CURRICULUM VITAE

Personal Information

Name: Xin-Gao GONG **Sex:** Male
Permanent Address: Dept. of Physics, Fudan University, Shanghai, 200434, China
Email: xggong@fudan.edu.cn
Tel: +86-21-65643932 (Office) **Fax:** +86-21-64104949
Website: http://www.physics.fudan.edu.cn/xggong
Website in Chinese Language(中文主页，last updated: Sep. 10th 2001):
http://www.physics.fudan.edu.cn/xggong/theoldbackup/index.html
Thesis Supervised: 16 Ph.D, 5 MS **Current Student:** 10 Ph.Ds

Education

1978 – 1982	Physics Department, Hunan Normal University	B.Sc.
1982 – 1985	Institute of Solid State Physics, Academia Sinica	M.Sc.
1991 – 1993	Institute of Solid State Physics, Academia Sinica	Ph.D.

Research Employment

1985 – 1987	Institute of Solid State Physics, Academia Sinica	Research Assistant
1987 – 1992	Institute of Solid State Physics, Academia Sinica	Assistant Professor
1992 – 1993	Institute of Solid State Physics, Academia Sinica	Associated Professor
1993 – 2005	Institute of Solid State Physics, Academia Sinica	Full Professor
2000 – 2005	Department of Physics, Fudan University	Full Professor
2005 – Now	Department of Physics, Fudan University	Distinguished Professor

Research Interesting

- Theoretical study of nano-particle and nano-structure
- Computational design of new materials
- Properties and defects of oxides and semiconductor
- Structure and dynamic properties of surfaces and interfaces
- Theoretical methods for multiscale modeling
- Computational method of electron structure of complex systems

Visiting Positions:

Long term:

January 1988-April 1991
International center for theoretical physics, Research fellow
July 1997-Januray 1998
Department of Physics, Ohio State University Visiting Professor
February 1999-July 1999

Department of Physics, Clark Atlanta University Visiting Professor
January 2000-June 2000,
Department of Physics, Chinese University of HK Visiting Professor

Short term:
International Center for theoretical Physics(1988, 1992, 1993, 1994, 1995), CBPF(Brazil, 1996), Tokyo University(1996), Kyoto University(1996),Nagoya University(1996), Keio University(1996), Oak ridge National lab (2002), University of Texas at Arlington(2002), Chinese University of HK(2005, 2008),University Sydney(2007), University College London(2008)

Previous and Present Responsibilities

1995 – 2004 Division head of theoretical physics, Institute of solid state physics, CAS
2002 – 2006 Deputy Director, Surface Science Lab (National Key) in Fudan Univ.
2003 – 2005 Deputy Director, Department of Physics, Fudan University
2005 – Now Dean of Research, Fudan University.
2009 – Now Director, Laboratory of Ministry of Education for Computational Physical Sciences
2006 – Now General Secretary and Vice president, Computational Materials Science Society of China
2006 – Now Communications in Computational Physics, Associate Editor
2006 – Now China Science Bulletin, Associate Editor

- Member of the International Organization Committee of Asian Workshop on First-Principles Electronic Structure Calculations (an annual workshop series). Served as Chairman of the 5th Workshop.
- Member of scientific committee: "International workshop on computational physics and materials sciences: total energy and force method" (workshop for every two years). Served as Chairman of the 2010-mini-workshop.
- Member of Program committee of Psi-k 2010
- General Secretary and vice president of Computational Materials Science of China
- Chairman of annual fall meeting of Chinese Physical Society for computational physics since 2004
- Co-Organizer: ICTP-NSFC-Asian/Pacific Regional School on Electronic Structure Methods and their Applications, July19-30, 2004 (Beijing)
- Committee member of NSF of China (2005-2008)

Invited talks

1. Applied Surface Modeling: Experiment, Theory and Simulations, Aug. 21-23, 2002, Cleveland, OH, USA
2. Computer Simulation of Cluster Diffusion on the Surface, 5th Chinese-American

