Final Report:

1. DOE award #: DE-FG02-03ER46027; Recipient: University of Utah

2. Project Title: "Group IV Nanomembranes, Nanoribbons, and Quantum Dots: Processing, Characterization, and Novel Devices"; PI: Feng Liu

3. Reporting Period: February 1, 2003 – April 30, 2013

4. Program Scope

This theoretical project has been carried out in close interaction with the experimental project at UW-Madison under the same title led by PI Max Lagally and co-PI Mark Eriksson. Extensive computational studies have been performed to address a broad range of topics from atomic structure, stability, mechanical property, to electronic structure, optoelectronic and transport properties of various nanoarchitectures in the context of Si and other solid nanomembranes. These have been done by using combinations of different theoretical and computational approaches, ranging from first-principles calculations and molecular dynamics (MD) simulations to finite-element (FE) analyses and continuum modeling.

5. Accomplishments.

We have made strong efforts in carrying out both atomic and continuum simulations to investigate fundamental sciences related to the growth, stability and electronic properties of semiconductor nanomembranes, nanoribbons, and their hybrid structures with quantum dots and molecular adsorbates. In total, we have published **58** papers fully or partially supported by this 11-year DOE-DMSE project, including **7** invited book chapters or review articles and **17** papers in high impact journals (**10** *Phys. Rev. Letters*, **1** Nature Mat., **1** Nature Commun., **3** Nano Letters and **2** ACS Nano). **Seven** postdoctoral research associates, **seven** PhD (**six** graduated) and **one** Master graduate student (graduated) have been fully or partially supported by this DOE project. In addition, **seven** visiting scholars/students have participated in the research of this project, mostly on their own funding. Benefited from the success of this project, during the funding period, the PI gave **171** invited talks, including **seventy two** invitations at national/international conferences and **sixty nine** departmental/institutional colloquium/seminar presentations.

PI has been elected Fellow of American Physical Society (2011), awarded Senior Humboldt Research Award (2008) and Australia Research Council International Professorial Fellowship (2007), and appointed Chair of Department of Materials Science and Engineering. The PI organized or co-organized two conferences/workshops: (1) "International Symposium on Clusters and Nanostructures" held in Richmond, VA on November 7-10, 2011; (2) Surface Kinetics International Conference, March 20-22, 2009, Salt Lake City, UT;

Our theoretical/computational studies have been done in close collaborations with experiments at University of Wisconsin-Madison (PI: Max Lagally) which are also funded by DOE. We published together **thirteen** papers, including **1** invited book chapter and **2** invited

review articles. Their experiments have provided new ideas stimulating theoretical studies, and in return our theory has explained some of their experimental results. In addition, we have had collaborations with other research groups around the world including **six** joint papers with groups in China.

