Final Report for Period: 07/2007 - 06/2008 **Submitted on:** 09/28/2008
Principal Investigator: Chou, Mei-Yin . **Award ID:** 0205328
Organization: GA Tech Res Corp - GIT
Submitted By:
Chou, Mei-Yin - Principal Investigator
Title:
ITR: Modelling and Simulations of Quantum Phenomena in Semiconductor Structures of Reduced Dimensions

Project Participants

Senior Personnel

Name: Chou, Mei-Yin
Worked for more than 160 Hours: Yes
Contribution to Project:
PI of the project

Name: Umrigar, Cyrus
Worked for more than 160 Hours: Yes
Contribution to Project:
Co-PI of the project

Name: Landman, Uzi
Worked for more than 160 Hours: Yes
Contribution to Project:
Co-PI of the project

Name: Wang, Xiao-Qian
Worked for more than 160 Hours: Yes
Contribution to Project:
Co-PI of the project

Post-doc

Name: Zhao, Xinyuan
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Mei-Yin Chou on Si nanowires in Years 1 and 2.

Name: Guclu, Devrim
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Cyrus Umrigar on quantum dots in Years 2 and 3.

Name: Felfli, Zineb
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang in Year 2 (July - August, 2003).

Name: Musin, Ryza
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang on nanowires in Years 2-4.

Name: a Beccara, Silvio
Worked for more than 160 Hours: Yes

Contribution to Project:
Worked with Cyrus Umrigar on quantum dots in Year 2.

Name: Scherbakov, Andrew
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Uzi Landman on quantum transport during Year 2.

Name: Yannouleas, Constantine
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Uzi Landman on quantum dots in Year 3.

Name: Toulouse, Julien
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Cyrus Umrigar on extending our new many-body wave function optimization methods to LCAO coefficients. This is an important ingredient for eliminating the fixed-node error in quantum Monte Carlo.

Name: Shen, Peiqing
Worked for more than 160 Hours: Yes
Contribution to Project:

Name: Geist, Wolfgang
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Mei-Yin Chou on quantum dots in Years 4 and 5.

Name: Yan, Jia-An
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Mei-Yin Chou on nanowires and graphene in Years 4-6.

Name: Ruan, Wen-Ying
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Mei-Yin Chou on graphene in Years 5 and 6.

Name: de Silva, Theja
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Cyrus Umrigar and Erich Muellller on cold gases in year 5

Name: Al-Saidi, Wissam
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Cyrus Umrigar on improved forms of wave functions in year 5

Name: Zhang, Chun
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Uzi Landman in Year 4.

Name: Baksmaty, Leslie
Worked for more than 160 Hours: Yes
Contribution to Project:

Worked with Uzi Landman in Year 4.

Name: Wang, Yan
Worked for more than 160 Hours: Yes
Contribution to Project:

Graduate Student

Name: Yang, Li
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Mei-Yin Chou on nanowires in Years 1-3.

Name: Romanovsky, Igor
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Uzi Landman on quantum transport in Years 1-3.

Name: Cupid, Damian
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang in Years 1 and 2.

Name: Nduwimana, Alexis
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang and Mei-Yin Chou on nanowires in Years 1-5.

Name: Cochran, Anthony
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang in Year 2.

Name: Fadiran, Oladipo
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang in Year 2.

Name: Yuan, Longping
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang as a Programmer in Year 3.

Name: Yarahmad, Taha
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with X. Q. Wang on computer simulations in Year 3.

Name: Li, Yuesong
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Uzi Landman in Years 3 and 4.

Name: Smith, Ainsley
Worked for more than 160 Hours: Yes
Contribution to Project:

Worked with Xiao-Qian Wang.

Name: Karunwi, Olukayode
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang in Year 5.

Name: Bellamy, Michael
Worked for more than 160 Hours: Yes
Contribution to Project:

Name: Zeng, Lang
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Mei-Yin Chou on quantum dots in Year 5.

Name: Petruzielo, Frank
Worked for more than 160 Hours: No
Contribution to Project:
Worked with Cyrus Umrigar learning the basics of quantum Monte Carlo methods

Name: Xian, Lede
Worked for more than 160 Hours: Yes
Contribution to Project:
First-year graduate student

Name: Ogunro, Olayinka
Worked for more than 160 Hours: No
Contribution to Project:

Undergraduate Student

Name: Tarrant, Jermaine
Worked for more than 160 Hours: Yes
Contribution to Project:
Worked with Xiao-Qian Wang on computer simulations.

Name: Akinduro, Tolulope
Worked for more than 160 Hours: Yes
Contribution to Project:

Technician, Programmer

Other Participant

Research Experience for Undergraduates

Organizational Partners

Other Collaborators or Contacts

Cyrus Umrigar (Co-PI) has the following collaborations:

a) Harold Baranger, Weitao Yang and Amit Ghosal at Duke, on disordered dots and on the transition from the weakly correlated to the strongly correlated regime. Harold and Weitao are faculty in physics and chemistry, respectively. Amit is a postdoc in physics.

b) Jainendra Jain and Gun-San Jeon (faculty and postdoc at Penn State) on using composite fermion wave functions, originally developed by Jain for the fractional quantum Hall effect to construct many-body wave functions for quantum Monte Carlo calculations of planar dots.

c) John Lawson and Charlie Bauschlicher at NASA, Ames, on studing the adsorption of molecules on nanotubes.

d) Francesco Pederiva, Enrico Lipparini and Omar Berto in Trento, Italy. First two are both physics faculty, Omar is a student.
The project is on spin response of quantum dots

e) John Wilkins at Ohio State and Richard Hennig in Materials Science at Cornell high-pressure phases of Si and defects in Si.

f) Kevin Leung and Peter Schultz at Sandia. Spin states of transition metal ions and ligand interactions.

g) Claudia Filippi, faculty in Leiden, Holland. Optimization of many-body wave functions by energy minimization.

h) Zhiyong Zhang, research associate at Stanford University. Adsorbtion of hydrogen on benzene.

a),b),c) d) are on low-dimensional systems and therefore relevant to the grant.

e),f) are on 3D systems and therefore possibly not relevant to the grant.

g) is a significant methodological improvement, relevant to any system.

