

"A Density Functional Tight Binding scheme with self-consistent dual density matrix"

Abstract:

A new Density Functional Tight Binding (DFTB) formalism has been developed by incorporating one-center exchange-like terms in the expansion of multicenter integrals. This goes beyond the Mulliken approximation and leads to a scheme which treats in a self-consistent way the fluctuations of the whole dual density matrix, and not only its diagonal elements (Mulliken charges). In my talk I will briefly introduce this scheme and its straightforward extension to linear response applications [Time dependent (TD)-DFTB]. Its performance for the description of hydrogen bonds and absorption spectra will be shown to improve upon traditional SCC-DFTB and TD-DFTB. The elapsed time for the computation of the vertical excitation energies of several molecules will be benchmarked against higher-level formalisms. I will finally discuss the implementation of orbital constraints within TD-DFTB to further reduce the computational time.