6. Publications:

1. "Geometry Constant Defining Shape Transitions of Carbon Nanotubes under Pressure", Ji Zang, Andrejs Treibergs, Y. Han, and **Feng Liu**, Phys. Rev. Lett. 92, 105501 (2004).
2. "Coulomb Sink: a novel Coulomb effect on coarsening of metal nanoclusters on semiconductor surface", Y. Han, J.Y. Zhu, **Feng Liu**, S.C. Li, J.F. Jia, Y.F. Zhang, and Q.K. Xue, Phys. Rev. Lett. 93, 106102 (2004).
3. "Theory of Equilibrium Shape of an Anisotropically Strained Island: Thermodynamic Limits for Growth of Nanowires", Amit Pradhan, N.-Y. Ma and **Feng Liu**, Phys. Rev. B 70, 193405 (2004).
4. "Towards Quantitative Understanding of Formation and Stability of Ge Hut Island on Si(001)", G.H. Lu and **Feng Liu**, Phys. Rev. Lett 94, 176103 (2005).
5. "Mechanical stability of ultrathin Ge/Si film on SiO2: The effect of Si/SiO2 interface", M.H. Huang, J.A. Nairn, **Feng Liu**, and **M.G. Lagally**, J. Appl. Phys. 97, 116108 (2005).
6. "Bending of Nanoscale Ultrathin Substrates by Growth of Strained Thin Films and Islands", M.H. Huang, P. Rugheimer, **M.G. Lagally**, and **Feng Liu**, Phys. Rev. B 72, 085450 (2005).
7. "First-principles study of strain stabilization of Ge(105) facet on Si(001)", G.H. Lu, Martin Cuma, and **Feng Liu**, Phys. Rev. B 72, 125415 (2005).
8. "Self-organization of Semiconductor Nanocrystals by Selective Surface Faceting", B. Yang, P. Zhang, D.E. Savage, **M. Lagally**, G.H. Lu, M.H. Huang, and **Feng Liu**, Phys. Rev. B 72, 235413 (2005).
9. "Modeling and Simulation of Strain-Mediated Nanostructure Formation on Surface", **Feng Liu**, in "Handbook of Theoretical and Computational Nanotechnology", eds. M. Rieth and W. Schommers, Chapter 10, 577-625 (2006). (invited book chapter).
10. "Surface Mobility Difference between Si and Ge and its Effect on Growth of SiGe Alloy Films and Islands", Li Huang, **Feng Liu**, Guang-Hong Lu and X. G. Gong, Phys. Rev. Lett. 96, 016103 (2006).
11. "Quantitative Prediction of Critical Size for the Formation of Semiconductor Quantum Dots", G.H. Lu and **Feng Liu**, in "Physics, J. Chinese Phys. Association", 35, 447 (2006). (invited review).
12. "Intrinsic current-voltage properties of nanowires with four-probe scanning tunneling microscopy: A conductance transition of ZnO nanowire", X. Lin, X.B. He, T.Z. Yang, W. Guo, D.X. Shi, H.-J. Gao, D.D. Ma, S.T. Lee, **Feng Liu**, and X.C. Xie, Appl. Phys. Lett. 89, 043103(2006).
13. "Directed Self-Assembly of Quantum Dots by Local Chemical Potential Control via Strain Engineering on Patterned Substrates", M-H Huang, **Feng Liu**, and **M. G. Lagally**, in Lateral Alignment of Epitaxial Quantum Dots, ed. Oliver G. Schmidt, Springer Series on Nanoscience and Technology 2007. (invited book chapter)
14. "Making a field effect transistor on a single graphene nanoribbon by selective doping", Bing Huang, Qimin Yan, Gang Zhou, Jian Wu, Bing-Lin Gu, Wenhui Duan, and **Feng Liu**, Appl. Phys. Lett. 91, 253122 (2007).
15. "Synthesis of Carbon Nanotubes by Rolling Up Patterned Graphene Nanoribbons Using Selective Atomic Adsorption", Decai Yu and **Feng Liu**, Nano Lett. 7, 3046 (2007).
16. "Bending of Si Nano-Cantilever Induced by Molecular Adsorption: A Modified Stoney Formula for the Calibration of Nanomechanochemical Sensors", Ji Zang and **Feng Liu**, Nanotechnology, 18, 405501 (2007).
17. "Intrinsic current-voltage characteristics of graphene nanoribbon transistors and effect of edge doping", Q. Yan, B. Huang, J. Yu, F. Zheng, J. Zang, J. Wu, B. Gu, **Feng Liu**, and W. Duan, Nano Lett. 7, 1469 (2007).
18. "Mechanism for Nanotube Formation from Self-Bending Nanofilms Driven by Atomic-Scale Surface-Stress Imbalance", Ji Zang, Minghuang Huang, and **Feng Liu**, Phys. Rev. Lett. 98, 146102 (2007).
19. "MD simulation of structural and mechanical transformation of single-walled carbon nanotubes under pressure", J. Zang, O. Aldás-Palacios and **Feng Liu**, Commun. Comput. Phys. 2, 451 (2007). (invited).
20. "Impurity mediated absorption continuum in single-walled carbon nanotubes", C. Zhang, J.C. Chao, X.G. Guo and **Feng Liu**, Appl. Phys. Lett. 90, 023106 (2007).