Mei-Yin Chou has the following collaborators:

Tai C. Chiang, University of Illinois at Urbana-Champaign
Ken Shih, University of Texas, Austin
C. M. Wei, Institute of Physics, Academia Sinica, Taiwan
Klaus Yvon, University of Geneva, Switzerland
Kai-Ming Ho, Iowa State University and Ames Laboratory
Cai-Zhuang Wang, Ames Laboratory

Activities and Findings

Research and Education Activities: (See PDF version submitted by PI at the end of the report)

Findings: (See PDF version submitted by PI at the end of the report)

Training and Development:
The students and postdocs have acquired experience in high-performance computer simulations and software development, including the areas of parallel computer architecture, fortran 90 coding, and materials theory. In particular, they are developing skills in using computers for performing atomistic simulations of nano-wire systems.

In addition, the students and postdocs are encouraged to present their work at national and regional scientific meetings:

Igor Romanovsky (graduate student), Xinyuan Zhao (postdoc), and Wolfgang Geist (postdoc) presented their work at the American Physical Society meeting, Austin, Texas, March 2003.

R. Musin (postdoc) made a presentation at the 55th Southeast Regional Meeting of the American Chemical Society, Nov. 16-19, 2003.

Devrim Guclu, Xinyuan Zhao, and Wolfgang Geist (postdocs)gave a contributed talk at the APS March in Montreal, 2004.

Li Yang (graduate student), Devrim Guclu (postdoc), Igor Romanovsky (graduate student), and Yuesong Li (graduate student) presented the results at the APS March meeting in Los Angeles, 2005.

Devrim Guclu and Julien Toulouse (postdocs) gave contributed talks at the APS March in Baltimore, 2006.

Jia-An Yan, Wen-Ying Ruan and Julien Toulouse(postdocs) gave contributed talks at the APS March in Denver, 2007.

Julien Toulouse (postdoc) gave invited talks at the 18th Annual Workshop on Recent Developments in Electronic Structure Methods at Ohio State, June 2006 and at the CECAM workshop on Advances in Continuum Quantum Monte Carlo Methods, Lyon, Aug., 2007.

Jia-An Yan and Wen-Ying Ruan (postdocs) gave contributed talks at the APS March in New Orleans, 2008.

Alexis Nduwimana (graduate student) gave a poster presentation at the 21th Annual Workshop on Recent developments in Electronic Structure Methods, Urbana-Champaign, Illinois, June 2008.

Olayinka Ogunro (graduate student) gave a poster presentation at the 2008 ISSSR Conference, Hoboken, New jersey, June 2008.

Outreach Activities:

Mei-Yin Chou (PI) worked with an REU student in summer 2003 and 2005. She is also hosting an intern from Atlanta Girls High School.

The training and support of minority graduate students is an important component of the project. Under this project, full and partial support has been provided to four (4) minority graduate students.

We held a mini-workshop (Nov. 2003) on Simulation of Alloys at Clark Atlanta University. Four minority students (Nduwimana, Cupid, Cochran, Robinson) attended the 2-day miniworkshop and have hands-up experience for Monte-Carlo calculations, simulated annealing, universal energy relations, etc.

Anthony Cochran attended the 2004 Annual Conference of the National Society of Black Physicists and Black Physics Students held at Washington D. C., Feb. 18-21, 2004.

A seminar series introducing the application of information technology to minority students is being run at Clark Atlanta University.

Chou and Umrigar serve on the steering committee of the annual 'Recent developments in electronic structure methods' workshop. The 2005 workshop was held at Cornell University, and Umrigar was the local organiser, along with Tomas Arias and Garnet Chan.

U. Landman delivered a few public lectures that were attended audiences from all walks of life, as well as lectures to civic and non-profit organizations.

Cyrus Umrigar taught quantum Monte Carlo methods at three summer and winter schools:
1) 'Quantum Monte Carlo from Minerals and Materials to Molecules', July 9-19, 2007, University of Illinois at Urbana-Champaign
2) 'Quantum Monte Carlo Methods in Physics and Chemistry', winter school at the International Center for Theoretical Physics, Trieste, Jan 21 - Feb. 1, 2008
3)CAMD summer school on 'Electronic Structure Theory and Materials Design', Lyngby, Denmark, August 17-29, 2008.
He was one of the organizers of the school in Trieste.

Journal Publications

A. Nduwimana, X. G. Gong and X. Q. Wang, "Relative Stability of Missing-Row Reconstructed (110) Surfaces of Noble Metals", Applied Surface Science, p. 129, vol. 219, (2003). Published,

I. Krive, I. Romanovsky, E.N. Bogachek and U. Landman, "Phase-Controlled Force and Magnetization Oscillations in Superconducting Ballistic Wires", Phys. Rev. Lett., p. 126802, vol. 92, (2004). Published,

X.Zhao, C. M. Wei, L. Yang, and M. Y. Chou, "Quantum Confinement and Electronic Properties of Silicon Nanowires", Phys. Rev. Lett., p. 236805, vol. 92, (2004). Published,

C. M. Chang and M. Y. Chou, "Alternative Low-Symmetry Structure for 13-Atom Metal Clusters", Phys. Rev. Lett., p. 133401, vol. 93, (2004). Published,

C. R. Handy and X. Q. Wang, "Spectral Bounds for the PT-breaking Hamiltonian", J. Phys. A, p. 11513, vol. 36, (2003). Published,

J. Gegella, G. Japaridze, and X. Q. Wang, "Power Counting in Relativistic Perturbation Theory", J. Phys. G, p. 2303, vol. 39, (2003). Published,

M. H. Upton, C. M. Wei, M. Y. Chou, T. Miller, and T.-C. Chiang, "Thermal Stability and Electronic Structure of Pb Films on Si(111)", Phys. Rev. Lett., p. 026802, vol. 93, (2004). Published,

Robert N. Barnett, Hannu Hakkinen, Andrew G. Scherbakov, and Uzi Landman, ""Hydrogen Welding" and "Hydrogen Switches" in a Mono-Atomic Gold Nanowire", Nano Lett., p. 1845, vol. 4, (2004). Published,

C.J. Umrigar, Claudia Filippi, "Energy and Variance Optimization of Many-Body Wave Functions", Phys. Rev. Lett., p. 150201, vol. 94, (2005). Published,

Amit Ghosal, C.J. Umrigar, Hong Jiang, Denis Ullmo, Harold U. Baranger, "Interaction Effects in Irregular Quantum Dots: A Quantum Monte Carlo Study", Phys. Rev. B., p. 241306, vol. 71, (2005). Published,