Beckman Frontiers of Science Symposium, Nov. 22-24, 2002, Irvine, USA

3. Constant Pressure Molecular Dynamics and Phase Transition in Finite System, International Workshop on Cluster Science and Nanotechnology, May 22-24, 2002, Nanjing
4. Some Recent Progress in the Studies of Atomic Cluster, University of Texas at Arlington, Sept. 2002
5. Pressure Induced Phase Transition in Carbon Nanotubes and Nanoclusters, Oak Ridge National Laboratory, Sept. 2002
6. Structural and Phase Transition in Nanocluster and Carbon Nanotubes, The 6th Asian Workshop of First-Principle Electronic Calculation, Nov. 10-12, 2003, Japan
7. Adatom and Cluster Diffusion on the Strained Surface., Hong-Kong Polytechnic University, Nov. 18, 2003
8. Oxidation of Small Metal Clusters and Carbon Nano-tube, The China-Germany Symposium of Cluster and Nano-particles, March 29-31, 2003,Nanjing, China
9. Cage-like Metal Cluster: Aun, XII International Symposium on Small Particles and Inorganic Clusters, 2004, Nanjing, China
10. Metallic Cage Clusters, 7th Asian Workshop on the First-Principles Electronic Structure Calculations Oct. 31- Nov. 3, 2004, Taipei
11. First-Principles Studies on Hafnia: Mechanical Stability, Lattice Vibrations and Al-related Defect Complexes, EuroMat2005, September 5-8, Prague, Czech Republic.
12. Constant Pressure MD for Finite System and its Application to Nanocluster and Nanotubes, The Croucher Foundation - Advanced Study Institute on Frontiers in Computational Methods and Their Applications in Physical Sciences，Dec. 9-15, 2005, Hong Kong
13. Pressure Induced Structural Transformation in Nano-particles and Carbon Nano-tubes， Slovak Technical University, Oct. 4, 2006
14. Structural Transition in Semiconductor Nanopaticles and Carbon Nano-tubes， 13th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, Jan. 11-13, 2007, ICTP, Trieste.
15. Structure and Properties of Nano-particles and Carbon nanotubes. Feb. 12, 2007, The University of Sydney
16. A New Scheme for Coupling Atomic and Continuum Simulations, Symposium on Frontier of Multiscale Modeling, July 5~ July 10, 2007, Fudan
17. Structure and Structural Transformation in Nano-particles and Carbon nano-tubes, University of Waikato, New Zealand, Aug. 17, 2007
18. Searching for the Ground State Structures of Nanoclusters and Nanowires, The 6th International Conference on Materials Processing for Properties and Performance Sept.14-16 2007
19. Searching for the Ground State Structures of Nanoclusters and Nanowires, Hong Kong Forum 2007 - Frontiers in Condensed Matter, Dec. 14-16, 2007
20. Nanostructures Under Pressure, Department of Chemistry and Center of Materials Research, University College London, Feb. 14, 2008

21. Searching for the Ground States of Nano-clusters and Nano-particles， International Symposium on the Multiscale Modeling and Simulation of Materials, July 7～11, 2008，Fudan, Shanghai
22. Gold Cluster Beyond Planar Structure, The Third Symposium on Size Selected Cluster, Mar. 8-13, 2009, Brand, Austria
23. Computational studies on the materials properties, 2009-symposium on the first-principles calculation the materials properties, April 2-3, Institute of applied physics and computational mathematics.

