

First Principles Modeling of Magnetic Tunnel Junctions

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I will discuss an aspect of nanoelectronic device theory, namely modeling nanoelectronics from atomic first principles. Some important issues of quantum transport theory in the atomic limit will be reviewed. I will then report a recent theoretical development for treating atomistic disorder in nonlinear and non-equilibrium quantum transport modeling. The theory uses non-equilibrium vertex corrections to handle the configurational average of random disorder at the density matrix level. Using this technique, we have analyzed spin injection in magnetic tunnel junctions with interface roughness as well as with oxygen vacancies in the tunnel barrier. Disorder effect is found to significantly alter spin polarized tunneling.