A.D. Guclu, C.J. Unrigar, "The Maximum Density Droplet to Lower Density Droplet Transition in Quantum Dots", Phys. Rev. B., p. 045309, vol. 72, (2005). Published,

R.N. Musin, Xiao-Qian Wang, "Structural and Electronic Properties of Epitaxial Core-Shell Nanowire Heterostructures", Phy. Rev. B., p. 155318, vol. 71, (2005). Published,

O. Ciftja, G. Japaridze, X.Q. Wang, "An Anyon Wave Function for the Fractional Quantum Hall Effect", J. Phys. Condensed Matter, p. 2977, vol. 17, (2005). Published,

I.Romanovsky, C. Yannouleas, and U. Landman, "Crystalline Boson Phases in Harmonic Traps: Beyond the Gross-Pitaevskii Mean Field", Phys. Rev. Lett., p. 230405, vol. 93, (2004). Published,

K. Yvon, G. Renaudin, C. M. Wei, and M.Y. Chou, "Hydrogenation-Induced Insulating State in the Intermetallic Compound LaMg2Ni", Phys. Rev. Lett., p. 066403, vol. 94, (2005). Published,

A. D. Guclu, Gun Sang Jeon, C. J. Umrigar, and J. K. Jain
, "Quantum Monte Carlo study of composite fermions in quantum dots: The effect of Landau-level mixing", Phys. Rev. B
, p. 205327, vol. 72, (2005). Published,

Gun Sang Jeon, A. D. Guclu, C. J. Umrigar, and J. K. Jain,
, "Composite-fermion antiparticle description of the hole excitation in a maximum-density droplet with a small number of electrons", Phys. Rev. B
, p. 245312, vol. 72, (2005). Published,

Arthur H. Edwards, Andrew C. Pineda, Peter A. Schultz, Marcus G. Martin, Aidan P. Thompson, Harold P. Hjalmarson, and Cyrus J. Umrigar
, "Electronic structure of intrinsic defects in crystalline germanium telluride", Phys. Rev. B
, p. 045210, vol. 73, (2006). Published,

X. Zhao, C. M. Wei, L. Yang, and M. Y. Chou, "Reply to Comment on Quantum Confinement and Electronic Properties of Silicon Nanowires", Phys. Rev. Lett., p. 219702, vol. 94, (2005). Published,

A. C. Cancio and M. Y. Chou, "Beyond the Local Approximation to the Exchange-Correlation Energy: the Role of the Laplacian of the Density", Phys. Rev. B (Rapid Communications), p. 081202, vol. 74, (2006). Published,

C.R. Hsing, M. Y. Chou, and T. K. Lee, "Exchange-Correlation Energy in Molecules: A Variational Quantum Monte Carlo Study", Phys. Rev. A, p. 032507, vol. 74, (2006). Published,

L. Yang, C. D. Spataru, S. G. Louie, and M. Y. Chou, "Enhanced Electron-Hole Interaction and Optical Absorption in a Silicon Nanowire", Phys. Rev. B (Rapid Communications), p. 201304, vol. 75, (2007). Published,

C. M. Wei and M. Y. Chou, "Band-Structure Contribution to the Quantum Size Effect in Pb(100) Films", Phys. Rev. B, p. 195417, vol. 75, (2007). Published,

J.-A. Yan, L. Yang, and M. Y. Chou, "Size and Orientation Dependence in the Electronic Properties of Silicon Nanowires", Phys. Rev. B, p. 115319, vol. 76, (2007). Published,

Arthur H. Edwards, Andrew C. Pineda, Peter A. Schultz, Marcus G. Martin, Aidan P. Thompson, Harold P. Hjalmarson, and Cyrus J. Umrigar, "Electronic structure of intrinsic defects in crystalline germanium telluride", Phys. Rev. B, p. 045210, vol. 73, (2006). Published,

Amit Ghosal, A. D. Guclu, C. J. Umrigar, Denis Ullmo, Harold U. Baranger, "Correlation-induced inhomogeneity in circular quantum dots", Nature Physics, p. 336, vol. 2, (2006). Published,

E. R. Batista, J. Heyd, R. G. Hennig, B. P. Uberuaga, R. L. Martin,
G. E. Scuseria, C. J. Umrigar, and J. W. Wilkins, "Comparison of screened hybrid density functional theory to
diffusion Monte Carlo in calculations of total energies of silicon phases and defects", Phys. Rev. B, p. 085411, vol. 75, (2007). Published,

W. Hellmann, R. Hennig, S. Goedecker, C. Umrigar, B. Delley, T. Lenosky, "Questioning the existence of a unique ground state structure for Si clusters", Phys. Rev. B, p. 085411, vol. 08411, (2007). Published,

C. J. Umrigar, Julien Toulouse, Claudia Filippi, S. Sorella, R. G. Hennig,
, "Alleviation of the Fermion-sign problem by optimization of many-body wave functions
", Phys. Rev. Lett.
, p. 110201, vol. 98, (2007). Published,

Julien Toulouse and C. J. Umrigar, "Optimization of quantum Monte Carlo wave functions by energy minimization", J. Chem. Phys., p. 084102, vol. 126, (2007). Published,

R. N. Musin and X. Q. Wang, "Quantum size effect in core-shell structured silicon-germanium nanowires", Phys. Rev. B, p. 165308, vol. 74, (2006). Published,

U. Landman, "Materials by Numbers: Computations as Tools of Discovery", Proc. Nat. Acad. Sci., p. 6671, vol. 102, (2005). Published,

Yeusong Li, C. Yannouleas, U. Landman, "From a few to many electrons in quantum dots under strong magnetic fields: properties of rotating electron crystallites with multiple rings", Phys. Rev. B, p. 075301, vol. 73, (2006). Published,

C. Ellenberger, T. Ihn, C. Yannouleas, U. Landman, K. Ensslin, D. Driscoll, and A.C. Gossard, "Excitation Spectrum of Two Correlated Electrons in a Lateral Quantum Dot with Negligible Zeeman Splitting", Phys. Rev. Lett., p. 126806, vol. 96, (2006). Published,

C. Yannouleas and U. Landman, "Symmetry Breaking and Wigner Molecules in Few Electron Quantum Dots", Physica status solidi (a), p. 1160, vol. 203, (2006). Published,