Organized conferences and workshops:

1. Conference of Chinese Materials Science: session of computational materials Science, , Oct.22-24 2002 ,Beijing Co-Chair
2. Symposium on computation and simulation of materials, July 15-20, 2002, Xiangtang, China, Chair
3. Symposium on computational materials, July 8-10, 2002, Interdisciplinary center of Chinese Academy of Sciences, Beijing, Chair
4. Workshop on the computation of physical properties, Aug. 15-21, 2003, Interdisciplinary center of Chinese Academy of Sciences, Beijing , Chair
5. 6th Chinese-American Beckman Frontiers of Science Symposium Oct.10-12,2003，Shanghai, Co-Chair
6. Symposium on the multiscale modeling and computation, May. 29 –Jun. 2,2004, Fudan, Shanghai, Chair
7. ICTP-NSFC-ICTS Asian/Pacific Regional School on Electronic Structure Methods and their Applications Jul.19-30, 2004，Directors: X.G. Gong, Yu LU, S. Scandolo, Beijing, China
8. CPS2004-Session of computational Physics, Sept.18-22,2004, Taiyuan, Chair
9. Workshop on the electronic structure calculation and their application. Jun.13-25,2005, Interdisciplinary center of Chinese Academy of Sciences, Beijing , Chair
10. 8th- Asian workshop on the first principle electronic structure calculation, Oct. 31-Nov.2,2005，2005, Fudan, Chair
11. CPS2005-Session of computational Physics, Sept 18-21, 2005, Wuhan, Co-Chair
12. 9th- Asian workshop on the first principle electronic structure calculation,Nov.6～8,2006，Seoul, Advisory committee member
13. CPS2006-Session of computational Physics Sept.2006, Bejing, Co-Chair
14. CPS2006-Session of computational Physics, Sept. 2007, Nanjing, Co-Chair
15. The 6th International Conference on Materials Processing for Properties and Performance, Sept. 14-16, Beijing, 2007, organizing committee member.
16. Workshop on the frontier of multiscale modeling and simulations，July 5-10, 2007，Shanghai, Chair
17. 10th- Asian workshop on the first principle electronic structure calculation, Oct. 29-Oct.31，2007, Hiroshima, Advisory committee member
18. 11th asian workshop on first principles electronic structure calculations, Oct.

29-31, Taiwan, Advisory committee member

19. International symposium on the multiscale modeling and simulation of materials July 7～11，2008， Fudan, Shanghai, Chair
20. CPS2008-Session of computational Physics, Sept. 18-20. 2007, Jinan, Co-Chair
21. Conference of Chinese Materials Science: session of computational materials Science，2008-11-19-23，Guangzhou.
22. 4th Fudan Conference on Quantum Control, July 8-9, 2009, Shanghai, Co-Chair
23. Sino-German Workshop on Computational Materials Science: Methods and Applications, Sept. 13-18, 2009, Shanghai, Co-Chair
24. International Workshop on Computational Physics and Materials Science Progress in Computational Electronic Structure Theory, 2010.1.10-12, Fudan, China, Chair

Published papers:

