Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Development of a non-equilibrium quantum transport calculation method based on constrained density functional\(^1\) HAN SEUL KIM, YONG-HOON KIM, Graduate School of EEWS, Korea Advanced Institute of Science and Technology — We report on the development of a novel first-principles method for the calculation of non-equilibrium quantum transport process. Within the scheme, non-equilibrium situation and quantum transport within the open-boundary condition are described by the region-dependent \(\Delta\) self-consistent field method and matrix Green’s function theory, respectively. We will discuss our solutions to the technical difficulties in describing bias-dependent electron transport at complicated nanointerfaces and present several application examples.

\(^1\)Global Frontier Program (2013M3A6B1078881), Basic Science Research Grant (2012R1A1A2044793), EDISON Program (No. 2012M3C1A6035684), and 2013 Global Ph.D fellowship program of the National Research Foundation. KISTI Supercomputing Center (KSC-2014-C3-021).

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Date submitted: 14 Nov 2014

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