C. Yannouleas and U. Landman, "Electron and Boson Clusters in Confined Geometries: Symmetry Breaking in Quantum Dots and Harmonic Traps", Proc. Nat. Acad. Sci. (USA), p. 10600, vol. 103, (2006). Published,

I. Romanovsky, C. Yannouleas, L.O. Baksmaty, U. Landman, "Bosonic Molecules in Rotating Traps", Phys. Rev. Lett., p. 090401, vol. 97, (2006). Published,

T. Ihn, C. Ellenberger, K. Ensslin, C. Yannouleas, U. Landman, D. Driscoll, and A.C. Gossard, "Quantum Dots Based on Parabolic Quantum Wells: Importance of Electronic Correlations", Int. J. Mod. Phys. B, p. 1316, vol. 21, (2007). Published,

A. Marchenkov, Z. Dai, C. Zhang, R. N. Barnett, U. Landman, "Atomic Dimer Shuttling and Two-Level Conductance Fluctuations in Nb nanowires", Phys. Rev. Lett., p. 046802, vol. 98, (2007). Published,

L. O. Baksmaty, C, Yannouleas, U. Landman, "Rapidly Rotating Boson Molecules With Long or Short Range Repulsion: An Exact Diagonalization Study", Phys. Rev. A, p. 023620, vol. 75, (2007). Published,

Z. Dai, C. Zhang, R. N. Barnett, A. Marchenkov and U. Landman, "Structural and Transport Peoperties of Nb Nanowires", Physica Status Solidi (a), p. 1712, vol. 204, (2007). Published,

Guclu, AD; Ghosal, A; Umrigar, CJ; Baranger, HU, "Interaction-induced strong localization in quantum dots", PHYSICAL REVIEW B, p. , vol. 77, (2008). Published, 10.1103/PhysRevB.77.04130

Ghosal, A; Gueclue, AD; Umrigar, CJ; Ullmo, D; Baranger, HU, "Incipient Wigner localization in circular quantum dots", PHYSICAL REVIEW B, p. , vol. 76, (2007). Published, 10.1103/PhysRevB.76.08534

Colletti, L; Pederiva, F; Lipparini, E; Umrigar, CJ, "Spin- and charge-density excitations in quantum dots via Quantum Monte Carlo simulation", PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS, p. 2317, vol. 244, (2007). Published, 10.1002/pssb.20067460

Ghosal, A; Guclu, AD; Umrigar, CJ; Ullmo, D; Baranger, HU, "Correlation-induced inhomogeneity in circular quantumdots", NATURE PHYSICS, p. 336, vol. 2, (2006). Published, 10.1038/nphys29

Guclu, AD; Jeon, GS; Umrigar, CJ; Jain, JK, "Quantum Monte Carlo study of composite fermions in quantum dots: The effect of Landau-level mixing", PHYSICAL REVIEW B, p. , vol. 72, (2005). Published, 10.1103/PhysRevB.72.20532

W. Geist and M. Y. Chou, "Variational Calculation of the Depolarization of the Maximum Density Droplet in Two-Dimensional Quantum Dots", Physical Review B, p. 235306, vol. 76, (2007). Published, 10.1103/PhysRevB.73.235306

Jia-An Yan, W. Y. Ruan, and M. Y. Chou, "Phonon Dispersions and Vibrational Properties of Monolayer, Bilayer, and Trilayer Graphene", Physical Review B, p. 125401, vol. 77, (2007). Published, 10.1103/PhysRevB.77.125401

L. Yang, R. N. Musin, X.-Q. Wang, and M. Y. Chou, "Quantum Confinement Effect in Si/Ge Core-Shell Nanowires", Physical Review B, p. 195325, vol. 77, (2007). Published, 10.1103/PhysRevB.77.195325

Li Huang, Ning Lu, Jia-An Yan, M. Y. Chou, Cai-Zhuang Wang, and Kai-Ming Ho, "Size- and Strain-Dependent Electronic Structures in H-Passivated Si [112] Nanowires", Journal of Physical Chemistry C, p. , vol. 112, (2008). Accepted, 10.1021/jp802591v

A. Nduwimana, R. Z. Musin, A. M. Smith, and X.-Q. Wang, "Spatial Carrier Confinement in Core-Shell and Multishell Nanowire Heterostructures", Nano Letters, p. , vol. 8, (2008). Accepted, 10.1021/nl8017725

X.-Q. Wang, "Twinned structure for shape memory: First-principles calculations", Physical Review B, p. 092103, vol. 78, (2008). Published,

X.-Q. Wang, "Structural and electronic properties of conjugated polymer wrapping around carbon nanotubes", Physical Review Letters, p. , vol. , (2008). Submitted,

Y. Wu, Andrey Malkovskiy, Xiao-Qian Wang, Alexei P. Sokolov, Marisabel, Lebron-Colon, Michael A. Meador, Yi Pang, "Polymer Conformation-Assisted Wrapping of Single-Walled Carbon Nanotube: The Impact of cis-Vinylene Linkage", ACS Nano, p. , vol. , (2008). Submitted,

A. Nduwimana and X.-Q. Wang, "Quantum Dipoles in Coaxial Semiconductor Nanowires", Nano Letters, p. , vol. , (2008). Submitted,

O. Ciftja and X.-Q. Wang, "Composite Abelian and Non-Abelian Semions: an Inhomogeneous Quantum Fluid", Journal of Physics: Condensed Matter, p. , vol. , (2008). Submitted,

O. O. Ogunro and X.-Q. Wang, "Charge transfer in noncovalent functionalization of carbon nanotubes", Journal of Chemical Theory and Computation, p. , vol. , (2008). Submitted,

Books or Other One-time Publications

F. Pederiva, M.H. Kalos, F. Reboredo, D. Bressanini, A.D. Guclu, L. Colletti, C.J. Umrigar, "The fixed hypernode method for the solution of the many body Schr\"odinger equation", (2006). Book, Published
Editor(s): Jambes B. Anderson and Stuart Rothstein
Bibliography: Pacifichem Symposium on Quantum Monte Carlo methods

X. Q. Wang, "Structural and Electronic Properties from First-Principles", (2007). Book, Published
Editor(s): Bozzolo, Guillermo; Noebe, Ronald D.; Abel, Phillip B.
Collection: Applied Computational Materials Modeling Theory, Simulation and Experiment
Bibliography: ISBN: 978-0-387-23117-4

Web/Internet Site

URL(s):
http://www.physics.gatech.edu/itr/

http://dcwww.fys.dtu.dk/~bligaard/School08/C_Umrigar_CAMDSchool08.pdf
Description:
This is the home page for this ITR project.