1. ZF Hou, GH Chen, XG Gong, Energetics and electronic structure of Aluminum point defects in HFO2: a first principle study, App. Phys. Accepted.
2. Yin WJ, Gong XG , Hybridized kinetic energy functional for orbital-free density functional method PHYSICS LETTERS A,373, 480(2009)
3. Chen, SY; Gong, XG; Walsh, A, Wei SH , Crystal and electronic band structure of Cu2ZnSnX4 (X=S and Se) photovoltaic absorbers: First-principles insights, , APPLIED PHYSICS LETTERS, 94 (4): Art. No. 041903 JAN 26 2009
4. Sun, DY; Chen, HY; Liu, JW, Gong XG, Liu ZF, Diffusion through a molecular ball check valve composed of a C-60 molecule and a nanotube cap,PHYSICAL REVIEW B, 79 (3): Art. No. 033403 JAN 2009
5. G.H. Chen, Z.H. Hou, X.G. Gong, Q. Li Effects of Y doping on the structural stability and defect properties of cubic HfO2, J. App. Physics, 104, 074101(2008)
6. X Gu, L Zhang, XG Gong, ZF Liu, Diffusion of Vinyl Bromide through the Crystals of p-Bu-t-calix[4]arene, J. Phys. Chem. B, 112, 14851(2008)
7. W. Fan, X.G. Gong, "A density functional theory study of magnetic anisotropies of one-dimensional Ni chain and magnetism of 3d transition metals on Au(110)-(1 × 2) surface, Surface Review Letters, 15, 567(2008).
8. G.H. Chen, Z.H. Hou, X.G. Gong, "Structural and electronic properties of cubic HfO2 surfaces", Computational Materials Science 44，46（2008）
9. W.J. Yin, X.G. Gong and S.H.Wei, Origin of the unusually large band-gap bowing and the breakdown of the band-edge distribution rule in the SnxGe1−x alloys, PHYSICAL REVIEW B 78, 161203 (2008). (Rapid Communication)
10. C.D. Dong and X.G. Gong,"Magnetism enhancd layer-like structure of small cobalt clusters", PHYSICAL REVIEW B, 78, 020409 (2008) (Rapid Communication)
11. Yuan DW, Gong XG, Wu RQ, "Peculiar distribution of Pd on Au nanoclusters: First-principles studies", PHYSICAL REVIEW B, 78, 035441(2008)
12. X. Ye, D.Y. Sun, and X.G. Gong , Pressure-induced structural transformation of CdSe nanocrystals studied with molecular dynamics, PHYSICAL REVIEW B, 77， 094108（2008）。

13. Li SF, Gao L, Gong XG,Guo ZX ,"No Cage, No Tube: Relative Stabilities of Nanostructures", JOURNAL OF PHYSICAL CHEMISTRY C 112 13200 JUN 2008
14. Yin WJ, Gu X and Gong XG, "Magic number 32 and 90 in metal clusters: A shell jellium model study",SOLID STATE COMMUNICATIONS 147 323 JUN 2008
15. Wei Huang, Min Ji, Chuan-Ding Dong, Xiao Gu, Lei-Ming Wang, Xin Gao Gong,and Lai-Sheng Wang' Relativistic Effects and the Unique Low-Symmetry Structures of Gold Nanoclusters， ACS NANO， 2, 897(2008)
16. X.G. Gong, LiHua Shen, Dier Zhang and Aihui Zhou, Finite element approximation for Schodinger Equations, J. Computational mathmatics, 26, 310(2008).
