Physical Review B* **98**, 115145 (2018)
25. J. Chen, Y.-K. Li, J.-H. Dai, and **Chao Cao**^{*}, Electronic structure and topological properties of centrosymmetric $\text{MoAs}_2/\text{WAs}_2$ from first principles, *Scientific Reports* **7**, 10491 (2017)
26. Chunyu Guo, **Chao Cao**, Michael Smidman, Fan Wu, Yongjun Zhang, Frank Steglich, Fu-Chun Zhang and Huiqiu Yuan*, Possible Weyl fermions in the magnetic Kondo system CeSb , *npj Quantum Materials* **2**, 39 (2017)
27. Yi Zhou*, **Chao Cao**, and Fuchun Zhang, Theory for superconductivity in alkali chromium arsenides $A_2\text{Cr}_3\text{As}_3$ ($A = \text{K, Rb, Cs}$), *Science Bulletin* **62**, 208 (2017)
28. C. Xu, J. Chen, G.-X. Zhi, Y.-K. Li, J.-H. Dai*, and **Chao Cao**^{*}, Electronic structures of transition metal dipnictides XPn_2 ($X = \text{Ta, Nb}$; $\text{Pn} = \text{P, As, Sb}$), *Physical Review B* **93**, 195106 (2016)
29. Y.-K. Li, Lin Li, J.-L. Wang, T.-T. Wang, X.-F. Xu, C.-Y. Xi, Chao Cao and J.-H. Dai, Resistivity plateau and negative magnetoresistance in the topological semimetal TaSb_2 , *Physical Review B* **94**, 121115 (2016)