In addition, various talks and computer exercises given at summer/winter schools are available on the internet, e.g.:
http://dcwww.fys.dtu.dk/~bligaard/School08/C_Umrigar_CAMDSchool08.pdf
http://dcwww.fys.dtu.dk/~bligaard/School08/Umrigar_Exercises.pdf

Other Specific Products

Contributions

Contributions within Discipline:
This project aims to advance the state of the art in algorithms for large-scale electronic-structure and atomistic simulations through the study of quantum phenomena in semiconductor structures of reduced dimensions. Electron confinement strongly affects the energy gap, optical absorption, electron-phonon coupling strength, exciton binding energy, and ballistic transport in these nanowires nanostructures. Our calculations of these quantities will shed light on the fundamental characteristics in these low-dimensional systems, where intriguing and sometimes exotic physics properties often occur. Our results will also provide detailed information on the growth and stability of these nanostructures. In addition, the results obtained through our research provide deep insights into the nature of highly correlated electron systems in quantum dots, and as such they are of significance and relevance to solid-state, spin-based, implementations of quantum logic gates, and quantum information.

Contributions to Other Disciplines:
The materials that we are studying have the potential to function as nanoscale devices such as light-emitting diodes, bipolar transistors, logic gates, photodetectors, and biological and chemical sensors. Other applications include integrated electronic and photonic circuits, optical switches, and interconnects, all of which have a substantial impact in future development of computer hardware.

In addition, a nonlinear optimization package written by Peter Nightingale and Cyrus Umrigar is now being used by James Sethna (Cornell faculty) in his research on biological networks.

The QMC methods developed under this project are now being used in a project on the study of deep earth materials. This project is funded jointly by the Earth & Atmospheric Sciences and the Mathematics divisions of the NSF.

Contributions to Human Resource Development:

The students and postdocs have acquired experience in high-performance computer simulations and software development, including the areas of parallel computer architecture, fortran 90 coding, and materials theory. In particular, they are developing skills in using computers for performing atomistic simulations of nano-wire systems.

Two undergraduate students, 15 postdocs and 18 graduate students have been involved in this project, including one female postdoc and three minority graduate students.

Contributions to Resources for Research and Education:

The grant has contributed to the ongoing development [in collaboration with Filippi(ex student, currently faculty in Leiden) and Toulouse (ex postdoc, currently faculty in Paris)] of a flexible and powerful package for doing quantum Monte Carlo calculations, named 'Cornell-Holland Abinitio Materials Package' (CHAMP, http://www.tc.cornell.edu/~cyrus/champ.html). This package is now being used by several collaborators in the US and Europe and recently a group in Japan expressed interest in collaboration, too.

Contributions Beyond Science and Engineering:

Categories for which nothing is reported:

Organizational Partners

Any Product

Contributions: To Any Beyond Science and Engineering

Research:

We are conducting first-principles simulations of the atomic configurations, electronic structure, dynamic properties, and transport in semiconductor nanowires and nanostructures using computational methods based on density functional theory and quantum Monte Carlo approaches. Specific projects include calculations of the band gap and optical properties of various semiconductor nanowires, transport in the presence of aluminum contact electrodes, vibrational and thermal properties of nanostructures, and electron correlation in two-dimensional quantum dots. We have also worked on the formulation of superconductivity-induced contributions to the cohesive energy and elongation-forces in metallic nanowires.

We have worked on the development, implementation and application of theoretical computational methods of high accuracy and efficiency for investigations of the properties of the geometric and spectral properties of highly correlated electrons in semiconductor nano-size two-dimensional lateral quantum dots. These methodologies include quantum Monte Carlo, exact diagonalization and unrestricted hartree-fock with subsequent (post HF) projection techniques. In addition, we have developed a specific method for treating fine trapped bosonic systems, based on a new formulation of an 'Unrestricted Bose Hartree-Fock' (UBHF) technique and applied it to investigation of a crystallization quantum phase-transition of a finite bose condensate.

Regarding the code development, we have extended the DMC program to treat periodic systems and tested it on bulk semiconductors. This will allow us to treat wires that are periodic in one dimension. We find that DMC gives better band gaps than other methods but in general has a tendency to overestimate excitation energies by 10 to 20%. We have also extended the VMC and DMC codes to allow complex wavefunctions and to do fixed-phase calculations.

Collaborations within the project:

1) Georgia Tech and Cornell: Chou and Umrigar are collaborating on the study of electron correlation in two-dimensional semiconductor quantum dots in the presence of a magnetic field. The method of diffusion quantum Monte Carlo is being used with the fixed phase approximation. The focus is on the transition of different spin states and development of electron localization as a function of magnetic field. A manuscript on the transition from the Fermi liquid phase to the Wigner molecule phase as the density varies is in preparation.

2) Georgia Tech and Clark Atlanta University: Chou and Wang are working together on a project studying Ge nanowires. The minority graduate student (Alexis Nduwimana) at Clark Atlanta University working on this project has since joined the Ph.D. program at Georgia Tech. A joined paper of core-shell nanowires has been published.

3) Within Georgia Tech: Chou and Landman are working on the molecular dynamics simulations of melting in Si nanowires.

Education:

These research activities provide educational opportunities for both students and postdocs. Two undergraduate students, 18 graduate students and 15 postdocs have been involved in these efforts. Uzi Landman taught a one-semester special course on 'The Physics of Small Systems' at Georgia Tech in Spring 2003-2008, which attracted a significant number of local students.

Invited talks and contributed lectures and posters at national and international meetings:

Contributed talk (X. Q. Wang), Applied Surface Modeling, Experiment, Theory, and Simulations, Cleveland, Ohio, August 2002.

Plenary talk (U. Landman), APS Computational Physics Conference, San Diego, August 2002.

Plenary talk (U. Landman), ISSPIC11, Strasburg, France, September 2002.

Invited talk (C. J. Umrigar), 'Time-evolution operators, with and without the fixed-node approximation', CECAM Workshop on The Diffusion Monte Carlo Method, Lyon, France, 19-21 September 2002.

Keynote speech (U. Landman), TNT 2002 (Trends in Nanotechnology), Santiago de Compostella, Spain, September 2002.

Keynote speech (U. Landman), Cabrerra Summer School, Miaflores, Spain, September 2002.

