

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Surface Green functions in molecular transport junctions: The generalization to interacting electrons in the leads¹ ALEKSEY KLETSOV, YURI DAHNOVSKY — The expression for current in transport junctions is generalized to interacting electrons in the leads. We derive a formula for the current where in the expression for line-width matrices the lead density of states is replaced by the surface spectral density matrix for arbitrary e - e interactions in the leads and in the bridge, respectively. This expression is only valid for small lead-bridge interactions. A novel computational method for a surface Green function matrix is introduced to find the surface spectral density (\sim the trace of the imaginary part of the surface Green function matrix). The proposed non-recursive approach results in the solution of the second order matrix equation for the spectral density matrix (the density of states for noninteracting electrons). The single and double principle layer models are studied for *aluminum* surfaces. We find that the peak in the spectral function is rather narrow (~ 2 eV). and can cause a peak in the Γ matrices resulting in a peak in the current-voltage characteristics. Beside the *aluminum* surface with *fcc*-structures, we study a *hexagonal* structure as well. Such surfaces exhibit a gap and two bands in the spectral density. The gap and the band widths depend on the parameters of the lead Hamiltonian. We show that the narrow gap and the narrow bands can result in large negative resistances in the conduction.

¹NFS grant CHE-0426090

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Date submitted: 20 Nov 2006

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