30. H.-M. Chen, J.-H. Yang, **Chao Cao**, L. Li *et al.*, Superconductivity in a new layered nickel selenide CsNi_2Se_2 , *Superconductor Science and Technology* **29**, 045008 (2016)
31. C.-Y. Shen, B.-Q. Si, **Chao Cao**, X.-J. Yang *et al.*, Two superconducting domes separated by a possible Lifshitz transition in $\text{LaFeAs}_{1-x}\text{P}_x\text{O}$, *Journal of Applied Physics* **119**, 083903 (2016)
32. H. Jiang, G.-H. Cao and **Chao Cao***, Electronic structure of quasi-one-dimensional superconductor $\text{K}_2\text{Cr}_3\text{As}_3$ from first-principles calculations, *Scientific Reports* **5**, 16054 (2015)
33. **Chao Cao***, Hao Jiang, Xiao-Yong Feng and Jianhui Dai, Reduced dimensionality and magnetic frustration in KCr_3As_3 , *Physical Review B* **92**, 235107 (2015)
34. Peayush Choubey, T. Berlijn, A. Kreisel, **Chao Cao**, and P. J. Hirschfeld*, Visualization of atomic-scale phenomena in superconductors: Application to FeSe, *Physical Review B* **90**, 134520 (2014)
35. P.-R. Huang, Y. He*, **Chao Cao**, and Z.-H. Lu, Impact of lattice distortion and electron doping on $\alpha\text{-MoO}_3$ electronic structure, *Scientific Report* **4**, 07131 (2014)
36. J.-Z. Ma, A. van Roekeghem, P. Richard, Z.-H. Liu, H. Miao, L.-K. Zeng, N. Xu, M. Shi, **Chao Cao**, J.-B. He, G.-F. Chen, Y.-L. Sun, G.-H. Cao, S.-C. Wang, S. Biermann, T. Qian, and H. Ding, Correlation-Induced Self-Doping in the Iron-Pnictide Superconductor $\text{Ba}_2\text{Ti}_2\text{Fe}_2\text{As}_4\text{O}$, *Physical Review Letters* **113**, 266407 (2014)
37. N. Zhou, Xiaofeng Xu*, J. R. Wang, J. H. Yang, Y. K. Li, Y. Guo, W. Z. Yang, C.-Q. Niu, B. Chen, **Chao Cao** and Jianhui Dai, Controllable spin-orbit coupling and its influence on the upper critical field in the chemically doped quasi-one-dimensional Nb_2PdS_5 superconductor, *Physical Review B* **90**, 094520 (2014)
38. Xiaofeng Xu*, W. H. Jiao, N. Zhou, Y. K. Li, B. Chen, **Chao Cao**, Jianhui Dai, A. F. Bangura and Guanghan Cao, Electronic nematicity revealed by torque magnetometry in $\text{EuFe}_2(\text{As}_{1-x}\text{P}_x)_2$, *Physical Review B* **89**, 104517 (2014)
39. Yuke Li*, Xi Lin, Lin Li, N. Zhou, X.-F. Xu, **Chao Cao**, Jianhui Dai, L. Zhang, Y.-K. Luo, Wenhe Jiao, Q. Tao, Guanghan Cao, and Zhu-an Xu, Electronic phase diagram in a new BiS_2 -based $\text{Sr}_{1-x}\text{La}_x\text{FBiS}_2$ system, *Superconductor Science and Technology* **27**, 035009 (2014)
40. C. Q. Niu, J. H. Yang, Y. K. Li, B. Chen, N. Zhou, J. Chen, L. L. Jiang, B. Chen, X.-X. Yang, **C. Cao**, Jianhui Dai and X.-F. Xu*, Effect of selenium doping on the superconductivity of $\text{Nb}_2\text{Pd}(\text{S}_{1-x}\text{Se}_x)_5$, *Physical Review B* **88**, 104507 (2013)
41. Xiaofeng Xu*, Bin Chen, W. H. Jiao, B. Chen, C.-Q. Niu, Y.-K. Li, J.-H. Yang, A.-F. Bangura, Q.-L. Ye, **C. Cao**, J.-H. Dai, Guanghan Cao and N. E. Hussey, Evidence for two energy gaps and Fermi liquid behavior in the SrPt_2As_2 superconductor, *Physical Review B* **87**, 224507 (2013)
42. Xiaojun Yang, Y.-K. Li, P. Zhang, H. Jiang, Y.-K. Luo, Q. Chen, C. M. Feng, **C. Cao**, Jianhui Dai, Q. Tao, Guanghan Cao and Zhu-An Xu*, K and Mn co-doped BaCd_2As_2 : A hexagonal structured bulk diluted magnetic semiconductor with large magnetoresistance, *Journal of Applied Physics* **114**, 223905 (2013)
43. P.-R. Huang, Yao He*, **Chao Cao**, and Z.-H. Lu, The origin of the high work function of chlorinated indium tin oxide, *Npg Asia Materials* **5**, e57 (2013)
44. Rashid Hamdan, A. F. Kemper, **Chao Cao** and Hai-Ping Cheng*, Structure and functionality of bromine doped graphite, *Journal of Chemical Physics* **138**, 164702 (2013)
45. **Chao Cao*** and Fuchun Zhang, Electronic structure of vacancy-ordered iron-selenide $\text{K}_{0.5}\text{Fe}_{1.75}\text{Se}_2$, *Physical Review B* **87**, 161105 (2013)
46. Yongkang Luo, **Chao Cao**, Bingqi Si, Yuke Li, Jinke Bao, Hanjie Guo, Xiaojun Yang, Chenyi Shen, Chunmu Feng, Jianhui Dai, Guanghan Cao and Zhu-an Xu*, Li_2RhO_3 : A spin-glassy relativistic Mott insulator, *Physical Review B* **87**, 161121 (2013)
47. Hui-Fei Zhai, Wen-He Jiao, Yun-Lei Sun, Jin-Ke Bao, Hao Jiang, X.-J. Yang, Z.-T. Tang, Q. Tao, X.-F. Xu, Y.-K. Li, **Chao Cao**, Jianhui Dai, Zhu-An Xu and Guang-Han Cao*, Superconductivity, charge- or spin-density wave, and metal-nonmetal transition in $\text{BaTi}_2(\text{Sb}_{1-x}\text{Bi}_x)_2\text{O}$, *Physical Review B* **87**, 100502(R) (2013)