Invited talk (M. Y. Chou), NSF Workshop on Opportunities in Materials Theory, Washington D.C., October 2002.

Contributed talk (X. Q. Wang), Annual Conference of the National Society of Black Physicists and Black Physics Students, Atlanta, GA, February 2003.

Four contributed talks (C. Umrigar, I. Romanovsky, X. Zhao, and W.Geist), APS meeting, Austin, Texas, March 2003.

Invited talk (U. Landman), Conference on Cluster and Nanoscale Science, Nanjing University, Nanjing, China, March 2003.

Keynote speech (U. Landman), Opening Ceremony of the Nano-Characterization Center, The Hebrew University, Jerusalem, Israel, April 2003.

Invited talk (M. Y. Chou), 'Electronic Quantum Size Effects in Metal Thin Films', 15th Annual Workshop in Electronic Structure Methods, Minneapolis, Minnesota, May 2003.
Plenary talk (U. Landman), Conference on Perspectives in Nanotechnology, Berlin, May 2003.

Invited talk (U. Landman), 3rd Stig Lunquist Symposium on Modern Trends in Condensed Matter Systems, Trietse, Italy, August 2003.

Invited talk (Cyrus Umrigar), 'Diffusion Monte Carlo study of excitation energies in solids and quantum dots', American Chemical Society National Meeting, New York City, 7-11 September, 2003.

Invited talk (Cyrus Umrigar), 'Quantum Monte Carlo study of quantum dots', Workshop on computational approaches towards the electronic properties of quantum dots, Chicago, 22-24 September, 2003.

Invited talk (U. Landman), Trends in NanoTechnology, Salamanca, Spain, September 2003.

Keynote speaker (U. Landman), Modeling of Nanosystems, Barcelona, October 2003.

Invited talk (U. Landman), Workshop on Modeling and Simulations, Brasilia, Brazil, December 2003.

Invited talk (U. Landman), Conference on Clusters and Nanostructures, Institute for Molecular Science, Okazaki, Japan, December 2003.

Invited talk (M. Y. Chou), APS March meeting, Montreal, March 2004.

Four contributed talks (A. D. Guclu, X. Zhao, R. Barnett, and W. Geist), APS meeting, Montreal, Canada, March 2004.

Invited talk (M. Y. Chou), Workshop on Methods in Computational Science, National Science Foundation, San Francisco, April 2004.

Invited talk (U. Landman), 'N+N – US/UK Computational Science Workshop,' Washington, D.C., April 2004.

Invited talk (M. Y. Chou), International Conference on Physics Education and Frontier Research, Shanghai, June 2004.

Invited talks (3) (U. Landman), ICTP School on Nanoscience, Trieste, Italy, June 2004.

Invited talk (U. Landman), Electronic Structure Simulations of Nanostructures 2004 – ESSN04, Jyvaskyla, Finland, June 2004.

Invited talk (M. Y. Chou), Asian/Pacific Regional School on Electronic Structure Methods and their Applications, Beijing, July 2004.

Invited talk (X. Q. Wang), 'Multiscale simulations for shape memory alloys', Glenn Research Center's HBCUs/OMUs Research Conference, July 2004.

Invited talk (C. J. Umrigar), Workshop on 'Electronic Structure Beyond Density Functional Theory', Leiden, Holland, July 2004.

Keynote lecture (M. Y. Chou), Fifth 'Trends in NanoTechnology' International Conference (TNT2004), Segovia, Spain, September 2004.

Plenary talk (U. Landman), ISSPIC 12, Nanjing, China, September 2004.

Keynote lecture (U. Landman), Conference on Nanoscience, Lanzhou, China, September 2004.

Keynote speaker (U. Landman), Kiwanis Club, Atlanta, October 2004.

Keynote speaker (U. Landman), Leadership Atlanta, Atlanta, October 2004.

Invited talk (C. J. Umrigar), Workshop on the Advances in Computational Many-Body Theory, Banff, January 2005.

Keynote lecture (U. Landman), 'North-South Nanotechnology Symposium', UNIDO, Trieste, February 2005.

Keynote lecture (U. Landman), 'Nanotechnology Symposium 2005', AAAS Annual Meeting, Washington D.C., February 2005.

Poster (R. N. Musin), 'Structural and electronic properties of core-shell nanowire heterostructures', ACS 229 National Meeting, Division of Physical Chemistry, San Diego, March 2005.

Invited talk (U. Landman), Symposium on Computations, Pre-March Meeting, DCOMP/ APS, Los Angeles, March 2005.

Invited talk (U. Landman), 'Rahman Prize Lecture', APS March Meeting, Los Angeles, March 2005.

Poster (T. Yarahmad), 'Multiscale modeling of materials', CAEFF at Clemson University, April 2005.

Invited talk (C. J. Umrigar), 'Correlations in quantum dots', Ab-initio simulation methods beyond density functional theory, CECAM, Lyon, France September 23-25, 2005.

Keynote lecture (U. Landman), Sixth 'Trends in NanoTechnology' International Conference (TNT2005), Keynote Lecture, Oviedo, Spain, September 2005.

Invited talk (M Y. Chou), Sixth 'Trends in NanoTechnology' International Conference (TNT2005), Keynote Lecture, Oviedo, Spain, September 2005.

Invited talk (U. Landman), 'Workshop on Multiscale Methods', Institute for Pure and Applied Mathematics (IPAM), UCLA, Los Angeles, October 2005.

Invited talk (U. Landman), Trends in Nanoscience, Irsee, Germany, October 2005.

Invited talk (M Y. Chou), Fall Meeting of the Materials Research Society, Boston, November 2005.

Invited talk (C. J. Umrigar), 'Optimization of nodes of many-body wave functions', International Chemical Congress of Pacific Basin Societies, Honolulu, December 15-20, 2005.

Distinguished lecturer (U. Landman), Simons Foundation, Stony Brook, NY, October 2005.

Invited talk (M Y. Chou), GE Computational Techniques for Nano-scale Physics Symposium, Niskayuna, New York, January 2006.

Invited talk (M Y. Chou), APS March Meeting, Baltimore, Maryland, March 2006.

Keynote lecture (U. Landman), ICONSAT (International Conference on Nano Science and Technology), New Delhi, India, March 2006.