17. Zhang D, Shen LH, Zhou AH, Gong XG,"Finite element method for solving Kohn-Sham equations based on self-adaptive tetrahedral mesh", PHYSICS LETTERS A 373, 5071(2008)
18. Dingwang Yuan, Xingao Gong, and RuQian Wu, Decomposition pathways of methanol on the PtAu(111) bimetallic surface: A first-principles study, J. Chemical Physics,. 1539-1543（2008）
19. Hou ZF, Gong XG, Li Q，" Al-induced reduction of the oxygen diffusion in HfO2: an ab-intio study", JOURNAL OF PHYSICS-CONDENSED MATTER,20,135206(2008)
20. Chen SY, Gong XG, Wei SH，Ground state structure of coherent lattice-mismatched zinc-blende A(1-x)B(x)C semiconductor alloys(x=0.25 and 0.75) ， PHYSICAL REVIEW B 073305（2008）
21. Shiyou Chen, X.G. Gong, and Su-Huai Wei, Crystal structures and mechanical properties of superhard BC$_2$N and BC$_4$N alloys: First-principles calculations, PHYSICAL REVIEW B,77，014113（2008）.
22. Xiao Gu, Satya Bulusu, Xi Li, X. C. Zeng,* Jun Li,* X. G. Gong,* and Lai-Sheng Wang*, Au34–: A Fluxional Core-Shell Cluster, J. Physics Chemistry , C 111(23) 8228-82232(2007).
23. Chen SY, Gong XG, Wei SH ，Band-structure anomalies of the chalcopyrite semiconductors CuGaX_2 versus AgGaX_2 (X=S and Se) and their alloys PHYSICAL REVIEW B 75 Art. No. 205209 FEB 2007
24. L. Huang, F. Liu and X.G. Gong, First-principles study of adsorption and diffusion on Ge/Si(001)-(2 x 8) and Ge/Si(105)-(1 x 2) surfaces , Surface Science, 601(14), 3067(2007)
25. Xiao Gu and X.G. Gong, Structural transitions of non-helical Au nanotubes induced by axial compression , J. Physics: Condensed Matter(letter), 19, 242205(2007)
26. J. X. Cao, X. G. Gong and R. Q. Wu, Giant piezoresistance and its origin in Si<111> nanowires： first-principles calculations, Physical Review B, 75, 233302(2007)
27. Shiyou Chen, X. G. Gong, and Su-Huai Wei, Band structure anomaly of chalcopyrite semiconductors CuGaX$_2$ versus AgGaX$_2$ (X=S and Se) and their alloys, Physical Review B, 75, 205209(2007)
28. L Huang, X. G. Gong and E. Gergert and F. Forster and A. Bendounan and F. Reinert and Zhenyu Zhang, Evolution of a Symmetry Gap and Synergetic Quantum Well States in Ultrathin Ag Films on Au(111) Substrates, Europhysics Letters, 78, 57003(2007)
29. D.Y. Sun, J.W. Liu, X.G. Gong, Zhi-Feng Liu，Empirical potential for the interaction between molecular hydrogen and graphite， PHYSICAL REVIEW B， 75， 075424(2007)
30. X.F. Wang, Q. Li, R.F. Egerton, R.F. J.Y. Dai, Z.F. Hou and X.G. Gong, Effect of Al addition on the microstructure and electronic structure of HfO2 films, JOURNAL OF APPLIED