48. Hui Chen, Xiaofeng Xu, **Chao Cao**^{*}, and Jianhui Dai, First-principles calculations of the electronic and phonon properties of APt_3P ($A=\text{Ca}$, Sr , and La): Evidence for a charge-density-wave instability and a soft phonon, *Physical Review B* **86**, 125116 (2012)
49. Y.-K. Li^{*}, X.-F. Xu, **C. Cao**, C.-Y. Shen, Y.-K. Luo, Q. Tao, X. Lin, L. Zhang, G.-H. Cao and Z.-A. Xu, Magnetic phase diagram in the Co-rich side of the $\text{LCo}_{1-x}\text{Fe}_x\text{AsO}$ ($L=\text{La}$, Sm) system, *Physical Review B* **86**, 104408 (2012)
50. **Chao Cao**^{*} and Jianhui Dai, Block Spin Ground State and Three-Dimensionality of $(\text{K}, \text{Tl})_y\text{Fe}_{1.6}\text{Se}_2$, *Physical Review Letters* **107**, 056401 (2011)
51. **Chao Cao**^{*} and Jianhui Dai, Electronic Structure of KFe_2Se_2 from First-Principles Calculations, *Chinese Physics Letters* **28**, 057402 (2011)
52. **Chao Cao**^{*}, Yan Wang, Hai-Ping Cheng and J.-Z. Jiang, Perfect spin-filtering and giant magnetoresistance with Fe-terminated graphene nanoribbon, *Applied Physics Letters* **99**, 073110 (2011)
53. **Chao Cao**^{*}, Yun-wen Chen, Yu-ning Wu, E. Deumens and Hai-Ping Cheng, OPAL: A Multiscale Multicenter Simulation Package Based on MPI-2 Protocol, *International Journal of Quantum Chemistry* **111**, 4020 (2011)
54. **Chao Cao**^{*} and Jianhui Dai, Electronic structure and Mott localization of iron-deficient $\text{TlFe}_{1.5}\text{Se}_2$ with superstructures, *Physical Review B* **83**, 193104 (2011)
55. Hua Chen, **Chao Cao** and Jianhui Dai^{*}, Block spin magnetism and metal-insulator transition in a two-dimensional Hubbard model with perfect vacancy superstructure, *Physical Review B* **83**, 180413 (2011)
56. **Chao Cao**^{*}, Min Wu, J. Z. Jiang and Hai-Ping Cheng, Transition metal adatom and dimer adsorbed on graphene: Induced magnetization and electronic structures, *Physical Review B* **81** 205424 (2010)
57. Min Wu, **Chao Cao** and J.-Z. Jiang^{*}, Light non-metallic atom (B, N, O and F)-doped graphene: a first-principles study, *Nanotechnology* **21**, 505202 (2010)
58. Yan Wang, **Chao Cao** and Hai-Ping Cheng^{*}, Metal-terminated graphene nanoribbons, *Physical Review B* **82**, 205429 (2010)
59. **Chao Cao**, Yuning Wu, R. Hamdan, Yun-Peng Wang and Hai-Ping Cheng^{*}, Accurate projected augmented wave datasets for BaFe_2As_2 , *New Journal of Physics* **12**, 123029 (2010)
60. Min Wu, **Chao Cao** and J.-Z. Jiang^{*}, Electronic structure of substitutionally Mn-doped graphene, *New Journal of Physics* **12**, 063020 (2010)
61. J. L. Palma, **Chao Cao**, X.-G. Zhang, P. S. Krstic, J. L. Krause and Hai-Ping Cheng^{*}, Manipulating I-V Characteristics of a Molecular Switch with Chemical Modifications, *Journal of Physical Chemistry C* **114**, 1655-1662 (2010)
62. A. F. Kemper, **Chao Cao**, P. J. Hirschfeld^{*}, and Hai-Ping Cheng, Effects of cobalt doping and three-dimensionality in BaFe_2As_2 , *Physical Review B* **80**, 104511 (2009)
63. S. Alkis, **Chao Cao**, Hai-Ping Cheng, and J. L. Krause^{*}, Molecular Dynamics Simulations of Au Penetration through Alkanethiol Monolayers on the Au(111) Surface, *Journal of Physical Chemistry C* **113**, 6360-6366 (2009)
64. **Chao Cao**, A. F. Kemper, L. Agapito, Jian-Wei Zhang, Yao He, A. Rinzler, Hai-Ping Cheng^{*}, Xiao-Guang Zhang, A. R. Rocha and S. Sanvito, Nonequilibrium Green's function study of Pd_4 -cluster-functionalized carbon nanotubes as hydrogen sensors, *Physical Review B* **79**, 075127 (2009)
65. **Chao Cao**^{*}, P. J. Hirschfeld and Hai-Ping Cheng, Proximity of antiferromagnetism and superconductivity in $\text{LaFeAsO}_{1-x}\text{F}_x$: Effective Hamiltonian from ab initio studies, *Physical Review B* **77**, 220506 (2008)
66. **Chao Cao**^{*}, S. Hill and Hai-Ping Cheng, Strongly correlated electrons in the $[\text{Ni}(\text{hmp})(\text{ROH})\text{X}]_4$ single molecule magnet: A DFT+U study, *Physical Review Letters* **100**, 167206 (2008)
67. **Chao Cao**, Yao He and Hai-Ping Cheng^{*}, First-principles simulations of dissociated and molecular H_2 adsorption on Pd_4 -cluster-functionalized carbon nanotubes, *Physical Review B* **77**, 045412 (2008)