21. "Nucleation-Mediated Lateral Growth on Foreign Substrate", D.J. Shu, M. Wang, **Feng Liu**, Z. Zhang, R.W. Peng, R. Zhang, N.B. Ming, *J. Phys. Chem. C,* 111, 1071 (2007).
22. "First-Principles Study of Adsorption and Diffusion on Ge/Si(001)-(2X8) and Ge/Si(105)-(1X2) Surfaces", Li Huang, Guang-Hong Lu, **Feng Liu**, and X. G. Gong, *Surf. Sci*. 601, 3067 (2007).
23. "First-principles study of electronic properties of biaxially strained silicon: Effects on charge carrier mobility", D. Yu and **Feng Liu**, Phys. Rev. B 78, 245204 (2008).
24. "Magnetism in Nanopatterned Graphite Film", L. Chen, D. Yu, **Feng Liu**, Appl. Phys. Lett. 93, 223106 (2008).
25. "Unified Design Rule for Nanomagnetism in Graphene", D. Yu, E. M. Lupton, H.J. Gao, C. Zhang and **Feng Liu**, Nano Res. 1, 497 (2008).
26. "Collective Magnetic Behavior of Graphene Nanohole Superlattices", D. Yu, E. M. Lupton, M. Liu, W. Liu and **Feng Liu**, Nano Res. 1, 56 (2008).
27. "Suppression of spin-polarization in graphene nanoribbon by edge defect and impurity", Bing Huang, **Feng Liu**, Jian Wu, Bing-Lin Gu, and Wenhui Duan, Phys. Rev. B 77, 153411 (2008).
28. "Coulomb sink effect on coarsening of metal nanostructures on surfaces", Y. Han and **Feng Liu**, Front. Phys. China, 3, 41 (2008). (Invited).
29. "Modified Timoshenko formula for bending of ultrathin strained bi-layer films", Ji Zang and **Feng Liu**, Appl. Phys. Lett. 92, 021905 (2008).
30. "Nanomechanical Architectures – Mechanics-Driven Fabrication Based on Crystalline Membranes", **F. Liu, M. G. Lagally**, and Ji Zang, MRS Bulletin 34, 190 (2009). (invited)
31. "Mechano-electronic Superlattices in Silicon Nanomembranes", Minghuang Huang, C. S. Ritz, B. Novakovic, D.C.Yu, Yu Zhang, F. Flack, D. E. Savage, I. Knezevic, P. G. Evans, **F. Liu,** and **M. G. Lagally**, ACS Nano 3, 721 (2009).
32. "Effects of Ge Adsorption on Dewetting and Thermal Agglomeration of Thin Silicon-on-Insulator", P.P. Zhang, B. Yang, P. Rugheimer, M. Roberts, D.E. Savage, **F. Liu**, and **M. G. Lagally**, J. Phys. D 42, 175309 (2009).
33. "Strain – band structure relationships in Si(001) and Si(110) nanomembranes", C. Euaruksakul, F. Chen, B. Tanto, C. S. Ritz, D. M. Paskiewicz, F. J. Himpsel, D. E. Savage, Zheng Liu, Yugui Yao, **Feng Liu**, and **M. G. Lagally**, Phys. Rev. B 80, 115323 (2009)
34. "Directed self-assembly of monodispersed platinum nanoclusters on graphene Moiré template", Y. Pan, M. Gao, L. Huang, **Feng Liu**, and H.-J. Gao, Appl. Phys. Lett. 95, 093106 (2009).
35. "Quantum Manifestations of Graphene Edge Stress and Edge Instability: A First-Principles Study", B. Huang, M. Liu, N. Su, J. Wu, W. Duan, B. Gu and **Feng Liu**, Phys. Rev. Lett. 102**,** 166404 (2009).
36. "Vacancy trapping mechanism for hydrogen bubble formation in metal", Y.-L. Liu, Y. Zhang, H.-B. Zhou, G.-H. Lu, **Feng Liu**, and G. -N. Luo, Phys. Rev. B 79, 172103 (2009).
37. "Mechanical Wave Propagation in Carbon Nanotubes Driven by an Oscillating Tip Actuator", M. Chen, J. Zang, D. Xiao and **Feng Liu**, J. Appl. Phys. 105, 026102 (2009).
38. "Highly Ordered, Millimeter-Scale, Continuous, Single-Crystalline Graphene Monolayer Formed on Ru (0001)", Y. Pan, H. Zhang, D. Shi, J. Sun, S. Du, **Feng Liu**, H.-J. Gao, Adv. Mat. 21, 2777 (2009).
39. "Electronic Phase Diagram of Silicon Single-Element Lateral 'Strain' Superlattice", Zheng Liu, Jian Wu, Wenhui Duan, **M. G. Lagally**, and **Feng Liu**, Phys. Rev. Letters 105, 016802 (2010).
40. "Atomic Layers of Hybridized Boron Nitride and Graphene Domains", L. Ci, L. Song, C. Jin, D. Jariwala, D. Wu, Y. Li, A. Srivastava, Z. F. Wang, K. Storr, L. Balicas, **Feng Liu**, and P. M. Ajayan, Nature Mat. 9, 430 (2010).
41. "Effect of Surface Bonding on Semiconductor Nanoribbon Wiggling Structure", Y. Zhang, M. Yu, D. E. Savage, **M. G. Lagally**, R. H. Blick, and **Feng Liu**, Appl. Phys. Letters 96, 111904 (2010).
42. "Manipulation of Electron Beam Propagation by Hetero-Dimensional Graphene Junctions", Z. F. Wang and **Feng Liu**, ACS Nano. 4, 2459 (2010).
43. "Tunable interfacial properties of epitaxial graphene on metal substrates", M. Gao, Y. Pan, C. Zhang, H. Hu, R. Yang, H. Lu, J. Cai, S. Du, **Feng Liu**, and H.-J. Gao, Appl. Phys. Lett. 96, 053109 (2010).
44. "Nanomechanical Architecture of Semiconductor Nanomembranes", M.H. Huang, F. Cavallo, **Feng Liu**, and **M.G. Lagally**, Nanoscale 3, 96 (2011) (invited).