PHYSICS, 101, 013514(2007)
31. D.W. Yuan, X.G. Gong and R.Q. Wu, Atomic configurations of Pd atoms in PdAu(111) bimetallic surfaces investigated using the first-principles pseudopotential plane wave approach, PHYSICAL REVIEW B, 75, 085428(2007)
32. X. Ye, D.Y. Sun, and X.G. Gong, Molecular dynamics study of radial pressure transmission in multiwalled carbon nanotubes, PHYSICAL REVIEW B， 75, 073406(2007)
33. Shiyou Chen, X.G. Gong, and Su-Huai Wei, Superhard pseudocubic BC$_2$N superlattices, PHYSICAL REVIEW LETTERS, 98, 015502(2007)
34. Y.H. Yao, X. Gu, M. Ji, Gong XG, Ding-sheng Wang, Structures and magnetic moments of Ni n (n=10~60) clusters, PHYSICS LETTERS A 360 (4-5): 629-631 (2007)
35. X. Ye, X. Gu, X.G. Gong, Z.F. Liu, A nanocontainer of the storage of hydrogen, Carbon, 45(2), 315(2007)
36. Cao JX, Gong XG, Zhong JX, Wu RQ, Sharp Corners in the Cross Section of Ultrathin Si Nanowires, PHYSICAL REVIEW LETTERS 97 (13): Art. No. 136105 (2006)
37. Li SF, Gong XG, Neutral and negatively charged Al12X (X=Si, Ge, Sn, Pb) clusters studied from first principles, PHYSICAL REVIEW B 74 (4): Art. No. 045432 (2006)
38. Li YH, Gong XG, Wei SH, Ab initio all-electron calculation of absolute volume deformation potentials of IV-IV, III-V, and II-VI semiconductors: The chemical trends, PHYSICAL REVIEW B 73 (24): Art. No. 245206 (2006)
39. Dalpian GA, Wei SH, Gong XG, da Silva AJR, Fazzio A, Phenomenological band structure model of magnetic coupling in semiconductors, SOLID STATE COMMUNICATIONS 138 (7): 353-358 (2006)
40. Li Q, Koo KM, Lau WM, Lee PF, Dai JY, Hou ZF, Gong XG, Effects of Al addition on the native defects in hafnia, APPLIED PHYSICS LETTERS 88 (18): Art. No. 182903 (2006)
41. Li SF, Xue XL, Jia Y, Zhao GF, Zhang MF, Gong XG, Stable cubic metal-semiconductor alloy clusters: X4Y4 (X=Cu,Ag,Au,Ti; Y=C,Si), PHYSICAL REVIEW B 73 (16): Art. No. 165401 (2006)
42. Wei SH, Huang L, Ji M, Gong XG, Structural and electronic properties of Al7In (n=1,2,3), CHEMICAL PHYSICS LETTERS 420 (1-3): 125-129 (2006)
43. Li YH, Gong XG, Wei SH, Ab initio calculation of hydrostatic absolute deformation potential of semiconductors, APPLIED PHYSICS LETTERS 88 (4): Art. No. 042104 (2006)
44. Huang L, Liu F, Lu GH, Gong XG, Surface mobility difference between Si and Ge and its effect on growth of SiGe alloy films and islands, PHYSICAL REVIEW LETTERS 96 (1): Art. No. 016103 (2006)
45. Cao JX, Gong XG, and Wu RQ, Adsorption, segregation and magnetization of a single Mn adatom on the GaAs(110) surface, Physical Review B 72, 153410 (2005)
46. Mi J, Gu X, Li X, Gong XG, Li J, Wang LS, Experimental and theoretical investigation of the electronic and geometric structure of Au32 cluster, Angew. Chem. Int. Ed. 2005, 44, 7119-7123,
47. Fan W, Gong XG “superheated melting of grain boundaries”, PHYSICAL REVIEW B 72 (6): Art. No. 064121 AUG 2005
48. Ye X, Sun DY, Gong XG “Pressure-induced structural transition of double-walled carbon nanotubes” PHYSICAL REVIEW B 72 (3): Art. No. 035454 JUL 2005

