

Final Report for Period 9/15/2003 to 11/15/2009

Grant Number: DE-FG02-03ER46095
DOE Computational Nanoscience Project:
Integrated Multiscale Modeling of Molecular Computing Devices

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1. BACKGROUND

Nanoscience has been one of the major research focuses of the U.S. and much of the world for the past decade, in part because of its promise to revolutionize many fields, including materials, medicine, and electronics. At the heart of this promise is the fact that nanostructured materials can behave radically differently than their macroscopic counterparts (e.g., bulk gold is such an inert metal that it has found applications in such diverse fields as jewelry, biomedical implants and dentistry, whereas gold nanoparticles are highly reactive and are thus useful as nanocatalysts) and have properties that are tunable due to a strong dependence on the size and surface area of the nanostructure. Thus, nanoscience offers a remarkable opportunity to develop new functional systems built around nanostructured materials with unusual and tunable properties and functionality.

The transition from nanoscience to nanotechnology becomes possible when nanostructured systems can be made reproducibly by processes that can be implemented on a large scale. The microelectronics industry is one example of an industry that has evolved into the realm of nanotechnology, since the exponential reduction in feature size in computer chips has resulted in feature sizes now under 50nm (45nm in production, 32nm demonstrated; feature size has been going down by a factor of approximately $1/\sqrt{2}$ every 18 months as chip density has doubled every 18 months according to Moore's law). Silicon-based microelectronics relies on etching features into a single-crystal silicon substrate by photolithography. As the feature size of silicon-based microelectronics continues to decrease, the continuation of Moore's law to below 20nm feature sizes is being questioned, due to limitations in both the physics of the transistors (leading to unacceptable power dissipation) and doubts about the scalability of top-down photolithography-based manufacturing to such small sizes.

There is no doubt that photolithography will some day reach a miniaturization limit, forcing designers of Si-based electronics to pursue increased performance by other means. Any other alternative approach would have the unenviable task of matching the ability of Si technology to pack more than a billion interconnected and addressable devices on a chip the size of a thumbnail. Nevertheless, the prospects of developing alternative approaches to fabricate electronic devices have spurred an ever-increasing pace of fundamental research. One of the promising possibilities is molecular electronics (ME), self-assembled molecular-based electronic systems composed of single-molecule devices in ultra dense, ultra fast molecular-sized components. This project focused on developing accurate, reliable theoretical modeling capabilities for describing molecular electronics devices. The participants in the project are given in Table 1.

2. OUTCOMES

The primary outcomes of this fundamental computational science grant are publications in the open scientific literature. As listed below, 62 papers have been published from this project. In addition, the research has also been the subject of more than 100 invited talks at conferences, including several plenary or keynote lectures. Many of the goals of the original proposal were completed. Specifically, the multi-disciplinary group developed a unique set of capabilities and tools for investigating electron transport in fabricated and self-assembled nanostructures at multiple length and time scales.

Table 1: Project participants. Key: AM = Applied Mathematics; CE = Chemical Engineering; CSM = Computer Science and Mathematics Division; M = Mathematics; P = physics

Institution	Name	Project Role
Vanderbilt University (VU)	Peter T. Cummings (PI), CE	Atomistic and mesoscale simulation, non-equilibrium methods, self-assembly
	Sokrates T. Pantelides, P	Quantum transport in nano devices and the connection to macroscopic electrodes
	Ron Schrimpf, EECE	Transition from nanoscale devices to engineering-level device/circuit modeling
North Carolina State University (NCSU)	Jerzy Bernholc, P	Multigrid electronic structure, $O(N)$ methods, quantum transport, multiscale, parallel computing
	Marco Buongiorno Nardelli, P	Quantum transport, optimized localized orbitals, electronic structure of nanoscale systems
Oak Ridge National Laboratory (ORNL)	Robert Harrison, CSM	Algorithms for large-scale electronic structure calculations, multiresolution methods
	George I Fann, CSM	Fast, $O(N)$, spectrally accurate, multiwavelet methods for computational chemistry
	Xiaoguang Zhang, CSM	Multiple scattering theory and Green's function method
	Vincent Meunier, CSM	Semi-empirical and first principles studies of nanoscopic materials
	Bryan Hathorn, CSM	Time-scale-spanning methods for atomistic simulations; Monte Carlo methods
	Phani Kumar Nukala, CSM	Multiscale methods in materials modeling
Princeton University (PU)	Weinan E., M and AM	Scale-spanning materials modeling, stochastic differential equations, complex energy landscapes
University of Colorado (CU)	Gregory Beylkin, AM	Multiresolution analysis, wavelet methods, non-uniform fast fourier transform
University of Michigan (UM)	Sharon Glotzer, CE	Atomistic and mesoscale materials modeling, hybrid materials, nano-interfaces
University of Tennessee Knoxville (UTK)	Tim Schultze, M	Kinetic Monte Carlo and related time-coarsening methods; mathematical analysis

Table 2. Publications from grant DE-FG02-03ER46095.

<ol style="list-style-type: none"> Hernandez, E., Meunier, V., Smith, B. W., Ruruli, R., Terrones, H., Nardelli, M. B., Terrones, M., Luzzi, D. E. and Charlier, J. C., "Fullerene coalescence in nanopeapods: A path to novel tubular carbon," Nano Letters, 3, 1037-1042 (2003). Krstic, P. S., Dean, D. J., Zhang, X. G., Keffer, D., Leng, Y. S. and Cummings, P. T., "Computational chemistry for molecular electronics," Computational Materials Science, 28, 321-341 (2003). Leng, Y. S., Keffer, D. J. and Cummings, P. T., "Structure and dynamics of a benzenedithiol monolayer on a Au(111) surface," J. Phy. Chem. B, 107, 11940-11950 (2003). Bernholc, J., Nardelli, M. B., Lu, W. C., Meunier, V., Nakhmanson, S. M. and Zhao, Q., "Simulations of nanotube-based structures and devices," In Foundations of Nanoscience 2004: Proceedings of Self-Assembled Architectures and Devices. Snowbird Cliff Lodge, Snowbird, UT, April 21-23, 2004.; J. Reif, Ed.; ScienceTechnica: 2004; pp 367-372. Bernholc, J., Nardelli, M. B., Lu, W. C., Meunier, V., Nakhmanson, S. M. and Zhao, Q., "Large-scale quantum-mechanical simulations of nanoscale devices and new materials," In Users Group Conference (DOD-UGC '04); R. E. Peterkin, Ed.; IEEE Computer Society: 2004; pp 34.

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