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Quantum mechanical pseudopotential atomistic simulations of nanosized CMOS devices LIN-WANG WANG, Lawrence Berkeley National Laboratory, XIANG-WEI JIANG, HUI-XIONG DENG, Semiconductor Institute, Chinese Academy of Science — We have used empirical pseudopotential to calculate the electronic structures of million atom CMOS systems. This is done by using the linear combination of bulk band (LCBB) method. For a nonequilibirum CMOS system with an applied source-drain bias, we have devised three different ways to calculate the inverse carrier charge densities and the corresponding currents. The first is to use partition functions extended from source and drain using their respective Fermi energies. The second is to use a spatially dependent local quasi-Fermi energy, and the third is to calculate the current using Bardeen's tunneling current formula. In this talk, we will compare the results of these three different methods. We will also compare the quantum mechanical results with classical simulation results. This work was supported by U.S. Department of Energy under Contract No. DE-AC02-05CH11231. It has also been supported by Chinese National Natural Science Foundation.

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