Very Large Scale MNDO-Like SCF Calculations

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A massively parallel SCF-program, EMPIRE, has been designed from scratch to allow full SCF calculations on up to 50,000 atoms on 1,000 cores. The program has exceeded its designed performance and has been used for up to 76,000 atoms. The program does not at present use linear scaling techniques, but performs the complete NDDO-SCF calculation without additional cutoffs or approximations in order to provide a benchmark for linear-scaling techniques. The design principles and implementation will be described and performance discussed.

EMPIRE has been used to simulate a field-effect transistor based on a self-assembled monolayer of organic molecules (SAMFETs) that combine the functions of insulator and semiconductor in one molecule. Snapshots from classical molecular dynamics simulations were used as geometries for single-point AM1 calculations to investigate the electronic properties of the device. Visualization of the local electron affinity and the local electronegativity helps interpret the observed electrical properties of the SAMFETs.

The planned future development of the program will also be discussed.