Density-Functional based tight-binding (DFTB) methodology within an SCF DFT framework

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The foundation of the density-functional tight-binding (DFTB) method is briefly reviewed. The approximations of the DFTB within the Kohn-Sham density functional theory (KS-DFT) are critically evaluated. We present a DFTB approach based on a self-consistent field (SCF) framework beyond the original second order self-consistent charge (SCC) DFTB. Several corrections are described and evaluated on selected test systems. The relation to traditional semiempirical quantum chemical methods is outlined.