45. "Formation of hydrogenated graphene nanoripples by strain engineering and directed surface self-assembly", Z. F. Wang, Y. Zhang, and **Feng Liu**, Phys. Rev. B 83, 041403(R) (2011)
46. "Maximum asymmetry in strain induced mechanical instability of graphene: Compression versus tension", Y. Zhang and **Feng Liu**, Appl. Phys. Lett. 99, 241908 (2011).
47. "Stable Nontrivial Z2 Topology in Ultrathin Bi (111) Films: A First-Principles Study", Z. Liu, C.-X. Liu, Y.-S. Wu, W.-H. Duan, **Feng Liu**, and J. Wu, Phys. Rev. Lett. 107, 136805 (2011).
48. "Chemical versus Thermal Folding of Graphene Edges", N. Su, M. Liu and **Feng Liu**, Nano Res. 4, 1242 (2011).
49. "Giant Magnetoresistance in Zigzag Graphene Nanoribbon", Z. F. Wang and **Feng Liu**, Appl. Phys. Lett. 99, 042110 (2011).
50. "Stabilizing Graphitic Thin Films of Wurtzite Materials by Epitaxial Strain", Dangxin Wu, **M.G. Lagally**, and **Feng Liu**, Phys. Rev. Letters 107, 236101 (2011).
51. "Conduction Band Structure and Electron Mobility in Uniaxially Strained Si via Externally Applied Strain in Nanomembranes", F. Chen, C. Euaruksakul, Zh. Liu, F. Himpsel, **Feng Liu**, and **M.G. Lagally**, J. Phys. D 44, 325107 (2011).
52. "Atomic chemisorption on graphene with Stone–Thrower–Wales defects", L. Chen, H. Hu, Yu. Ouyang, H.Z. Pan, Y.Y. Sun, and **Feng Liu**, Carbon 49, 3356 (2011).
53. "Edge Stability of BN sheets and Its Application for Designing Hybrid BNC Structures", B. Huang, H. Lee, B.-L. Gu, **Feng Liu**, and W. Duan, Nano Res. 5, 62 (2012).
54. "Fractal Landau-Level Spectra in Twisted Bilayer Graphene", Z. F. Wang, **Feng Liu**, and M. Y. Chou, Nano Lett. 12, 3833 (2012).
55. "Topological and electronic transitions in a Sb(111) nanofilm: The interplay between quantum confinement and surface effect", P. Zhang, Z. Liu, W. Duan, **Feng Liu**, and J. Wu, Phys. Rev. B 85, 201410 (R) (2012).
56. "Mechanical properties of graphene oxides", L. Liu, J. Zhang, J. Zhao and **Feng Liu**, Nanoscale 4, 5910 (2012).
57. "Electronic Strengthening of Graphene by Charge Doping", C. Si, W. Duan, Z. Liu, and **Feng Liu**, Phys. Rev. Lett. 109, 226802 (2012).
58. "Creation of Helical Dirac Fermions by Interfacing Two Gapped Systems of Ordinary Fermions", Z.F. Wang, M.-Y. Yao, W. Ming, L. Miao, F. Zhu, C. Liu, C. L. Gao. D. Qian, J.F. Jia, and **Feng Liu**, Nature Communications 4, 1384 (2013).

7. People working on the project:

Postdoctoral Associates: Guanghong Lu, Naiyang Ma, Decai Yu, Elisabeth Lupton, Dangxin Wu, Zhengfei Wang, Zheng Liu
PhD students: Ji Zang, Yong Han, Junyi Zhu, Yu Zhang, Miao Liu, Ninghai Su, Wenmei Ming
Master students graduated: Amit Pradhan
Visiting Scholars and students: Li Chen, Si Chen, Min Chen, Hao Hu, Lizhao Liu, Wei Liu, Zheng Liu,

8. Unexpended funds: This DOE-BES project was combined with another DOE-BES account (Grant # DEFG02-04ER46148) last year. Partly because the ending dates of the two accounts differ by one month, our university accounting missed to transfer a small amount of ~$1400.00 funds from this account to the new joint account on time, so they returned ~$1400.00 to the DOE Chicago office. The account is balanced now with no unexpended funds left.