49. Chen G, Gong XG, Chan CT “Theoretical study of the adsorption of H-2 on (3,3) carbon nanotubes” PHYSICAL REVIEW B 72 (4): Art. No. 045444 JUL 2005
50. Wang Y, Gong XG “first principles study of neutral and charged silver clusters” EUROPEAN PHYSICAL JOURNAL D 34 (1-3): 19-22 JUL 2005
51. Li SF, Gong XG “First-principles studies on the reaction of O-2 with silicon clusters” JOURNAL OF CHEMICAL PHYSICS 122 (17): Art. No. 174311 MAY 1 2005
52. Wei SH, Gong XG, Dalpian GM, Wei SuHuai,”First-principles study of the Mn-induced local magnetic moments in host semiconductor” PHYSICAL REVIEW B 71 (14): Art. No. 144409 APR 2005
53. Sun DY, Shu DJ, Ji M, Liu F, Wang M, Gong XG, “Pressure-induced hard-to-soft transition of a single carbon nanotube” PHYSICAL REVIEW B 70 (16): Art. No. 165417 OCT 22 2004
54. Gu X, Ji M, Wei SH, Gong XG, “AuN clusters (N=32, 33, 34, 35): Cagelike structures of pure metal atoms” PHYSICAL REVIEW B 70 (20): Art. No. 205401 NOV 2 2004
55. Huang L, Liu F, Gong XG, Strain effect on adatom binding and diffusion in homo- and heteroepitaxies of Si and Ge on (001) surfaces PHYSICAL REVIEW B 70 (15): Art. No. 155320 OCT 22 2004.
56. Zhang HY, Gu X, Zhang XH, Ye X, Gong XG “Structures and Properties of Ni Nanowires” PHYSICS LETTERS A 331 (5): 332-336 OCT 25 2004
57. Zhang XH, Liu ZF, Gong XG Comment on ``Collapse of single-wall carbon nanotubes is diameter dependent'' PHYSICAL REVIEW LETTERS 93 (14): Art. No. 149601 SEP 27 2004
58. Li Q, Gong XG, Wang CR, Wang J, Ip K, Hark S “Size-dependent periodically twinned ZnSe nanowires” ADVANCED MATERIALS 16 (16): 1436-1440 2 Sep 2004
59. Li SF, Gong XG “Charge-induced structural changes in Al12C clusters” PHYSICAL REVIEW B 70 (7): Art. No. 075404 AUG 9 2004
60. Zhang XH, Sun DY, Liu ZF, Gong XG “Structure and phase transitions of single-wall carbon nanotube bundles under hydrostatic pressure” PHYSICAL REVIEW B 70 (3): Art. No. 035422 JUL 30 2004
61. Fan W, Gong XG “Monte Carlo simulation of surface de-alloying of Au/Ni(110)” SURFACE SCIENCE 562 (1-3): 219-225 AUG 1 2004
62. Zhang QM, Wells JC, Gong XG, Zhang ZY “Adsorption of a carbon atom on the Ni38 magic cluster and three low-index nickel surfaces: A comparative first-principles study” PHYSICAL REVIEW B 69 (20): Art. No. 205413 MAY 28 2004
63. Ji M, Sun DY, Gong XG “Ab initio molecular dynamics simulation on nano-system under external pressure” SCIENCE IN CHINA SER. A MATHEMATICS 47 (Supp.): 92-100 APR 1 2004
64. Zhang LB, Chen SY, Li XL, Cao JW, Zhang WS, Gong XG “Teracluster LSSC-II: Its designing principles and applications in large scale numerical simulations” SCIENCE IN CHINA SER. A MATHEMATICS 47 (Supp.): 53-68 APR 1 2004
65. Chen G, Liu ZF, Gong XG “Ab initio study on structural and electronic properties of BanOm clusters” JOURNAL OF CHEMICAL PHYSICS 120 (17): 8020-8024 MAY 1 2004
66. Wu J, Zang J, Larade B, Guo H, Gong XG, Liu F “Computational design of carbon nanotube electromechanical pressure sensors” PHYSICAL REVIEW B 69 (15): Art. No. 153406 APR

