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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 Δ 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.

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Han Seul Kim
Graduate School of EEWS,
Korea Advanced Institute of Science and Technology

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