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Recent progress in computational electronics: disorder effects in nonequilibrium quantum transport[1]

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Realistic nanoelectronic devices inevitably have some disorder which affect device operation. Unintentional impurities sit at unpredictable locations and any predicted quantum transport property should be averaged over the impurity configurations. Impurity atoms are also intentionally doped into device material where the average is also necessary. One may generate many impurity configurations, calculate all and average the results. Such a brute force approach is not practical for first principles analysis as it is computationally too costly. I shall present the theory of nonequilibrium vertex correction (NVC) [1] where the configurational average is analytically done resulting to a NVC self-energy contributing to the nonequilibrium density matrix. NVC accounts for multiple impurity scattering at nonequilibrium. By integrating NVC with the density functional theory (DFT) and Keldysh nonequilibrium Green's functions (NEGF), nonequilibrium quantum transport in nanoelectronic systems having atomistic disorder can be carried out. By further integrating a recently proposed semi-local exchange potential that accurately determines band gaps [2], semiconductor nanoelectronics can now be analyzed from atomic first principles. Several examples will be presented including disorder scattering in Fe/MgO/Fe magnetic tunnel junction, electronic structure of $In_xGa_{1-x}N$ with varying concentrations x for solar cells, and quantum transport properties of doped Si membrane.

[1] Youqi Ke, Ke Xia and Hong Guo, Phys. Rev. Lett. 100, 166805 (2008); *ibid* (in print, 2010).
[2] Fabien Tran and Peter Blaha, Phys. Rev. Lett. 102, 226401 (2009).

[1]Work in collaboration with Youqi Ke and Ke Xia.