16 2004

67. Ji M, Gong XG “Ab initio molecular dynamics simulation on temperature-dependent properties of Al-Si liquid alloy” JOURNAL OF PHYSICS-CONDENSED MATTER 16 (15): 2507-2514 APR 21 2004
68. Chan SP, Ji M, Gong XG, Liu ZF “Pressure-driven confinement of hydrogen molecules between graphene sheets in the regime of van der Waals repulsion” PHYSICAL REVIEW B 69 (9): Art. No. 092101 MAR 5 2004
69. Chan SP, Chen G, Gong XG, Liu ZF, “Oxidization of carbon tubes by singlet O_2, PHYSICAL REVIEW LETTERS 90 (8): art. no. 086403 FEB 28 2003
70. G. Chen, Z. F. Liu and X. G. Gong, “Structural Transition in Ba_nO_m clusters”, PHYSICAL REVIEW B 67 (20): art. no. 205415 MAY 15 2003
71. W. Fan and X. G. Gong, “Simulation of Ni cluster diffusion on Au(1 1 0)-(1 × 2) surface”, Apllied Surface Science, 219, 117(2003)
72. X. M. Duan, D.Y. Sun, and X.G, Gong,”Local bias potential for COMPUTATIONAL MATERIALS SCIENCE 27 (3): 375-380 MAY 2003
73. Yim WL, Gong XG, Liu ZF “Chemisorption of NO2 on carbon nanotubes” J PHYS CHEM B 107 (35): 9363-9369 SEP 4 2003
74. Nduwimana A, Gong X.G, , Wang X.Q.,“Relative stability of missing-row reconstructed (1 1 0) surfaces of noble metals” Apllied Surface Science, 219, 129(2003)
75. Chan SP, Yim WL, Gong XG, et al. “Carbon nanotube bundles under high oressre: transformation to low-symmetry structures” PHYS REV B 68 (7): Art. No. 075404 AUG 15 2003
76. Fan W, Gong XG, Lau WM, “ Instability of an atomic chain arising from lattice misfit”, PHYSICAL REVIEW B 66 (11): art. no. 115418 SEP 15 2002
77. Sun DY, Gong XG , “A new constant-pressure molecular dynamics method for finite systems ”, JOURNAL OF PHYSICS-CONDENSED MATTER 14 (26): L487-L493 JUL 8 2002
78. Liu YB, Sun DY, Gong XG, “Local strain induced anisotropic diffusion on (23x root 3)-Au(111) surface ”, SURFACE SCIENCE 498 (3): 337-342 FEB 10 2002
79. Sun Q, Wang Q, Gong XG, Kumar V, Kawazoe Y, “Structures and stability of Al7C and Al7N clusters” EUROPEAN PHYSICAL JOURNAL D 18 (1): 77-81 JAN 2002
80. Chen G, Liu ZF, Gong XG, “Structure and growth modes of (BaO)(n) (n <= 9) clusters”,JOURNAL OF CHEMICAL PHYSICS 116 (4): 1339-1342 JAN 22 2002
81. DJ Shu, F. Liu and X. G. Gong，“ A simple generic method for predicting the effect of strain on surface diffusion” Phys Rev. B 64 24 (24): 5410-+ DEC 15 2001
82. Chan SP, Chen G, Gong XG, Liu ZF, "Chemisorption of hydrogen molecules on carbon nanotubes under high pressure", Phy. Rev. Lett., 87: 5502-+ NOV 12 2001
83. Chen G, Liu ZF, Gong XG, "Sturcture and its evolution of Ban (n=2~14) clusters", Eur. J. Physics D, 16 (1-3): 33-36 SEP 2001.
84. Shu DJ, Gong XG, " Curvature effect on surface diffusion: The nanotube", J CHEM PHYS 114 (24): 10922-10926 JUN 22 2001.
85. Duan HM, Gong XG, Zheng QQ, et al., " Electronic structure and magnetic properties of Ni clusters", J APPL PHYS 89 (11): 7308-7310 Part 2 JUN 1 2001

86. Sun DY, Gong XG, Wang XQ, "Soft and hard shells in metallic nanocrystals - art. no. 193412", PHYS REV B 63 (19): 3412-+ MAY 15 2001
87. Duan XM, Sun DY, Gong XG, " Hypermolecular dynamics simulations of monovacancy diffusion", COMP MATER SCI 20 (2): 151-156 FEB 2001.
88. X. G. Gong and V. Kumar, Atomic shell covering on C60, to appear Chem. Phys. Lett, 334，238(2001)
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92. Y. Xiang, D. Y. Sun and X. G. Gong, " Generalized simulated annealing studies on Ni clusters",J. Phys. Chem., 104 2746(2000).
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94. Y. Xiang and X.G. Gong, " The efficiency of generalzed simulated annealing",Phys. Rev. E, 61, 4473(2000)
95. M. Duan and X. G. Gong, "Surface trapping of hyperthermal particles", Phys. Stat. Solidi B, 220, (2000)
96. D.Y. Sun, X. G. Gong, "Cluster on the fcc(111) surface: structure, stability and diffusion", SURF SCI, 42, 445 41(2000).
97. H. Wu, Q.Q. Zheng, X. G. Gong, "Electronic structure study of the magnetoresistance material CaCu3Mn4O12 by LSDA and LSDA+U", Phys. Rev. B, 61, 5217(2000).
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