Invited talk (C. J. Umrigar), 'Systematic elimination of fixed-node error by optimization of nodes of many-body wave functions', New Developments in Quantum Monte Carlo, Tempe, Arizona, May 14-17, 2006.

Invited talk (U. Landman), 50 Years Jubilee Conference on Nano Science and Technology, Bar-Ilan University, Ramat Gan, Israel, May 2006.

Invited talk (C. J. Umrigar), 'Systematic elimination of fixed-node error by optimization of nodes of many-body wave functions', Recent Developments in Electronic Structure Methods, Ohio State University, June 2006.

Invited talk (Julien Toulouse), 'Multideterminantal density functional theory', Recent Developments in Electronic Structure Methods, Ohio State University, June 2006.

Invited talk (M Y. Chou), The 18th Annual Workshop on Recent Developments in Electronic Structure Methods, Columbus, Ohio, June 2006.

Plenary talk (M. Y. Chou), International Conference on Physics Education and Frontier Research, Taipei, Taiwan, June 2006.

Invited talk (X. Q. Wang, D. Cupid, and O. Sowemino), 'Electronic structures of shape memory alloys', NASA Glenn Research Center, HBCU/MI Research Conference, Cleveland Ohio, July 2006.

Poster (A. H. Smith, M. Bellamy, and X. Q. Wang), 'Quantum phenomena in nanowires', NASA Glenn Research Center, HBCU/MI Research Conference, Cleveland Ohio, July 2006.

Invited talk (U. Landman), International Conference on Nanoscience and Technology, Basel, Switzerland, July-August 2006.

Contributed talk (A. H. Smith, M. Bellamy, and X. Q. Wang), 'Quantum confined states and charge separations in nanowires', Morehouse College, Third International Conference on Neural, Parallel, and Scientific Computations, Morehouse College, Atlanta, August 9-12, 2006.

Invited talk (C. J. Umrigar), 'Energy optimization of many-body wave functions', Density functional theory meets strong correlation, Brookhaven National Laboratory, September 5-8, 2006.

Keynote lecture (U. Landman), TNT 2006, Grenoble, France, September 2006.

Invited talk (U. Landman), Multiscale Modeling, Freiburg, Germany, September 2006.

Invited talk (U. Landman), Donaldson Lectures, University of Minnesota, Minnesota, September 2006.

Invited talk (U. Landman), Workshop on 1D Nanostructures, MPI Schloss Ringberg, Germany, October 2006.

Invited talk (C. J. Umrigar), 'Energy optimization of many-body wave functions', Mathematical and Numerical Aspects of Quantum Chemistry Problems', Oberwolfach, Germany, October 22-28, 2006.

Invited talk (M Y. Chou), Symposium on the Physics and Chemistry of Metallic Quantum Sized Films and Related Nanostructures, Hong Kong, November 2006.

Plenary talk (C. J. Umrigar), 'Quantum Monte Carlo study of correlations in planar quantum dots in magnetic fields', International Workshop on Computational Methods for Nanoscale Systems, Hong Kong, China, December 11-13, 2006.

Invited talk (M Y. Chou), U.S.-Taiwan Joint Workshop on Frontiers in Nanoscience, Taipei, December 2006.

Invited talk (U. Landman), U.S.-Taiwan Joint Workshop on Frontiers in Nanoscience, Taipei, December 2006.

Plenary talk (U. Landman), 6th EBASI (Edward Bouchet Abdus Salam Institute) Conference, Cape Town, South Africa, January 2007.

Plenary talk (U. Landman), USA-Africa Workshop on Nanoscience, Cape Town, South Africa, January 2007.

Invited talk (C. J. Umrigar), 'Quantum Monte Carlo methods for correlated systems, Correlation Issues in Electronic Structure Calculations, Sapporo, Japan, Feb. 14-17, 2007.

Contributed talk (R. N. Musin and X. Q. Wang), 'Core-shell structured nanowires: Charge distribution and band offsets', The 233rd ACS National Meeting, Chicago, IL, March 25-29 (2007).

Keynote lecture (U. Landman), 'Trends in Nanotechnology (TNT) '07', San Sebastian, Spain, September 2007.

Invited talk (U. Landman), 'African Regional College on Science at the Nanoscale', Cape Town, South Africa, November 2007.

Plenary talk (U. Landman), 'Nanoscience and Technology Conference', Dublin, Ireland, December 2007.

Minority postdoctoral researcher and graduate students supported

An important component of the project involves the support, training, and mentoring of underrepresented minority students. We have made an effort to recruit, train, and support minority students for participation in the research projects. Two African American students (Alexis Nduwimana and Olayinka Ogunro) participated in this project. One of them, Dr. Alexis Nduwimana, joined the Clark Atlanta group as a postdoc after graduation. Both of them have been presenting the research results at conferences.

a) Umrigar and Filippi have developed a simple, robust and efficient method for constructing many-body wave functions by optimizing the expectation value of the energy. The basic idea is to add terms to the straightforward expression for the Hessian of the energy that have zero expectation value, but that cancel much of the statistical fluctuations for a finite Monte Carlo sample. The method was tested on two systems. For the smaller one it resulted in more than 3 orders of magnitude gain in efficiency compared to a straightforward implementation of the Newton method (a method used by some researchers), and, for the larger system it resulted in 5 orders of magnitude gain in efficiency.

b) Ghosal, Umrigar, Jiang, Ullmo and Baranger have studied interaction effects in irregular quantum dots. They find that that in comparison to LSDA, DMC predicts a somewhat larger spin gap and a stronger even/odd effect in the addition spectra.

c) Guclu and Umrigar have demonstrated that Jastrow factors are a very efficient way to include Landau-level mixing in wave functions for quantum dots in magnetic fields. For large numbers of electrons or for very high angular momentum states even the number of determinants in the first Landau level can be very large. In this case, Guclu, Jeon, Umrigar and Jain have shown that composite fermion wave functions (times a Jastrow factor) are a highly efficient and accurate alternative to first Landau-level wave functions.

d) Calculations that we have performed for two electrons in an elliptic quantum dot, using symmetry breaking at the unrestricted Hartree-Fock level and subsequent restoration of the broken parity via projection techniques, have shown that the electrons can localize and form a molecular dimer, described by a Heitler-London type wave function. The calculated singlet-triplet splitting (J) as a function of the magnetic field (B) agrees with cotunneling measurements. Knowledge of the dot shape and of J(B) allows determination of the degree of entanglement in the ground state of the dot, which is of interest for the implementation of quantum logic gates and in the field of quantum information. The theoretical value agrees with the experimental estimates.