68. Yunwen Chen, **Chao Cao** and Hai-Ping Cheng*, Finding stable α -quartz (0001) surface structures via simulations, *Applied Physics Letters* **93**, 3021398 (2008)
69. L. A. Agapito*, **Chao Cao** and Hai-Ping Cheng, First-principles determination of the effects of intermolecular interactions on the electronic transport through molecular monolayers, *Physical Review B* **78**, 155421 (2008)
70. Yao He, **Chao Cao**, S. B. Trickey, and Hai-Ping Cheng*, Predictive first-principles simulations of strain-induced phenomena at water-silica nanotube interfaces, *Journal of Chemical Physics* **129**, 011101 (2008)
71. S. Graser, G. R. Boyd, **Chao Cao**, Hai-Ping Cheng, P. J. Hirschfeld and D. J. Scalapino, Determining gap nodal structures in Fe-based superconductors: Theory of the angle dependence of the low-temperature specific heat in an applied magnetic field, *Physical Review B* **77**, 180514 (2008)
72. Yao He, Chun Zhang, **Chao Cao**, and Hai-Ping Cheng*, Effects of strain and defects on the electron conductance of metallic carbon nanotubes, *Physical Review B* **75**, 235429 (2007)
73. **Chao Cao**, Yao He, J. Torras, E. Deumens, S. B. Trickey and Hai-Ping Cheng*, Fracture, water dissociation, and proton conduction in SiO₂ nanochains, *Journal of Chemical Physics* **126**, 211101 (2007)
74. K. Muralidharan, **Chao Cao**, Yingxia Wan, K. Runge and Hai-Ping Cheng*, Environment dependent dynamic charge potential for silica: Application to nanoscale silica structures, *Chemical Physics Letters* **437**, 92-98 (2007)
75. Yao He, **Chao Cao**, Yingxia Wan, and Hai-Ping Cheng*, From cluster to bulk: Size dependent energetics of silica and silica-water interaction, *Journal of Chemical Physics* **124**, 024722 (2006)
76. J. Torras, Yao He, **Chao Cao**, K. Muralidharan, E. Deumens, Hai-Ping Cheng and S. B. Trickey*, PUPIL: A systematic approach to software integration in multi-scale simulations, *Computer Physics Communications* **177**, 265-279 (2007)
77. Hai-Ping Cheng*, Lin-Lin Wang, Maohua Du, **Chao Cao**, Y.-X. Wan, Y. He, K. Muralidharan, G. Greenlee, and A. Kolchin, Quantum, classical, and multi-scale simulation of silica-water interaction: molecules, clusters, and extended systems, *Journal of Computer-Aided Materials Design* **13**, 161 (2006)

