Final Report of the DOE grant:
Integrated Multiscale Modeling of Molecular Computing Devices

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1. Summary of progress. The main bottleneck in modeling transport in molecular devices is to develop the correct formulation of the problem and efficient algorithms for analyzing the electronic structure and dynamics using, for example, the time-dependent density functional theory. We have divided this task into several steps. The first step is to developing the right mathematical formulation and numerical algorithms for analyzing the electronic structure using density functional theory. The second step is to study time-dependent density functional theory, particularly the far-field boundary conditions. The third step is to study electronic transport in molecular devices. We are now at the end of the first step.

Under DOE support, we have made subtantial progress in developing linear scaling and sub-linear scaling algorithms for electronic structure analysis. Although there has been a huge amount of effort in the past on developing linear scaling algorithms, most of the algorithms developed suffer from the lack of robustness and controllable accuracy. We have made the following progress:

1. We have analyzed thoroughly the localization properties of the wavefunctions. We have developed a clear understanding of the physical as well as mathematical origin of the decay properties. One important conclusion is that even for metals, one can choose wavefunctions that decay faster than any algebraic power.

2. We have developed algorithms that make use of these localization properties. Our algorithms are based on non-orthogonal formulations of the density functional theory. Our key contribution is to add a localization step into the algorithm. The addition of this localization step makes the algorithm quite robust and much more accurate. Moreover, we can control the accuracy of these algorithms by changing the numerical parameters.

3. We have considerably improved the Fermi operator expansion (FOE) approach. Through pole expansion, we have developed the optimal scaling FOE algorithm.

2. Student support: Two graduate students (Lin Lin and Jianfeng Lu) and two visitors (Weiguo Gao and Lexing Ying).

3. Talks: The work was the main topic discussed in my invited lecture at the International Congress of Industrial and Applied Mathematics in Zurich in July of 2007.

4. Publications:

W. E and J. Lu, "The continuum limit and QM-continuum approximation of quantum mechanical models of solids," *Comm. Math. Sci.*, vol. 5, no. 3, pp. 679-696, 2007.

W. E and J. Lu, "The elastic continuum limit of the tight binding model," *Chinese Ann. Math. Ser. B*, vol. 28, no. 6, pp. 665-676, 2007.

C. Garcia-Cervera, J. Lu and W. E, "A sub-linear scaling algorithm for computing the electronic structure of materials", *Comm. Math. Sci.*, vol. 5, No. 4, 999-1026, 2007.

L. Lin, J. Lu, L. Ying, R. Car and W. E, "Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems," *Comm. Math. Sci.*, vol. 7, pp. 755–777, 2009.

L. Lin, J. Lu, R. Car and W. E, "Multipole representation of the Fermi operator with application to electronic structure analysis of metallic systems," *Phys. Rev. B*, vol. 79, no. 11, pp. 115133–115113-10, 2009.

W. Gao and W. E "Orbital minimization with localization," *Discrete and Continuous Dynamical Systems*, vol. 23, no. 1-2, pp. 249–264, 2009.