Surface Green function calculations in the infinite number of principal layer approach: A non-recursive scheme[1] ALEKSEY KLETSOV, YURI DAHNOVSKY, VINZ ORTIZ — A novel computational method for a surface Green function matrix is determined for the calculation of electrical current in molecular wires. The proposed non-recursive scheme approach allows one to find the imaginary part of the surface Green matrix by the method that includes the infinite number of principal layers. It is shown that the solution of the second order matrix equation gives the spectral density matrix which for noninteracting electrons determines the density of states. Single and double principle layer models are studied both analytically and numerically.

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