e) We have shown that a supersolid phase, exhibiting simultaneously solid and superfluid behavior, properly describes the finite electron crystallites that form in two-dimensional quantum dots under high magnetic fields. These crystallites rotate already in their ground state and exhibit a nonclassical rotational inertia. They are precursors to a supersolid crystal in the lowest Landau level. We use exact numerical diagonalization, calculations employing analytic many-body wave functions, and a newly derived analytic expression for the total energies that permits calculations for arbitrary number of electrons.

f) Strongly-interacting bosons in two-dimensional harmonic traps were treated by us through a method that allows breaking of rotational symmetry at the Hartree-Fock level and subsequent symmetry restoration via projection techniques, thus incorporating correlations beyond the Gross-Pitaevskii (GP) solution. The bosons localize and form polygonal-ringlike crystalline patterns, both for a repulsive contact potential and a Coulomb interaction, as revealed via conditional-probability-distribution analysis. For neutral bosons, the total energy of the crystalline phase saturates in contrast to the GP

solution, and its spatial extent becomes smaller than that of the GP condensate. For charged bosons, the total energy and dimensions approach the values of classical pointlike charges in their equilibrium configuration. These results predict a quantum phase-transition for two-dimensional trapped Boson systems, and are thus the analogue of the 1D Tonk-Girardeau gas-to-crystal phenomenon. We trust that our result will provide the impetus for experimental verification of our predictions.

g) We investigate the structural, electronic, and optical properties of hydrogen-passivated silicon nanowires along [110] and [111] directions with diameter d up to 4.2 nm from first principles. The size and orientation dependence of the band gap is investigated and the local-density gap is corrected with the GW approximation. Quantum confinement becomes significant for d < 2.2 nm, where the dielectric function exhibits strong anisotropy and new low-energy absorption peaks start to appear in the imaginary part of the dielectric function for polarization along the wire axis.

h) We have extended our new wave function optimization method to optimize both the Jastrow and the determinantal parameters simultaneously. This allows one to systematically reduce the fixed-node error to the point that it is negligible for many systems. It is impossible to predict the magnitude of this error in advance, e.g. if the determinantal part of the wave function is the best possible single determinant then the fixed-node error is only 0.05 eV for Si_2 but 1 eV for C_2! Employing 120 determinants for C_2 in the new optimization method results in perfect agreement with experiment. This development is an important advance not only for the nanosystems that are the subject of this grant, but also for essentially all quantum Monte Carlo computations.

i) In collaboration with the Baranger group we have studied loocalization in 2-dimensional planar quantum dots for r_s upto 60. The correlation-induced inhomogeneities appear to be quite different from that in the bulk. First, the absence of translational symmetry in the radial direction introduces radial localization of the electrons in rings well before individual electrons localize. Second, the transition between the weak and strong correlation regimes is surprisingly broad. Third, some spin excitations become very low in energy, but in general we find that Hund's first rule is quite robust. Fourth, in the addition energy, which is the observable that is most readily accessible in experiments, there is a clear cross-over from shell structure to classical features caused by the localized electrons.In order to get these results we took advantage of our new optimization methods developed in a) and h) and we developed a new floating Gaussian form of the wave function.

j) We have carried out first-principles calculations of Pb(100) films up to 22 monolayers to study variations in the surface energy and work function as a function of film thickness. An even-odd oscillation is found in these two quantities, while a jellium-like model for this s-p metal predicts a periodicity of about three monolayers. This unexpected result is explained by considering a coherent superposition of contributions from quantum-well states centered at both the Gamma and M points in the two-dimensional Brillouin zone, demonstrating the importance of crystal band structure in studying the quantum size effect in metal thin films.

k) We have studied the correlated electron-hole states in semiconductor nanowires and their influence on the optical absorption spectrum. Calculations are performed for a hydrogen-passivated silicon nanowire of a diameter of 1.2 nm. The quasiparticle states are calculated employing a many-body Green's function approach within the GW approximation to the electron self-energy, and the effects of the electron-hole interaction to optical excitations are evaluated by solving the Bethe-Salpeter equation (BSE). The enhanced Coulomb interaction in this confined geometry results in an unusually large binding energy (1-1.5eV) for the excitons, which dominate the optical absorption spectrum. Our results predict general features in the optical absorption spectrum of semiconductor nanowires that may impact future applications of these nanostructures.

l) Chou and Wang have collaborated on the studies of quantum confinement and charge separation of nanowires The electronic structure of Si/Ge core-shell nanowires along the [110] and [111] directions are studied with first-principles calculations. We identify the near-gap electronic states that are spatially separated within the core or the shell region, making it possible for a dopant to generate carriers in a different region. The confinement energies of these core and shell states provide an operational definition of the "band offset", which is not only size dependent but also component dependent. The optimal doping strategy in Si/Ge core-shell nanowires is proposed based on these energy results.

m) We further considered the strain effects on the core-shell and multishell heterostructures. We have investigated two prototype semiconductor nanowires with type-II band alignments: Ge/Si with a 4 % lattice mismatch and GaN/GaP with a 20 % mismatch. We have derived an analytical effective-mass model and employed first-principles density functional theory to study the spatial confinement of carriers in core-shell and multishell structured semiconductor nanowires. The band offset is analyzed based on the subband charge density distributions, which is strongly dependent upon the strain relaxation. First-principles calculation results for spatially confined Si/Ge and GaN/GaP nanowires indicate accumulation of a Ge-core hole gas and a GaN-core electron gas, respectively, in agreement with experimental observations.

n) We have derived an analytical fermion wave function for the fractional quantum Hall states at filling factor 2/(4p+1). The lowest Landau level fermion wave function is a composite of a Laughlin-type Abelian semion and a charge neutral non-Abelian semion, along with 2p flux attachment. Monte Carlo simulations for the quantum Hall state at 2/5 show that the ground-state energy of the composite semion wave function is not only lower than Jain's composite fermion one, but also lower than the energy of a Laughlin-type semion wave function. This wave function describes an inhomogeneous quantum fluid and represents a bound fermion state of composite semions. The composite semions wave function is based on the use of a so-called Schur's Pfaffian which is charge neutral for a 2D electronic system. The properties of the resultant inhomogeneous quantum fluid system have been studied with use of intensive Monte Carlo calculations.