TEACHING

@ Hangzhou Normal University: Fundamental Physics course for science-education majored undergraduate students, using *Sears and Zemansky's University Physics*; Frontiers of Condensed Matter Physics course for Physics majored graduate students.

PROFESSIONAL SERVICES

Referee of

- APS journals (Physical Review B, Physical Review Letters, Physical Review X)
- Chinese Physics Letters

Organization committee member and **academic secretary** of 2011 National Conference on Superconductivity (China)

RESEARCH GRANTS

- National Science Foundation of China, General Project, Grant No. 11874137, *First-principles study of quasi-one-dimensional noncentrosymmetric CrAs-based superconductors*, **PI**, 2019.01 - 2022.12, RMB 630,000
- National Science Foundation of China, General Project, Grant No. 11274006, *First-principles study of vacancy-ordering modulated frustrated systems*, **PI**, 2013.01 - 2016.12, RMB 750,000
- National Science Foundation of China, Young Scientist Project, Grant No. 10904127, *Atomic level study of electronic structure and magnetism of graphene interface/surface*, **PI**, 2010.01 - 2012.12, RMB 200,000

- National Key Basic Research Program of China (973), Grant No. 2014CB648400, *Design and synthesis of novel ultraviolet/deep ultraviolet borate-based nonlinear optical materials*, **2/5**, 2014.01 - 2018.12, RMB 5,500,000
- Zhejiang Natural Science Foundation, Excellent Young Scientist Project, Grant No. LR12A04003 *First principles study of novel iron-based superconducting materials*, **PI**, 2012, RMB 300,000

INVITED PRESENTATIONS

International Conferences

2020.03 APS March Meeting, 36 min invited presentation, From Trivial Kondo Insulator $\text{Ce}_3\text{Pt}_3\text{Bi}_4$ to Nodal-line Semimetal $\text{Ce}_3\text{Pd}_3\text{Bi}_4$

2015.05 Asian-Pacific Workshop on Strongly Correlated System, 30 min invited presentation, Electronic Structure of Quasi-1D Superconductor $\text{K}_2\text{Cr}_3\text{As}_3$

2014.02 Sannibel Symposium, 30 min invited presentation, Application of First-principles Methods in Iron-Selenide Superconductors

2013.09 Montauk Conference on High-Tc superconductors, 30 min invited presentation, Electronic structure of vacancy-ordered iron-selenides: First-principles perspective

2013.05 Hangzhou Quantum Matter International Workshop, 30 min invited presentation, First-Principles study of Li_2RhO_3

2011.10 11th National Conference on Superconductivity, 25 min invited presentation, First-Principles Study of $(\text{Tl},\text{K})_y\text{Fe}_{2-x}\text{Se}_2$ Electronic Structures

2009.3 APS March Meeting, 36 min invited presentation, Understanding Nano-Scale Electronic Systems via Large Scale Computation

Domestic Conferences

2015.07 First National Conference on Condensed Matter Physics, 30 min invited presentation, Electronic Structure of Quasi-1D $\text{K}_x\text{Cr}_3\text{As}_3$

2015.04 14th National Symposium on Low Temperature Physics

2013.03 13th National Symposium on Low Temperature Physics